METAL- AND MATERIAL PHYSICS

METALL- UND MATERIALPHYSIK (MM)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture rooms IFW A, IFW B, IFW D)

Invited Talks

MM 1.1	Mon	09:30	(IFW A)	**Fundamentals of Severe Plastic Deformation**, Michael Zehetbauer
MM 6.1	Mon	14:00	(IFW A)	**Solid-State Physics with Fast Heavy Ions**, Siegfried Klaumünzer
MM 11.1	Tue	09:30	(IFW A)	**The Materials Challenge for Hydrogen Storage**, Züttel Andreas
MM 16.1	Tue	14:00	(IFW A)	**Electron Holography - New Possibilities for Materials Characterization with (sub-)nanometer Resolution**, Michael Lehmann
MM 26.1	Thu	09:30	(IFW A)	**Ion Tracks in Solids: An Overview of Technological Applications**, Hardev Singh Virk
MM 32.1	Thu	14:00	(IFW A)	**From First-Principles Calculations to Precipitate Microstructure Evolution in Alloys**, Long-Qing Chen
MM 39.1	Fri	10:15	(IFW A)	**Effect of High Magnetic Field on Crystallographic Texture and Grain Microstructure Evolution in Non-Ferromagnetic Metals**, Dmitri A. Molodov

Sessions

MM 1	**Invited talk Zehetbauer (SYSPD)**	Mon 09:30–10:00	IFW A	MM 1.1–1.1
MM 2	**Symposium Severe Plastic Deformation I**	Mon 10:15–12:45	IFW A	MM 2.1–2.5
MM 3	**Symposium Modern Metallic Materials Design I**	Mon 10:15–12:45	IFW B	MM 3.1–3.8
MM 4	**Phase transitions I**	Mon 10:15–11:15	IFW D	MM 4.1–4.4
MM 5	**Phase transitions II**	Mon 11:45–13:00	IFW D	MM 5.1–5.5
MM 6	**Invited talk Klaumünzer**	Mon 14:00–14:30	IFW A	MM 6.1–6.1
MM 7	**Symposium Severe Plastic Deformation II**	Mon 14:45–17:30	IFW A	MM 7.1–7.5
MM 8	**Symposium Modern Metallic Materials Design II**	Mon 14:45–16:30	IFW B	MM 8.1–8.7
MM 9	**Interfaces**	Mon 14:45–16:15	IFW D	MM 9.1–9.6
MM 10	**Intermetallic phases**	Mon 16:30–17:45	IFW D	MM 10.1–10.5
MM 11	**Invited talk Züttel**	Tue 09:30–10:00	IFW A	MM 11.1–11.1
MM 12	**Symposium Severe Plastic Deformation III**	Tue 10:15–12:45	IFW A	MM 12.1–12.4
MM 13	**Symposium Modern Metallic Materials Design III**	Tue 10:15–13:15	IFW B	MM 13.1–13.10
MM 14	**Hydrogen in Metals I**	Tue 10:15–11:15	IFW D	MM 14.1–14.4
MM 15	**Hydrogen in Metals II**	Tue 11:45–12:45	IFW D	MM 15.1–15.4
MM 16	**Invited talk Lehmann**	Tue 14:00–14:30	IFW A	MM 16.1–16.1
MM 17	**Symposium Severe Plastic Deformation IV**	Tue 14:45–17:30	IFW A	MM 17.1–17.7
MM 18	**Materials Design**	Tue 14:45–16:00	IFW B	MM 18.1–18.5
MM 19	**Electronic Properties I**	Tue 16:30–17:45	IFW B	MM 19.1–19.5
MM 20	**Amorphous and Liquid Materials I**	Tue 14:45–16:00	IFW D	MM 20.1–20.5
MM 21	**Amorphous and Liquid Materials II**	Tue 16:30–17:45	IFW D	MM 21.1–21.5

MM 22	**Electronic Properties II**	Wed 14:00–15:30	IFW A	MM 22.1–22.6
MM 23	**Mechanical Properties I**	Wed 14:00–15:15	IFW B	MM 23.1–23.5
MM 24	**Quasicrystals**	Wed 14:00–15:15	IFW D	MM 24.1–24.5
MM 25	**Poster Session**	Wed 15:30–17:30	P4	MM 25.1–25.45
MM 26	**Invited Talk Virk**	Thu 09:30–10:00	IFW A	MM 26.1–26.1
MM 27	**Diffusion I**	Thu 10:15–11:15	IFW B	MM 27.1–27.4
MM 28	**Amorphous and Liquid Materials III**	Thu 11:45–13:00	IFW B	MM 28.1–28.5
MM 29	**Poster Session (SYNW)**	Thu 10:00–11:00	P4	MM 29.1–29.6
MM 30	**Symposium Nano Wires (SYNW)**	Thu 11:00–13:15	IFW D	MM 30.1–30.9
MM 31	**Symposium Materials Modelling I**	Thu 10:15–13:00	IFW A	MM 31.1–31.6
MM 32	**Invited Talk Chen (SYMM)**	Thu 14:00–14:30	IFW A	MM 32.1–32.1
MM 33	**Symposium Materials Modelling II**	Thu 14:45–16:30	IFW A	MM 33.1–33.6
MM 34	**Symposium Materials Modelling III**	Thu 17:00–18:45	IFW A	MM 34.1–34.7
MM 35	**Growth**	Thu 14:45–16:30	IFW B	MM 35.1–35.7
MM 36	**Amorphous and Liquid Materials IV**	Thu 16:30–18:00	IFW B	MM 36.1–36.6
MM 37	**Nanostructured Materials I**	Thu 14:45–16:15	IFW D	MM 37.1–37.6
MM 38	**Nanostructured Materials II**	Thu 16:30–18:00	IFW D	MM 38.1–38.6
MM 39	**Invited Talk Molodov**	Fri 10:15–10:45	IFW A	MM 39.1–39.1
MM 40	**Nanostructured Materials III**	Fri 11:00–12:00	IFW D	MM 40.1–40.4
MM 41	**Nanostructured Materials IV**	Fri 12:30–13:15	IFW D	MM 41.1–41.3
MM 42	**Diffusion II**	Fri 11:00–12:00	IFW B	MM 42.1–42.4
MM 43	**Diffusion III**	Fri 12:30–13:30	IFW B	MM 43.1–43.4
MM 44	**Mechanical Properties II**	Fri 11:00–12:00	IFW A	MM 44.1–44.4
MM 45	**Mechanical Properties III**	Fri 12:30–13:30	IFW A	MM 45.1–45.4

Symposium: Nano Wires, see SYNW, continuation Thursday session MM30, poster session Thursday MM29
Symposium: Dynamics of electron transfer, see SYET
Symposium: Multiferroic Materials, see SYMM

Annual General Meeting of the Section Metal- and Material Physics

Tue 18:00–19:00 IFW A

Agenda
1. Reports from the chairmans of the FV MM and the AGMM
2. Spring Meeting 2005 Dresden, contributions and statistics
3. New subjects and symposia for the next spring meeting
4. Suggestions for invited talks for the next meeting
5. others

Sessions

– Invited, Keynote, Contributed Talks and Posters –

MM 1 Invited talk Zehetbauer (SYSPD)

Time: Monday 09:30–10:00 Room: IFW A

Invited Talk MM 1.1 Mon 09:30 IFW A

Fundamentals of Severe Plastic Deformation — •Michael Zehetbauer — Institiut für Materialphysik, Universität Wien, Boltzmanngasse 5, A-1090 Wien

The lecture addresses the special features of Severe Plastic Deformation (SPD) which distinguishes SPD from other methods to produce nanostructured materials and from conventional plastic deformation. These features are intimately connected with the unique properties of SPD nanometals revealing high ductility and/or superplasticity, large fracture toughness, an increased reate of hydrogen ad- and desorption, and changes in phase existencies as compared to equilibrium phase diagrams. The lecture reports on several competing explanations which have been subject of a vital discussion going on at present, in order to elucidate the physical background of these features/properties being typical of SPD.

MM 2 Symposium Severe Plastic Deformation I

Time: Monday 10:15–12:45 Room: IFW A

Keynote Talk MM 2.1 Mon 10:15 IFW A

Accumulative Roll-Bonding of Aluminium and Aluminium Alloys — •Irena Topic, Christine Klösters, Heinz-Werner Höppel, and Mathias Göken — Friedrich-Alexander-University Erlangen-Nuremberg, Department of Materials Science and Engineering, Institute of General Material Properties (WW1), Martensstraße 5, 91058 Erlangen, Germany

The interest in ultrafine-grained (UFG) materials has increased strongly during the past decade due to their superior strength and ductility. One of the ways to obtain an UFG microstructure is by accumulative roll-bonding (ARB). This is a severe plastic deformation process capable of obtaining an average grain size below 1um. During the ARB process, the 1mm aluminium strips are wire brushed, stacked, rolled together with a thickness reduction of 50% and at the end halved. The whole process was repeated up to 12 times for technically pure aluminium and up to 10 times for the aluminium alloy AA6016. The biggest advantage of this process is that it can be adopted in the industry to produce large scale UFG metal sheets. Due to the significantly increased specific strength paired with a high ductility, UFG sheet metals processed by ARB have a strong potential for prospective engineering applications in the transportation industry. In order to qualify the ARB process for these purposes detailed investigations on the robustness of the process, mechanical properties and the microstructural evolution are being carried out.

Keynote Talk MM 2.2 Mon 10:45 IFW A

Recent developments in optimization of mechanical properties of mechanically alloyed/ball milled nanostructured materials — •Jürgen Eckert, Sergio Scudino, and Shankar Venkataraman — Physical Metallurgy Division, Department of Materials and Geo Sciences, Darmstadt University of Technology, Petersenstr. 23, D-64287 Darmstadt, Germany

One of the areas of research on nanostructured materials that has received extensive study is their mechanical behavior. The great interest in the mechanical behavior of nanostructured materials originates from the unique mechanical properties observed and/or predicted when the critical length-scale of the microstructure/phases approaches the nanoscale. Such features include increased hardness and strength as well as the expectation of enhanced ductility, and perhaps even superplastic behavior at low homologous temperatures. While some of these observations and predictions have been verified, some have been found to be due to high porosity or other processing artefacts, and not inherent properties of the nanostructured materials. This presentation reviews recent developments in the development of mechanically alloyed/ball milled nanostructured metals and alloys and addresses the limitations to ductility in nanocrystalline materials. Examples of recent breakthroughs wherein both high strength and good ductility are observed will be presented and discussed in the light of possible functional and structural applications for nanostructured materials. This work was supported by the German Science Foundation (DFG).

Keynote Talk MM 2.3 Mon 11:45 IFW A

New Routes to obtain Massive Nanostructured Materials — •Gerhard Wilde — Forschungszentrum Karlsruhe, Institute of Nanotechnology, P.O.B. 3640, 76021 Karlsruhe, Germany

Synthesizing massive nanocrystalline materials that are free from residual porosity and free from contaminations of the interior interfaces still presents a challenge to basic research as well as to application-related processing efforts. Severe plastic deformation (SPD) processes have frequently been applied to synthesize massive ultrafine-(submicron)-grained or disk-shaped nanostructured pure metals and alloys. New opportunities might be based on combining different non-equilibrium processing routes sequentially such that an initially metastable state is continuously energized and successively driven farer away from thermodynamic equilibrium. One example is given by plastically deforming metallic glasses. Another way to obtain specimens, e.g. of pure metals with extremely small average grain sizes and with quantities in the gram range is given by repeated cold-rolling and folding. The microstructure evolution as well as the limits of this technique in comparison to conventional SPD methods will be discussed. Additionally, sequentially combining different processing pathways that are based on continuous strain energy input present new routes for nanostructure formation. The available permutations offer a wide range of options for tailoring the microstructure and the shape and quantity of the product nanostructure and, at the same time, present a wide field yet to be explored. The support of this work by the DFG is gratefully acknowledged.

MM 2.4 Mon 12:15 IFW A

Synthesis of nanostructured Al-Y-Fe using SPD processing — •Nancy Boucharat[1], Rainer Hebert[1,2], Harald Rösner[1], and Gerhard Wilde[1] — [1]Forschungszentrum Karlsruhe, Institute of Nanotechnology, P.O.B. 3640, 76021 Karlsruhe, Germany — [2]University of Wisconsin-Madison, Department of Materials Science and Engineering, Madison, WI 53706, USA

A common way to produce nanostructures from Al-rich glass-forming alloys is to apply low temperature isothermal treatments. However, plastic deformation can also induce crystallization in metallic glasses. Thus, deformation at large strains might present an alternative route for producing bulk nanostructures of adjustable grain size. We report here structural analyses of an Al-Y-Fe glass that has been subjected to high-pressure torsion straining at room temperature. The results show a remarkably high number density of Al-nanocrystals compared to the values obtained after annealing at low temperatures or after cold rolling at moderate strains, respectively. The nanocrystals appear to be distributed homogeneously throughout the sample without any evidence of strong coarsening. Moreover, the comparison between deformation-mediated nanocrystallization by applying either high pressure torsion straining or cold rolling is discussed with respect to the likely mechanisms underlying the nanocrystallization during deformation. These results form the basis for the development of advanced processing strategies for producing new nanostructures with high nanocrystal number densities giving rise to increased stability and improved performance of the nanoscale microstructure. Support by the DFG is gratefully acknowledged.

MM 2.5 Mon 12:30 IFW A

Downscaling the ECAP process — •Aikaterini Zi, Ralph J. Hellmig, and Yuri Estrin — Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal, Agricolastr. 6, 38678 Clausthal–Zellerfeld

Equal Channel Angular Pressing (ECAP) is a well–known severe plastic deformation method used to produce ultra–fine grained materials. The dimensions of ECAP specimens are usually in the centimetre range. Downscaling the ECAP process may be a viable option for producing high strength wires or fibres in the millimetre range. A multi channel die with channel diameter of 2 mm was used for that purpose. Microstructure investigations demonstrating significant grain refinement confirm the viability of this approach.

MM 3 Symposium Modern Metallic Materials Design I

Time: Monday 10:15–12:45 Room: IFW B

MM 3.1 Mon 10:15 IFW B

Modern Metallic Materials Design — •Ze Zhang[1], Dieter Herlach[2], and Knut Urban[3] — [1]Beijing University of Technology, 100022 Beijing, P.R. China — [2]German Aerospace Center, D-51170 Köln, Germany — [3]Research Center Jülich, D-52425 Jülich, Germany

Since 2002 the Sino-German Science Center for Research Promotion Beijing, the Natural National Science Foundation of China (NNSFC) and the German Research Foundation (DFG) are supporting a priority programme on Modern Metallic Materials Design (MMMD) of Chinese and German groups. Modern materials science ranges from tailoring of structures in nanodimensions to the optimization of technical materials by the application of new physical concepts reflecting the growing atomistic insight into structure and properties of matter. The project aims on joint work in projects on metals and alloys, which are of great topicality and therefore can be considered as interesting and challenging for materials science institutions in China as well as in Germany. One group of projects concerns the solidification of metals and alloys from the melt. Another group of projects concerns metallic glasses. This field has recently seen intensive expansion after new multicomponent systems have been developed which permit to obtain bulk materials. A group of metallic alloys, which has been pioneered by Chinese scientists is quasicrystalline materials. Finally the current project addresses the new field of structurally complex alloy phases. The science of these alloys exhibiting properties between those of conventional intermetallics and those of quasicrystals. The symposium MMMD consists mainly of reports of the research done within this programme.

MM 3.2 Mon 10:30 IFW B

Complex intermetallic alloys in the Al-rich region of the ternary Al-Pd-Ni system — •Mariya Yurechko and Philipp Ebert — Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich

The phase diagram and the liquidus surface projection of the ternary Al-Pd-Ni system in the range of 50 to 100 at.% Al was determined using SEM, EDX, XRD, ICP-OES, and TEM. Isothermal sections between 750 and 1100 degrees Celsius illustrate that the binary Al-Pd intermetallic ϵ phase (known also as ξ' phase) is stable up to 15 at.% Ni. Furthermore, the binary AlPd and AlNi compounds with CsCl structure as well as the hexagonal Al_3Pd_2 and Al_3Ni_2 compounds form continuous ranges of solid solutions, labeled β and δ phases, respectively. No exclusively ternary phase was observed to be stable in the system. The results are compared with the ternary Al-Pd systems containing Mn, Fe, Co, Ru, Rh, or Re and the similarities are discussed. Finally, the growth paths of single crystals of the different phases are derived.

MM 3.3 Mon 10:45 IFW B

Atomic Structure Determination of Phason Planes in the ξ'-Al-Pd-Mn Phase — •H. Tian[1], W. Sun[2], and Z. Zhang[2] — [1]Institute of Physics and Center for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China — [2]Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, 100 Pingle Yuan, Chao Yang District, Beijing 100022, China

The atomic structures of specific types of linear defects (phason lines) [1] and planar defects (phason planes) [2,3] in the complex metallic alloy phase ξ'-Al-Pd-Mn were determined by means of high-resolution electron microscopy (HREM) and theoretical HREM simulation. The results show that a representational atomic structural model for phason planes can be constructed by introducing a shift between two parts of the perfect crystalline structure using a translation vector of $r = \frac{1}{2}\alpha + \frac{1}{2\tau}\chi$. This typical phason plane is normally parallel to the (001) plane of the ξ'-Al-Pd-Mn phase and consists of phason lines which are arranged side-by-side with their linear direction parallel to the [010] axis. HREM simulations based on the structural model for both edge-on and inclined types of phason lines agree well with the experimental results. Taking into account the fact that the structural difference between various curved phason planes is due to the variation in the arrangement of individual phason lines, the atomic structures of the edge-on and inclined phason lines can be used to explain the various curved and broaden phason planes frequently observed in the ξ'-Al-Pd-Mn phase.

[1] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phys. Rev. Lett. 82 (1999) 3468. [2] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phys. Rev. Lett. 82 (1999) 3468. [3] H. Klein, M. Feuerbacher, K. Urban, Mat. Sci. Eng. 294 (2000) 769.

MM 3.4 Mon 11:00 IFW B

Atomic Structure Determination of structurally complex alloy Ψ Al-Pd-Mn Phase — •H. Tian[1], W. Sun[2], and Z. Zhang[2] — [1]Institute of Physics and Center for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China — [2]Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, 100 Pingle Yuan, Chao Yang District, Beijing 100022, China

Base on the study of two-dimensional planar defects [1,2] (phason planes) in the complex metallic alloy phase ξ'-Al-Pd-Mn, the atomic structure of the-Al-Pd-Mn phase [3] was determined by means of high-resolution electron microscopy (HREM) observations and theoretical HREM simulations. The Ψ-Al-Pd-Mn phase has an orthorhombic unit cell with lattice parameters of a =23.54 Å, b =16.56 Å, and c =56.98 Å. The structure of the Ψ-Al-Pd-Mn phase can be characterized as stacking of phason planes in the ξ'-Al-Pd-Mn phase [4] along the c axis. The dimension along the c axis for the Ψ-phase is $\tau + 3$ times larger than that of the ξ'-phase. A close comparison between the experimental and simulated diffraction pattern, based on phason-plane stacking model, shows that both of the position and intensity distribution of the simulated diffraction pattern agree well with the experimental result. Furthermore, the simulated HREM image of the Ψ-Al-Pd-Mn phase based on above structure model matches also very well with the experimental results. All of the agreements indicate that the structural model of the Ψ-Al-Pd-Mn phase we proposed here is reasonable.

[1] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phys. Rev. Lett. 82 (1999) 3468. [2] H. Klein, M. Feuerbacher, K. Urban, Mat. Sci. Eng. 294 (2000) 769. [3] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phil. Mag. Lett. 80 (2000) 11. [4] H. Klein, M. Feuerbacher, Phil. Mag. 83(2003) 4103.

MM 3.5 Mon 11:45 IFW B

Single-crystal growth of complex metallic alloy phases — •Michael Feuerbacher[1], Marc Heggen[1], Carsten Thomas[1], Ze Zhang[2], and Ke Hsin Kuo[2] — [1]Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — [2]Beijing Laboratory of Electron Microscopy, 100080 Beijing, China

Complex metallic alloys represent a new field in materials science recently attracting increasing interest. The characteristic features of this class of materials are large lattice parameters, a high number of atoms per unit cell, and a local order which is determined by a cluster substructure frequently involving icosahedral atom configurations. The physical properties of these materials are widely unexplored, which is mainly due to the unavailability of high-quality sample materials. The growth of complex metallic alloys is in many cases difficult as the phases solidify incongruently, their primary solidification area in the phase diagrams are small, etc. Therefore, advanced growth methods have to be applied. We have developed single-crystal growth routes for a variety of complex metallic alloy phases employing Czochralski-, Bridgman,- and self-flux growth techniques. The spectrum of phases produced covers different

structure types, different types of local order and elemental constituents and represents a solid materials basis for the experimental exploration of the physical properties of this class of materials. In the present contribution we report on the current state-of-the-art in materials production of complex metallic alloy phases.

MM 3.6 Mon 12:00 IFW B

Single-crystal growth of the complex metallic alloy β-Al-Mg. — •Marta Lipińska-Chwałek, Sergiy Balanetskyy, Carsten Thomas, and Michael Feuerbacher — Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

β-Al3Mg2 phase is a complex metallic alloy based on a giant unit cell (a=2.8 nm) containing approximately 1168 atoms. The material is very interesting also because of its low specific weight (2.2 g/cm3). Hardly any studies have been carried out on the physical properties of β-Al3Mg2. This is most probably due to the fact that until recently, high-quality single crystalline sample material was unavailable. We present the development of a single-crystal growth route for β-Al3Mg2. The phase diagram was probed in the vicinity of the existence range of β-phase. We approached the growth employing various techniques, the most successful of which turned out to be Czochralski- and self-flux-growth. With both of them we reproducibly achieved single crystals of several cubic centimeters. While the Czochralski technique allows for the production of deliberately oriented single crystals, the self-flux technique is capable of the production of very large single grains. The size of which is only limited by the crucible volume. The material produced is now successfully used for the physical property investigations.

MM 3.7 Mon 12:15 IFW B

The complex metallic alloy phase $Al_{13}Co_4$: Plastic deformation properties and defects — •Marc Heggen[1], Dewei Deng[1,2], Michael Feuerbacher[1], Ze Zhang[2], and Ke Hsin Kuo[2] — [1]Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, D-52425 Juelich — [2]Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, Beijing, People's Republic of China

Plastic deformation experiments were performed on single crystals of the orthorhombic $Al_{13}Co_4$ complex metallic alloy phase in a temperature range between 600 and 800 °C. The stress-strain curves show a pronounced yield-drop effect followed by a regime of weak work hardening. Incremental experiments like stress-relaxation tests and temperature changes are conducted in order to determine thermodynamic activation parameters of the deformation process.

Microstructural investigations by means of transmission electron microscopy reveals that dislocation motion on (0 0 1) planes is the basic mechanism of plastic deformation in $Al_{13}Co_4$. Dislocation cores and attached planar defects were investigated by lattice fringe imaging and interpreted in terms of a tiling model. The planar defects are thin shear zones involving a phase transformation from the orthorhombic to a structurally closely related monoclinic phase. The dislocations cores are closely related to those of the metadislocations recently suggested by Feuerbacher and Heggen (Phil. Mag., 2005, in press) and possess the same Burgers vector of 2.9 Å.

MM 3.8 Mon 12:30 IFW B

Icoshedral connections in complex metallic alloy phases — •Ke Hsin Kuo[1], Z.B. He[1], Ze Zhang[2], Michael Feuerbacher[3], and K. Urban[3] — [1]Beijing Laboratory of Electron Microscopy, Institute of Physics, 100080 Beijing, China — [2]Beijing University of Technology, 100022 Beijing, China — [3]Institut für Festkörperforschung, Forschungszentrum Jlich GmbH, 52425 Jülich, Germany

The crystal structures of a number of complex metallic alloy (CMA) phases in Al-Cr-Si alloys have been determined by X-ray and electron crystallography. The basic structural unit in these structures is the icosahedron with the smaller and minor Cr atom at its center and the somewhat larger Al atom at its vertices. Icosahedra can be connected by mutual penetration along their fivefold axis to form icosahedral chains displaying a pseudo fivefold symmetry. Icosahedra can also be connected by face- and edge-sharing, thus forming chains displaying three- and twofold symmetry. Consequently, such CMA can form icosahedral/decagonal quasicrystals after very rapid solidification or the crystalline approximants with either cubic (point group m3), hexagonal (6/mmm), orthorhombic (mmm) or monoclinic (2/m) symmetry of these quasicrystals after slow solidification. These structural characteristics will be analyzed with the new structures under investigation.

MM 4 Phase transitions I

Time: Monday 10:15–11:15 Room: IFW D

MM 4.1 Mon 10:15 IFW D

AFM, TEM and SEM studies of nano-scale plate-like precipitates — •Dietmar Baither[1], Ihor Sobchenko[1], Josef Pesicka[1], Thomas Pretorius[1], Volker Mohles[2], Werner Stracke[3], Rudolf Reichelt[3], and Eckhard Nembach[1] — [1]Institut fuer Materialphysik, Universitaet Muenster — [2]Institut fuer Metallkunde und Metallphysik, RWTH Aachen — [3]Institut fuer Medizinische Physik und Biophysik, Universitaet Muenster

The high strength of many structural materials derives from coherent nano-scale precipitates of secondary phases, for example Guinier-Preston zones in aluminium based alloys or γ' precipitates in nickel based superalloys. Their shape, size and volume fraction crucially determine the strengthening effect. An alloy with the composition $Ni_{69}Co_9Al_{18}Ti_4$ was used as model system to determine these parameters for nano-scale plate-like precipitates. Such precipitates of the disordered γ phase arise in the $L1_2$-long-range ordered γ' phase of the matrix after 333 h annealing treatment at 1173 K. From TEM micrographs an approximate mean edge length of 400 nm and a thickness of 40 nm of the precipitates were determined. A precise description of their shape was derived using superellipses. The main task was to attain comparable results by AFM. These investigations revealed that the electrolytic etching of the surface attacks preferentially the plate-like precipitates so that deep dimples are formed. Problems and limitations of the AFM characterization of this morphology will be discussed.

MM 4.2 Mon 10:30 IFW D

Coarsening dynamics in elastically anisotropic alloys — •Bastian Pfau[1], Lorenz-Mathias Stadler[1], Bogdan Sepiol[1], Richard Weinkamer[2], Federico Zontone[3], and Gero Vogl[1] — [1]Fakultät für Physik der Universität Wien, Strudlhofgasse 4, A-1090 Wien, Austria — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, D-14424 Potsdam, Germany — [3]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

With the availability of coherent X-rays at third-generation synchrotrons it became possible to investigate the very slow dynamics of precipitate coarsening in phase separating alloys by utilising the emerging method of X-ray photon correlation spectroscopy [1]. Here, we present an in-situ study of coarsening dynamics in elastically anisotropic alloys [2]. Fluctuating speckle intensities in time series of coherent small-angle X-ray diffraction images are analysed for two different Ni–Al–Mo samples with different lattice misfit between precipitates and matrix. The detected long-term correlations depend not only on the norm but strongly on the direction of the scattering vector. The experimental findings are compared with results from Monte Carlo simulations. Our experiments together with the simulations indicate that in alloys with high elastic misfit, precipitate coarsening proceeds almost exclusively within {100} planes. Furthermore, our data suggest that plate-like precipitates are formed by coalescence of smaller particles.

[1] L.-M. Stadler et al., Phys. Rev. B **68**, 180101(R), (2003).
[2] B. Pfau et al., Europhys. Lett., to be submitted.

MM 4.3 Mon 10:45 IFW D

Monte Carlo Simulation of Phase Separation Including Elastic Relaxations — •Rolf Anders and Ferdinand Haider — Univ. Augsburg, Institut f. Physik

We developped a real space technique which includes local atomic relaxation during each atomic jump, allowing thus to study phase transformations with strong elastic contributions. For each atomic jump, the activation energy is computed using phenomenological interaction potentials. After a succesful jump the atomic coordinates in the vicinity of the jumping atom are relaxed in order to minimise the total energy.

Using this method we studied different binary Lennard-Jones alloys. At suitable potential parameters oriented precipitates were forming due to the elastic anisotropy of the material. We also observed an asymmetric microstructure with respect to components if the atom sizes are different. This is caused by the different elastic properties, which are directly related to the atom size in the LJ potential.

MM 4.4 Mon 11:00 IFW D

Time dependent phenomena in the athermal martensite $Ni_{63}Al_{37}$ — •Benno Ludwig, Leonard Müller, and Uwe Klemradt — II. Physikalisches Institut, RWTH Aachen University

The unexpected finding of time-dependent behaviour in athermal martensitic transformations above the M_S temperature [1] has prompted further experimental studies of so called incubation time (waiting time). Several theoretical models have been put forward, which, however, disagree with each other on the detailed transformation mechanism [1,2].

In order to contribute to the ongoing discussion measurements employing different in-situ methods combined with a excellent temperature stability of ±4 mK over several days were conducted. Results clearly show the existence of incubation times between 50 s up to 112000 s despite the fact that the M_S temperature is not a constant but rather a fluctuating variable on a superimposed trend. In addition the obtained data suggests a strong dependence on the thermal history of the sample. The results will be discussed in view of the competing theoretical notions.

[1] Mat. Sci. Eng. **A273-275** 21-39 (1999) and ref. within
[2] Scripta Mat. **50** 181-186 (2004), Scripta Mat. **45** 145-152 (2001)

MM 5 Phase transitions II

Time: Monday 11:45–13:00 Room: IFW D

MM 5.1 Mon 11:45 IFW D

Formation of competing γ-Fe and ϕ-phase in undercooled Nd-Fe-B alloys investigated by in-situ diffraction experiments using synchrotron radiation — •Thomas Volkmann[1], Joern Strohmenger[2], Oliver Heinen[1], Dirk Holland-Moritz[1], Jianrong Gao[3], Sven Reutzel[2], and Dieter M. Herlach[1] — [1]Institut für Raumsimulation, Deutsches Zentrum für Luft- und Raumfahrt (DLR), D-51170 Köln, Germany — [2]Institut für Experimentalphysik IV, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [3]Key Lab of Electromagnetic Processing of Materials, Northeastern University, Shenyang 110004, P.R. China

Nd-Fe-B alloys are used for the development of advanced permanent magnets that are based on the $Nd_2Fe_{14}B_1$-phase (ϕ-phase). Under equilibrium solidification conditions of alloys near the stoichiometric composition the ϕ-phase is formed by a peritectic reaction from pro-peritectic γ-Fe. The electromagnetic levitation technique was combined with the diagnostic means at the European Synchrotron Radiation Facilitiy (ESRF) to study in-situ phase formation in the undercooled melt by energy dispersive diffraction experiments during solidification. It was found that the γ-Fe-phase crystallizes primarily in the undercooled melt even at temperatures below the peritectic temperature at which γ-Fe is metastable while the stable ϕ-phase solidifies in a subsequent step.

The work was financially supported by the Deutsche Forschungsgemeinschaft under contract no. HE1601/14. The support from the ESRF in Grenoble is gratefully acknowledged.

MM 5.2 Mon 12:00 IFW D

Effect of melt convection on microstructure evolution of Nd-Fe-B alloys using a forced crucible rotation technique — •Kaushik Biswas[1], Regina Hermann[1], Joerg Acker[1], Gunter Gerbeth[2], Janis Priede[2], and Victor Shatrov[2] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany — [2]Forschungszentrum Rossendorf e.V., Institut für Sicherheitsforschung, Germany

The forced crucible rotation technique has been applied to the solidification of Nd-Fe-B alloys. Specially sealed samples were subjected to well-defined forced rotation during induction heating and solidification. The resulting microstructure of the Nd-Fe-B alloys in consideration of melt convection has been investigated using scanning electron probe microscopy. The determination of the a-Fe volume fraction by measuring the magnetic moment in a vibrating sample magnetometer (VSM) resulted in a distinct reduction of the a-Fe volume fraction in samples with high crucible rotation frequencies. Furthermore, the investigation has been extended the peritectic Ti-Al system. It could be shown that the secondary dendritic arm spacing of the properitectic phase reduces with increasing forced sample rotation frequency.

MM 5.3 Mon 12:15 IFW D

Solute trapping during rapid solidification of alloys: A phase-field study — •Denis Danilov and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

The effect of nonequilibrium solute trapping by growing solid under rapid solidification conditions is studied by a phase-field model. Considering a continuous steady-state concentration profile across the diffuse solid-liquid interface, a new definition of the nonequilibrium partition coefficient in the phase-field context is introduced. This definition leads to a better description of the available experimental data, especially at high growth velocities, in comparison with other diffuse-interface and sharp-interface predictions.

MM 5.4 Mon 12:30 IFW D

Experimental and Theoretical Studies of Solidification in Undercooled Fe-Ni and Fe-Co Droplets — •T.G. Woodcock, H.-G. Lindenkreuz, R. Hermann, and W. Loeser — IFW Dresden, PO Box 270116, D-01171 Dresden, Germany

Fe-Ni and Fe-Co based alloys have important applications as soft magnetic materials. The solidification of such alloys is therefore of interest. Droplets of Fe-Ni and Fe-Co alloys were electromagnetically levitated enabling very high melt undercooling (maximum approx. 300 K). The temperature of the samples was monitored during the solidification process using a two-colour pyrometer and a Si diode with a very fast reaction rate. The recalescence during solidification showed a transition from single step to double step at a critical value of undercooling. The double step recalescence was caused by formation of a metastable bcc phase and subsequent transformation to the equilibrium fcc phase in both Fe-Ni and Fe-Co alloys. A thermodynamic database was used to generate values of the enthalpy of formation for the fcc and bcc phases in three different Fe-Co alloys. Based on classical nucleation theory, the free energy of formation of a spherical nucleus was calculated. Calculation of the nucleation rate of these two phases showed that below a critical undercooling, the metastable bcc phase can have a higher nucleation rate than the equilibrium fcc phase.

MM 5.5 Mon 12:45 IFW D

Primary crystallization of the hypoeutectic Ni-17at.% P alloy by ASAXS — •Rainer Kranold[1], Dragomir Tatchev[2], Günter Goerigk[3], and Stephan A. Armyanov[2] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, PF 1913, D-52425 Jülich, Germany

During the primary crystallization of a hypoeutectic Ni-P alloy, according to the equilibrium phase diagram, crystallites of pure Ni should be precipitated until the matrix reaches the eutectic composition with 19 at.% P. However, several authors assume that the precipitating Ni particles contain a certain P amount. We investigated with anomalous small-angle X-ray scattering (ASAXS) the primary crystallization of Ni(P) particles in the amorphous hypoeutectic Ni-17 at.% P alloy. Using the maximum entropy method, the particle size distribution, the size dependence of the particle composition and the amorphous matrix composition could be found simultaneously. The size distribution consists of a peak at particle radius of 1 nm and a tail spanning from 2 to 15 nm. The composition of the particles of the peak changes from 14 to 2 at.% P as their radius grows from 0.7 to about 3 nm. The particles in the tail of the size distribution (2-15 nm) have nearly constant P content in the range of 0-2 at.%. The matrix composition tends to the eutectic one at the end of the primary crystallization process. Our experimental results comply the predictions of a new nucleation theory developed recently [1]. [1] D. Tatchev et al., J. Appl. Cryst. 38 (2005) 787

MM 6 Invited talk Klaumünzer

Time: Monday 14:00–14:30 Room: IFW A

Invited Talk MM 6.1 Mon 14:00 IFW A

Solid-State Physics with Fast Heavy Ions — •Siegfried Klaumünzer — Ionenstrahllabor, Hahn-Meitner-Institut, Glienicker Str. 100, 14091 Berlin, Germany

Fast heavy ions in solids create a narrow cylindrical track of strongly heated matter. The most obvious response of amorphous materials to this kind of excitation is a change in shape (ion hammering). After a brief outline of this phenomenon two examples will be presented in more detail to demonstrate how high-energy ion beams can contribute to solid-state physics. The first example addresses the longstanding question of liquid polymorphism in silicon, i.e. the existence of a liquid silicon phase with coordination number 4 in comparison with common liquid silicon, which has a coordination number of 6. Exploiting the effect of ion hammering it could be shown that a tetrahedrally coordinated liquid silicon phase must exist on a time scale of about 100 ps. The second example deals with texture modification of nanocrystalline titanium. Starting again from ion hammering it will be argued that a collective rotation of crystalline grains is possible if the grain boundaries are amorphous. The experiments could provide a direct access to the dynamic behavior of grain boundaries.

MM 7 Symposium Severe Plastic Deformation II

Time: Monday 14:45–17:30 Room: IFW A

Keynote Talk MM 7.1 Mon 14:45 IFW A

Determination of long-range internal stresses in cyclically deformed Ni with submicro-crystalline grain structure — •Ellen Hieckmann[1], Lutz Hollang[2], and Werner Skrotzki[2] — [1]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

It is well accepted that, in fcc metals with a submicro- to nanocyrstalline grain structure, the typical dimensions of deformation induced dislocation arrangements are determined by the size of grains/subgrains. In this context, the long-range internal stresses considered here are assumed to be the mean stresses in grains/subgrains and in dislocation structure elements, respectively. These stresses can arise from granular constraints caused by the sample production processes and from heterogeneous plastic deformation from grain to grain during the subsequent cycling. The latter should lead to a change of the long-range internal stresses during one loading cycle. A concept is proposed to determine these stresses from their contribution to the broadening of Bragg-diffraction profiles. The basic idea is to analyse the changes of the profile shape within a mechanically stabilized loading cycle in comparison with the diffraction profile in the as-produced state of the specimen. Results of high resolution X-ray diffraction measurements are presented for Ni samples, where the submicro-crystalline grain structure is produced by equal-channel angular pressing or by electrodeposition.

MM 7.2 Mon 15:15 IFW A

Vacancy type defects in severely plastically deformed Ni — •Erhard Schafler, Gerd Steiner, Elena Korznikova, Heinrich Schindler, Michael Kerber, and Michael Zehetbauer — Institut für Materialphysik, Universität Wien, Boltzmanngasse 5, A-1090 Wien

Ni of two different purities have been deformed to different strains by high pressure torsion at room temperature using two different hydrostatic pressures. For comparison, some investigations by conventional deformation (rolling, compression) have been carried out, too. The material has been investigated by X-ray diffraction Bragg profile analysis, differential scanning calorimetry as well as residual electrical resistivity. The X-ray method gives information about the dislocation density and their arrangement, and the size and distribution of the smallest structural elements (coherently scattering domains). While the X-ray method detects the dislocations solely, the two other (annealing) methods are sensitive to both vacancies and dislocations. Therefore the proper combination of the results enables to analyse and quantify the evolution of vacancy type defects [1]. Similarly as in the case of Cu, the vacancy concentrations induced by SPD processing are definitely higher than those from conventional plastic deformation [2]. The resulting concentrations of vacancies are discussed in view of their dependencies on the deformation strain, the hydrostatic pressure and the purity of the material used.

[1] M. Zehetbauer, E. Schafler, T. Ungar, Z. Metallk., Vol 96(9) (2005) 1044-1048 [2] E.Schafler, G.Steiner, E.Korznikova, M.Zehetbauer, Mater.Sci Eng. A,410-411, (2005) 169-173.

Keynote Talk MM 7.3 Mon 15:30 IFW A

Tracing microstructure and mechanical properties evolution in ECAP: experiment vs. simulation — •Ralph J. Hellmig and Yuri Estrin — Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal, Agricolastr. 6, 38678 Clausthal–Zellerfeld

Equal channel angular pressing (ECAP) is a well–known method to produce ultra–fine grained bulk materials. In this process, a specimen is pressed through an angular channel leading to structural refinement, which results in a beneficial change of mechanical properties. Using dislocation density related constitutive modelling it is possible to trace the microstructure evolution as well as the variation of the mechanical properties during ECAP deformation. A comparison of experimental results and simulations for various materials will be given to demonstrate the capabilities of the model itself and the simulation technique applied.

Keynote Talk MM 7.4 Mon 16:30 IFW A

Texture development during equal channel angular pressing — •Werner Skrotzki — TU Dresden, Institut für Strukturphysik

Plastic deformation of polycrystalline materials is one of the main processes of texture formation which may lead to an anisotropy of properties. Therefore, texture studies on materials, which have undergone severe plastic deformation, are of particular interest from the scientific as well as technological point of view. A review will be given on the recent understanding of texture development during equal channel angular pressing (ECAP) of fcc metals. Emphasis will be put on the effect of process and material parameters like friction, temperature, starting texture and stacking fault energy. The experimental ECAP textures will be compared with simulations.

Keynote Talk MM 7.5 Mon 17:00 IFW A

Diffusion in nanocrystalline materials — •Wolfgang Sprengel — Institut für Physikalische Elektronik, Universität Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart, Germany; sprengel@ipe.uni-stuttgart.de

Atomic diffusion represents a key issue for nanocrystalline materials since it controls both, their physical properties, such as plasticity, and their structural stability. Diffusion in nanocrystalline solids substantially differs from diffusion in coarse-grained or single-crystalline materials. In nanocrystalline solids the high fraction of crystallite interfaces provides paths of high diffusivity. Due to the correlation between the diffusion behavior and the interface structure, diffusion measurements can serve as an important tool to solve the controversial debate to what extent interface structures in nanostructured materials differ from those of conventional grain boundaries. An overview will be given on atomic diffusion in nanocrystalline materials prepared by various synthesis routes including crystallization, crystallite condensation and compaction, and severe plastic deformation. The role of intergranular amorphous phases and of interfacial structural relaxation will be addressed. Diffusion studies in nanocrystalline alloys which show an intergranular melting transition will be presented [1,2].

[1] M. Eggersmann et al., Interface Science **9**, 337 (2001).
[2] W. Sprengel et al., J. Appl. Phys. **98**, 074314 (2005).

MM 8 Symposium Modern Metallic Materials Design II

Time: Monday 14:45–16:30 Room: IFW B

MM 8.1 Mon 14:45 IFW B

Investigation of the phase boundary and site occupation of atoms in pure and doped TiAl/Ti3Al intermetallic by means of the tomographic atom probe (TAP) — •Torben Boll[1], Talaat Al-Kassab[1], Yong Yuan[2], and Zhi-Guo Liu[2] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China

Dual-phase TiAl/Ti3Al alloys consisting of a lamellar structure, comprising γ-phase plus a small amount of α2-phase, with addition of 1 and 5at.%Nb were prepared. The samples were investigated by means of the field ion microscopy (FIM), the tomographic atom probe (TAP) and supporting TEM, HRTEM analysis. The influence of Nb-alloying on the variation of the field evaporation and microstructural parameters in the γ-phase as studied by FIM and TAP will be reported in this contribution. A new data treatment approach based on TAP results was developed to evaluate the site occupancies in such ordered structures. The Nb-atomic site occupancies, as well as any clustering and/or ordering of Nb atoms will be reported. In addition, computer modeling and simulation of the field evaporation behavior of the different species including the next neighbor interaction in a FIM specimen are performed for the first time. From these simulations, a structural order parameter and binding energies for the different species can be estimated. A comparison of the results, obtained with this model, to the experimental data will be presented and discussed for the site occupancy of Nb in these alloys.

MM 8.2 Mon 15:00 IFW B

Computer simulation of the field evaporation in TiAl with additions of Nb — •Torben Boll[1], Talaat Al-Kassab[1], Yong Yuan[2], and Zhi-Guo Liu[2] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China

The formation of an image in the field ion microscope and subsequently the field assisted evaporation of the upper most surface atoms from the atomic layers as originated in the tomographic atom probe were simulated. As a model system we have selected the ordered structure of the γ-TiAl-phase with a $L1_0$-unit cell containing various additions of Nb. For the first time in such a computer modeling next neighbor (NN)-binding energies have been used. The effect of site occupation and concentration of Nb on the process of field evaporation and its influence on the TAP- and FIM-results were investigated as well. Further algorithms were developed to explore the vicinity around selected species and hence to analyze the degree of order based on TAP results. These processes were tested on experimental as well as on simulated data. In this contribution the computer model will be presented and discussed. In particular the focus will be emphasized on the approach to estimate NN-binding energies and order parameters by comparing the simulations with experimental data.

MM 8.3 Mon 15:15 IFW B

TEM investigations of TiAl-based intermetallic compounds — •Yong Yuan[1], Zhi-Guo Liu[1], Torben Boll[2], and Talaat Al-Kassab[2] — [1]Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China — [2]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

TiAl based intermetallic alloys are promising high-temperature structural materials. Nb addition can enhance the strength, and precipitation hardening can improve the strength and creep-resistance of the alloys.

Dissociation of super-dislocations in Ti-48at.%Al-1at.%Nb and Ti-48at.%Al-10at.%Nb has been studied by HRTEM. Corresponding superlattice intrinsic stacking fault (SISF) energies in γ-TiAl were determined to be about 63 mJ/m^2 and 34 mJ/m^2, respectively. It is concluded that Nb addition can decrease the SISF energy, which may contribute to the strengthening effect. The microstructure of Ti-48 at.% Al-10 at.% Nb aged at 1073 K was also investigated by TEM. Needle-like γ1-$Ti_4Nb_3Al_9$ precipitates in the γ-TiAl matrix predicted before were for the first time observed. Their morphology and the orientation relationship was characterized.

The precipitation reaction of $L1_2$-$(Al,Ag)_3Ti$ in an $L1_0$ -TiAl(Ag) based Ti-54at.%Al-2at.%Ag alloy has been studied by TEM, HRTEM and supporting micro-hardness test preliminarily. The maximum hardness appeared in the samples with an average precipitate diameter of about 40 nm. The morphological evolution of the precipitates was discussed.

MM 8.4 Mon 15:30 IFW B

Monte-Carlo-Simulation of Nucleation of GP-Zones in Al-Cu-Alloys — •Andreas Lammerschop, Volker Mohles, and Günter Gottstein — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, Kopernikusstr. 14, 52056 Aachen

Age-hardening by precipitation is one of the most important mechanisms for strengthening of Al-alloys. We present an atomistic Monte-Carlo-Model for calculations on an f.c.c.-lattice. Diffusion is implemented by a vacancy mechanism. The thermodynamic driving force is represented as a regular solution model based on the bonding energies of the nearest and next nearest neighbours. The elastic energy model is based on the concept proposed by Eshelby and Khachaturyan. As to be expected from experiments, the simulations show that precipitations nucleate parallel to {100}-planes. This is actually caused by the elastic energy. In these MC-simulations, the thermodynamic energetics used have been based on experiments. The coupling of this model with quantum theory calculations (DFT) will improve the understanding of the formation process. Moreover it will enable true predictions on the precipitation kinetics in other f.c.c.-alloys.

MM 8.5 Mon 15:45 IFW B

First-principles studies on the precipitation thermodynamics of Al-Cu alloys — •Shaoqing Wang and Hengqiang Ye — Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

The technique of precipitation hardening is widely used for strengthening alloy materials in metallurgical industry. We studied the structure and ground-state energetics of Guinier-Preston (GP) precipitates in Al-Cu alloys. An atom-scale mechanism for the formation and structure evolution of GP zones in Al-Cu alloys was proposed [1]. The precipitation is a thermodynamic phenomenon. For a thorough understanding of the matter, it is essential to investigate the thermodynamic aspect of the process. In present work, we study the precipitation thermodynamics of Al-Cu alloys by first-principles response-function calculation [2]. The optimized atomic configurations of Al-Cu superlattices [1] for different Cu content are adopted as the starting point. We firstly calculate the dynamical matrices of Al-Cu superlattices for a set of special q-points. Then the full phonon spectrum is obtained by the Fourier interpolation algorithm of dynamical matrices [3]. From these full phonon spectrums, the temperature dependences of Helmholtz free energy and entropy of these Al-Cu superlattices are calculated. The structure evolution of GP precipitation as temperature decreases is reasonably interpreted.

[1] S. Q. Wang, M. Schneider, H. Q. Ye, G. Gottstein, Scripta Mater. 51, 665 (2004).
[2] X. Gonze, Phys. Rev. B 55, 10337 (1997).
[3] S. Baroni et al., Rev. Mod. Phys. 73, 515 (2001).

MM 8.6 Mon 16:00 IFW B

Are Guinier-Preston Zones in Al-Alloys stabilized by GrowninStructural Vacancies — •Torsten E.M. Staab, Michael Roebel, and Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik,Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16,D-53115 Bonn, Germany

Aluminum alloys obtain their strength by nanometer-sized precipitations of their alloying elements, which are effectively hindering the dislocation motion. The morphology of precipitations varies from spherical via ellipsoidal to plate- or needle-like structures. Recent ab-initio calculations on a plane of 14 Cu atoms – not containing any vacancies – in aluminum showed that this structures are unstable [1]. However, structural vacancies may be found in precipitations as-grown after solution heat treatment, quenching to water, and subsequent ageing. By the SIESTA ab-initio code we calculate the formation energies for vacancies in aluminum and their binding energy to substitutional atoms of the alloying elements for Al-Ag, Al-Cu and Al-MgSi. Additionally, we determine the formation and binding energies for vacancies inside the precipitations in

these materials, since important classes of technical alloys used in outer shell plates of airplanes are based on AlCu or AlMgSi. The results of the ab-initio calculations will be compared to positron annihilation experiments on AA2024 and AA6013 alloys.
[1] M. Röbel, Dissertation University Bonn, 2005

MM 8.7 Mon 16:15 IFW B

Analyse of frequency spectrum in the austenitic steel sample — •Remus Zagan, Petre Petculescu, and Niculae Peride — Ovidius University of Constanta, Mamaia Ave. 124, 900527, Constanta, Romania

This paper presents some experimental results in order to evaluate the effect of wavelet transform (WT) filtering on ultrasonic spectral analysis. By applying WT, the authors proved that it is possible to compress and filter the ultrasonic signal buried in noise, without any loss of accuracy in the time measurement. The experiments were made on an austenitic stainless steel sample 16Mo3. For the peak frequency the following values were found: 4.11 MHz by power spectrum (PS) and 4.111 MHz by power spectrum density (PSD). In this paper, we have used the power spectrum (PS) and power spectral density (PSD) for the determination of the frequency values of the spectrum and spectrum resonance spacing domains (SRSD). The experimental results presented here were obtained by the direct contact method using silicon gel as the coupling medium by pulse-echo technique. The instrumentation consisted of an IPR-100 pulser-receiver, a A/D-90 converter and a SMC-4 from Physical Acoustic Corporation, a sampler and a spectral analyzer. Keywords: ultrasounds, wavelets, power spectrum,power spectral density.

MM 9 Interfaces

Time: Monday 14:45–16:15 Room: IFW D

MM 9.1 Mon 14:45 IFW D

Ab-initio based multiscale calculations of low-angle grain boundaries in Aluminum. — •Liverios Lymperakis and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf

It is commonly accepted that grain boundaries have a central role in grain growth and recrystallization, and have significant contribution to the physical and mechanical properties of materials. A major challenge in describing extended defects such as low-angle grain boundaries is the large range of different length scales: The boundary consists of an array of dislocations where the core structure of each dislocation is rather localized, while the strain field is long range. In a previous study we have developed an ab-initio based multiscale approach that combines elements of density functional theory (DFT), empirical potentials, and continuum elasticity theory[1]. In the present study we have extended the formalism to an infinite array of ordered dislocations as realized in a low angle grain boundary. Based on this approach we have derived a diagram which predicts the energetically most stable boundary as function of the misorientation angle, the relevant displacement between the two grains, and the boundary-boundary separation distance. Based on this diagram we address the issue of grain boundary stability and we discuss recent experimental results.
[1] Phys. Rev. Lett. 93, 196401 (2004).

MM 9.2 Mon 15:00 IFW D

Structure and reactivity at the Ti-Si boundary — •Sibylle Gemming[1,2], Andrey Enyashin[1,2], and Michael Schreiber[2] — [1]Physikalische Chemie und Elektrochemie, Technische Universität, D-01062 Dresden. — [2]Institut für Physik, Technische Universität, D-09107 Chemnitz.

The density-functional band-structure investigation of several supercell models for the Ti(0001)|Si(111) interface reveals that an atomically flat interface is quite unstable due to the large lattice mismatch between the two constitutents. The most realistic supercell model with a remaining strain of 1% yields a very low interface energy of only 0.28 J/m^2 with respect to fracture into the two unrelaxed surfaces. This adhesion is mainly due to an interfacial electron transfer from Ti to Si. Other possible model structures with higher local strains are even non-bonding, which indicates the pronounced influence of the elastic interactions. Density-functional molecular dynamics at an elevated temperature of 600 K, however, shows, that a silicide interlayer is formed at the interface, which significantly strengthens the interface and doubles the interface energy. Further investigations on the interfaces between Ti or Si and the reaction product $TiSi_2$ confirm, that the silicide layer at the interface is beneficial for the mechanical stability of the contact.

MM 9.3 Mon 15:15 IFW D

Modelling and Characterisation of Interface Reactions between Diamond and Active Brazing Alloys — •Chunlei Liu[1,2], Ulrich E. Klotz[1], Peter J. Uggowitzer[2], and Jörg F. Löffler[2] — [1]Empa, Materials Science and Technology, Laboratory of Joining and Interface Technology, CH-8600 Dübendorf, Switzerland — [2]Laboratory of Metal Physics and Technology, Department of Materials, ETH-Zürich, CH-8093 Zürich, Switzerland

Diamond brazing has been deemed an effective route to the manufacture of high-performance diamond abrasive tools, and knowledge of the microstructure evolution of the interfacial area and the filler metal during the brazing process is of prime interest to enhance performance and to overcome existing problems. To reveal the microstructure evolution during the brazing process, we used a combination of thermodynamic modelling and sophisticated experimental techniques. A consistent thermodynamic database of the Cu-base filler metals was developed using the CALPHAD (Calculation of Phase Diagram) approach. The thermodynamic calculation and the experimental results show good agreement. Several alloy compositions and brazing temperatures were then selected according to the thermodynamic calculation for brazing trials. The interfacial structures were examined using FIB (Focused Ion Beam) and TEM (Transmission Electron Microscopy). The morphology of the reaction layers and nano-sized carbides grown at the interface between diamond and the alloy matrix were also studied to illustrate the reaction mechanism. These results are finally used for kinetic simulations, with the aim of achieving better properties in brazed diamond tools.

MM 9.4 Mon 15:30 IFW D

Examination of Grain Rotation Kinetics by Orientational Imaging Microscopy (OIM) — •M. Ziehmer[1], A. Tschöpe[1], C. Krill[2], and R. Birringer[1] — [1]Technische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Elektrotechnik, Universität Ulm, 89081 Ulm

The specific grain boundary energy γ depends on the misorientation θ of the adjacent grains. As a consequence, a torque which is proportional to the derivative of γ with respect to θ is acting on the grains . Sufficient thermal energy provided, this torque results in a rotation of the grains into local energy minimum configurations.

There are several open questions concerning the functional form of γ with respect to θ and the influence of grain boundary spatial extent on the rotation rate and the rotation mechanisms, which could all be enlightened by examining the rotation kinetics of individual grains.

We report on measurements of grain rotations in terms of the established method of spheres sintered onto a flat substrate. Both substrate and spheres are made of single crystalline copper. We take advantage of the progress in experimental techniques and use OIM for the measurement of the relative orientation of sphere and substrate. This method enables to study the rotations of single spheres over several orders of magnitude in grain boundary extent.

MM 9.5 Mon 15:45 IFW D

Paradoxical grain-growth kinetics observed in Al under compression — •Kejing Yang and Carl Krill — Materials Division, Albert-Einstein-Allee 47, University of Ulm, D-89081 Ulm, Germany

The mobility of grain boundaries in metals depends on stress in an intuitively reasonable manner: namely, compression slows the rate of boundary migration relative to that in the uncompressed state. Volkert and Lingk's discovery of *enhanced* boundary mobility in compressed Al films therefore came as a great surprise [1]. These authors attributed the faster grain growth in compressed regions to planarization of the film surface, which would be expected to reduce the pinning forces associated with grain-boundary grooving. We have tested this hypothesis in microcrystalline Al foils prepared by melt spinning. Since our samples are

much thicker than the initial average grain size, a clear distinction can be drawn between surface and volume-related effects. Characterization by EBSD confirms the mobility enhancement induced by compression, but cross-sectional analysis suggests that the greatest increase in growth rate occurs in the center of the sample rather than at the surface! We discuss possible explanations for this observation in terms of mechanisms for boundary migration.

[1] C. A. Volkert and C. Lingk, *Appl. Phys. Lett.* **73** (1998) 3677.

MM 9.6 Mon 16:00 IFW D

MD simulations about ordering and dynamics in Zr-crystal Ni_xZr_{1-x}-melt interfaces — •M. Guerdane and H. Teichler — Institut f. Materialphysik d. Univ. Göttingen, 37077 Göttingen

The contribution reports results from molecular dynamics (MD) simulations about local order and dynamics in binary Ni_xZr_{1-x} melts in contact with Zr crystalline solid. The crystalline interface induces a local order in the way that the trigonal-prismatic structure elements (tp-elements), inherent to the Ni_xZr_{1-x}-melt, are attached to the crystalline wall in an ordered way. (110)-crystal interfaces show a marked roughness compared with (100)-interfaces, which can be attributed to a better adaptation of the tp-elements to the (100)- than to the (110)-surface. Atoms in the liquid surface layer have a lower energy than those in the crystal and in the interior of the melt. The ordered arrangement of the tp-elements in the liquid layer near the interface influences the atomic dynamics and seems to dominate the crystallization kinetics in the crystal/liquid couples. (Funded by the DFG, SPP 1120)

MM 10 Intermetallic phases

Time: Monday 16:30–17:45 Room: IFW D

MM 10.1 Mon 16:30 IFW D

Anomalous equilibrium volume change of magnetic Fe-Al crystals — •Martin Friák and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany

Iron aluminides represent a very promising class of intermetallic materials with great potential for substituting stainless steels at elevated and high temperatures. Recent experiments observed an anomalous equilibrium-volume behaviour as a function of concentration in Fe-rich compounds [1]. This effect has been tentatively assigned to be due to an order-disorder transition.

In order to clarify this point we have studied the role of magnetism in Fe-Al crystals employing density functional theory (DFT) within the generalized gradient approximation (GGA). The excess energies, equilibrium lattice parameters and magnetic states have been determined for a dense set of different iron concentrations and a large variety of atomic configurations. Both external and internal relaxations were allowed.

The spin-polarized calculations for *ordered* ferromagnetic Fe-rich compounds nicely reproduce the anomalous volume behaviour, i.e. the effect is *not* related to an order-disorder transition. Analyzing different magnetic states we identified the change in magnetism to be the driving force. In fact, performing the same calculations but switching off magnetism removed the anomalous volume dependence and showed a clear linear dependence. Based on these results the importance of order-disorder transition in Fe-Al systems is revisited.

[1] R. A. Buckley and S. Kaviani, *Mat. Sci. Eng.* **A258**, 173 (1998).

MM 10.2 Mon 16:45 IFW D

Detecting low-temperature intermetallic compounds in the Ag-Pd-system - a first principles study — •E. Winning, S. Bärthlein, and S. Müller — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

Similar to Cu-Pd and Au-Pd, Ag-Pd-compounds form long-periodic superlattices (LPS) based on the $L1_2$-structure at 25at.% Pd. Experimentally Ag-Pd is known to form mutually miscible disordered solid solutions down to $\sim$ 800 K, but at lower temperatures no experimental data is available up to now. With the help of total-energy DFT calculations and a mixed-space cluster-expansion (MSCE) in conjunction with genetic algorithms (GA) [1], effective multi-body interactions are designed, that permit us to study millions of possible ground-states (GS) over the full concentration range. We thus find some new GS compared to earlier studies [2]. Most notably we predict the LPS3 as GS at $x_{Pd} = 0.25$. At $x_{Pd} = 0.5$ we can confirm earlier results by also predicting $L1_1$ as ground state, although a similar structure lies almost degenerately above. Like in the case of Cu-Pd 2D- and 3D-LPS are taken into consideration to confirm the LPS3-structure as GS. By applying Monte Carlo simulations we predict the phase transition temperatures and the short-range order behaviour.

[1] G.L.W. Hart et al., Nat. Mater. **4**, 391 (2005)
[2] S. Müller and A. Zunger, Phys. Rev. Lett. **87**, 165502 (2001)

MM 10.3 Mon 17:00 IFW D

Electric conductivity of long-range ordered FeAl alloys clarified by ab-initio calculations — •Wilfried Wunderlich[1], Raimund Podloucky[2], Wolfgang Püschl[3], and Wolfgang Pfeiler[3] — [1]Nagoya Institute of Technology, Japan — [2]Institut für Physikalische Chemie, Universität Wien — [3]Institut für Materialphysik, Universität Wien

Complicated resistivity behaviour in near-stoichiometric FeAl was interpreted as a transient establishment of local order on the way to a homogeneous equilibrium state of long-range order. In order to get more insight into the resistivity of short-range and long-range ordered states in this material, ab-initio studies were performed by extending previous band structure calculations from the literature. Spin-dependent VASP calculations were done for FeAl model crystals both defect-free and containing vacancies and antisite defects. From the curvature of bands near the Fermi level the effective electron mass was determined. The results are discussed in the framework of the Kubo-Greenwood formalism with reference to the experimental findings.

MM 10.4 Mon 17:15 IFW D

The Re-containing Inconel 706 Alloy: 3DAP Measurements — •Vitaliy Kindrachuk[1], Nelia Wanderka[1], John Banhart[1], Dominique Del Genovese[2], and Joachim Rösler[2] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany — [2]Institut für Werkstoffe, TU Braunschweig, Langer Kamp 8, 38106 Braunschweig, Germany

Inconel 706 is a wrought Ni-Fe base superalloy which is used for applications at service temperatures up to 600°C. The good mechanical properties are caused by precipitation of intermetallic phases γ' (L12 structure) and γ'' (DO22 structure). Re is known to stabilize the microstructure of Ni-based superalloys at higher temperature. Therefore, the influence of Re on Inconel 706 was investigated in the present study.

The microstructure evolution of 0.6 at.% Re-alloyed Inconel 706 was studied after ageing at 750°C for 750 h and 5000 h by three-dimensional atom probe tomography and by TEM.

The modified stabilization heat treatment (MST) produces individual γ' and γ'' precipitates and γ'/γ'' co-precipitates with average sizes of about 15 nm. Re concentrates mostly in the matrix (about 0.8 at. %), whereas the intermetallic phases contain 0.2 - 0.3 at.%. Large γ'' plates with sizes of about 50 - 100 nm are formed after ageing at 750°C for 750 h. Their Re-content is very small (0.07 at.%).

After ageing for 5000 h only one type of precipitates remains, namely η plates embedded into the matrix. Therefore, the Re-alloyed Inconel 706 loses its mechanical properties. Unexpectedly Re does not stabilize the microstructure of the alloy at 750°C.

MM 10.5 Mon 17:30 IFW D

Metastable phase formation in Ti-Al-Nb undercooled melts — •Olga Shuleshova, H-Günther Lindenkreuz, Regina Hermann, Thomas George Woodcock, Wolfgang Löser, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Metastable phase formation processes in ternary Ti-Al-Nb turbine blade alloys have been studied by containerless electromagnetic levitation for melt undercooling up to 300 K below the liquidus temperature. The

recalescence behaviour of $Ti_{45}Al_{45}Nb_{10}$ indicates β-phase formation with subsequent β to α transformation, whereas from the double-recalescence events of $Ti_{40}Al_{50}Nb_{10}$, $Ti_{45}Al_{50}Nb_5$ melts metastable β-phase formation is inferred beyond critical undercooling in the range of 150 K. Dendrite growth velocities of 10 to 20 m/s for highly undercooled Ti-Al-Nb melts are consistent with primary β-phase formation, which is promoted by Nb addition. For $Ti_{45}Al_{50}Nb_5$ and $Ti_{40}Al_{50}Nb_{10}$ alloys a second recalescence near 1300°C attributed to an α to γ solid state transformation was observed in the pyrometer trace. The γ-phase formation was suppressed in favour of a homogeneous α_2-phase in undercooled $Ti_{45}Al_{45}Nb_{10}$ samples quenched onto a chill substrate. Whereas, in $Ti_{40}Al_{50}Nb_{10}$, high undercooling enabled a direct γ-phase solidification.

MM 11 Invited talk Züttel

Time: Tuesday 09:30–10:00 Room: IFW A

Invited Talk MM 11.1 Tue 09:30 IFW A

The Materials Challenge for Hydrogen Storage — •Züttel Andreas — University of Fribourg, Physics Department, Pérolles, CH-Fribourg, Switzerland

The intense use of fossil hydrocarbons as energy carriers has caused an increase of CO_2 in the atmosphere. Furthermore, the reserves of fossil fuels on earth are finite and no matter how long they will last, an energy system independent of fossil fuels has to be developed for the future. Hydrogen exhibits the greatest heating value (39.4 kWh/kg) of all chemical fuels. Hydrogen can be produced by electrolysis from renewable energy, and is therefore regenerative and environment friendly. Hydrogen is stored by six different methods:

•high pressure gas cylinders (up to 800 bar)
•liquid hydrogen in cryogenic tanks (at 21 K)
•adsorbed hydrogen on materials with a large specific surface area (at $T < 100K$)
•absorbed on interstitial sites in a host metal (at ambient pressure and temperature)
•chemically bond in covalent and ionic compounds (at ambient pressure)
•oxidation of reactive metals and complex hydrides e.g. Li, Na, with water

Each method has its specific properties and limitations. The physical boundaries and the potentials will be outlined especially in view of the materials challenges.

MM 12 Symposium Severe Plastic Deformation III

Time: Tuesday 10:15–12:45 Room: IFW A

Keynote Talk MM 12.1 Tue 10:15 IFW A

Scaling Effects on the Plasticity of ECAP Nickel — •Lutz Hollang[1], Ellen Hieckmann[2], Dieter Brunner[3], Carl Holste[1], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [3]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The influence of grain size on the interaction mechanisms between dislocations governing the plastic behaviour of fcc metals at low temperatures was studied by means of thermal activation analysis. For this purpose the plastic behaviour of sub-microcrystalline (smc) nickel processed by equal-channel angular pressing (ECAP) was investigated in tension at constant temperatures between 4 K and 320 K. Stress-relaxation experiments performed during the tensile tests were used to determine the rate sensitivity of the material as a function of the flow stress. In all cases the relationship is found to be linear revealing that the mean dislocation spacing influences both, the athermal and thermal contribution to the flow stress in the same manner as predicted by the Cottrell-Stokes law. The effect of grain size on the flow stress can be attributed to a constant additive athermal stress contribution. Moreover, the thermal activation analysis indicates that at temperatures below 100 K a local single slip mechanism governs the plastic behaviour of smc ECAP nickel. At higher temperatures other thermally activated slip processes become rate controlling. They are probably connected with the thermally activated dissolution of the initial ECAP structure.

Keynote Talk MM 12.2 Tue 10:45 IFW A

Large plastic deformation of binary FeCr alloys - a new approach to understand the creep properties of tempered martensite ferritic steels — •Gunther Eggeler — Institut für Werkstoffe, Ruhr-Universität Bochum, Germany

In the present study we use equal channel angular pressing (ECAP) to strongly deform a binary Fe10Cr alloy. The ECAP parameters are adjusted such that the Fe10Cr alloy develops an ultra fine grained microstructure which appears to be very similar to the microstructure of a tempered martensite ferritic reference steel (German grade X20). We use transmission (TEM) and scanning electron microscopy with orientation imaging (SEM&OIM) to investigate grain sizes, grain shapes and grain orientations in both materials. While the two materials show very similar ultra fine grain microstructures, the grain boundaries of X20 are stabilized by carbides. We perform creep experiments on both materials and compare creep curves as well as the evolution of microstructures during creep. The results show how imported boundary carbides are in providing the good creep resistance of tempered martensite ferritic steels. The martensitic transformation (accompanied by strong internal stresses and strains) which represents an essential first step in the heat treatment of tempered martensite ferritic steels and the subsequent aging result microstructures which in the absence of a martensitic transformation can only be established by severe plastic deformation.

Keynote Talk MM 12.3 Tue 11:45 IFW A

Fatigue Behaviour of Ultrafine Grained BCC and FCC Materials — •Hans J. Maier[1] and Heinz Werner Höppel[2] — [1]Lehrstuhl für Werkstoffkunde, Universität Paderborn — [2]Lehrstuhl Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg

The present study reports on the fatigue behaviour of ultrafine grained materials with BCC (interstitial free (IF) steel) and FCC (copper and aluminium) structure. The ultrafine microstructures were obtained using equal channel angular extrusion (ECAE) at room temperature. Low-cycle fatigue tests were conducted in total strain-controlled fully reversed push-pull loading. Transmission electron microscopy was employed to characterize microstructural evolution. Cyclic stress-strain response was monitored both in constant amplitude tests and incremental step tests. Stable cyclic stress-strain response was observed for optimized ECAE routes. For ultrafine grained FCC materials, ECAE processing is commonly reported to result in an increase in cyclic strength but a decrease in fatigue life when compared with unprocessed material. By contrast, a more than two-fold increase in strength and number of cycles to failure was observed after optimum ECAE processing of the IF steel in the current study. In addition, in-situ fatigue tests were conducted in an environmental SEM to understand the substantially different fatigue behavior of the ECAE-processed materials. The implications of the damage mechanisms observed are discussed with respect to optimization of ultrafine microstructures.

Keynote Talk MM 12.4 Tue 12:15 IFW A

Cylic Deformation Behaviour and Fatigue Life of Ultrafine-Grained Aluminum — •Dorothea Amberger, Johannes May, Heinz-Werner Höppel, and Mathias Göken — Lehrstuhl Allgemeine Werkstoffeigenschaften, Martensstrasse 5, 91058 Erlangen

Bulk ultrafine-grained (UFG) metals with grain sizes in the submicrometer range can be produced by Equal Channel Angular Pressing. Generally UFG materials exhibit extraordinary mechanical properties [1,2], and show also an enhanced strain rate sensitivity (SRS). The mechanisms responsible for the SRS, like Coble creep, grain boundary sliding or thermally activated annihilation of dislocations [1,2,3,4], are still unclear. This work focuses on the influence of the strain rate of UFG Al

under cyclic loading. The obtained stress amplitudes for the tests performed at a smaller strain rate are only smaller within the first hundred cycles. This is in accordance to the observations under monotonic loading. After the first hundred cycles no significant differences between the obtained stress amplitudes with respect to the strain rate were found. Based on these results it can be concluded that grain boundary sliding or coble creep cannot be the relevant mechanisms for SRS, as there is no reasonable explanation for the diminishing of the difference in the stress amplitudes during cycling. In contrast, annihilation of dislocations can quite reasonably explain these results.

[1] RZ Valiev, IV Alexandrov; J Mater Res 2002 17 (1) 5 [2] HW Höppel, J May, M Göken; Adv Eng Mater 2004 6 781 [3] YJ Li, XH Zeng, W Blum; Acta Mater 2004 52 5009 [4] J May, HW Höppel, M Göken; Scripta Mater 2005 53 189

MM 13 Symposium Modern Metallic Materials Design III

Time: Tuesday 10:15–13:15 Room: IFW B

MM 13.1 Tue 10:15 IFW B

Formation and properties of Ce-based Metallic Plastics — •Bo Zhang and Wei Hua Wang — Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P. R. China

We report the formation and unique properties of the polymerlike Ce-based bulk metallic glasses. Ternary Ce-Al-Cu(Co,Ni) glassy rods of 1-3 mm in diameter can be easily formed in a wide composition range by a conventional copper-mold cast method. Substituting Ce with low cost Ce-rich misch metal (MM), MM-Al-Cu bulk glasses have the similar glass forming ability (GFA) as that of Ce-Al-Cu. With minor addition of extra elements like Fe, Co, Ni, Nb, Zn and Si, the critical diameter of full glassy rods of the matrix Ce-Al-Cu can be remarkably enhanced from 2 mm to at least 3-10 mm. It is found that the often-cited empirical criteria for bulk metallic glass formation cannot interpret the formation and addition effect on GFA in the metallic glasses. The striking effect and mechanism of the microalloying on the GFA of the metallic glasses are studied. These materials with extremely low glass transition temperature Tg (341 K - 439 K, even below the boiling temperature of water) and excellent deformability at low temperatures, which can be regarded as metallic plastics, should have potential applications.

MM 13.2 Tue 10:30 IFW B

Ductile Cu-Zr- base bulk metallic glasses — •J. Das[1,2], M.B. Tang[3], K.B. Kim[1], B.C. Wei[4], W.H. Wang[3], and J. Eckert[1] — [1]FG Physikalische Metallkunde, FB 11 Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany — [2]IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany — [3]Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China — [4]Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

Usually bulk metallic glasses exhibit strength values superior to conventional crystalline alloys, often combined with a large elastic limit and rather low Young's modulus. However, the major drawback for engineering applications is their limited room temperature ductility and toughness due to the localized deformation processes linked to shear banding. In this work we report on a new class of metallic glass in a simple Cu-base alloy. Addition of 5 at.% Al increases the glass-forming ability of binary Cu50Zr50. The resulting Cu47.5Zr47.5Al5 glass exhibits high strength (2265 MPa) together with large room temperature ductility up to 18%. After yielding a strong increase in the flow stress is observed during deformation. The interaction and intersection of shear bands increases the flow stress of the material with further deformation, leading to a "work hardening"-like behaviour and yields a continuous rotation of the shear angle up to fracture resulting in a high compressive ductility. This work was funded by the Chinesisch-Deutsches Zentrum für Wissenschaftsförderung (Grant No. GZ032/7) and the Deutsche Forschungsgemeinschaft (Grant Ec111/12)

MM 13.3 Tue 10:45 IFW B

Local amorphization/nanocrystallization in a bulk Ni45Cu5Ti33Zr16Si1 alloy during solidification — •K. B. Kim[1], S. Yi[2], H. Choi-Yim[3], J. Das[1,4], W. Xu[1], W. L. Johnson[5], and J. Eckert[1,4] — [1]FG Physikalische Metallkunde, FB 11 Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany — [2]Department of Materials Sciences and Metallurgy, Kyungpook National University, 1370 Sankyuk-dong, Buk-gu, Daegu 702-701, Korea — [3]Department of Physics, Sookmyung Women*s University, Seoul 140-742, Korea — [4]IFW Dresden, Institute für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany — [5]Keck Laboratory of Engineering Materials, California Institute of Technology, Pasadena, California 91125, USA

A local amorphization/nanocrystallization at the interfaces between B2 ordered Ni(Ti,Zr) phase and NiTiZr phase with P63/mmc has been investigated in a multicomponent Ni45Cu5Ti33Zr16Si1 alloy during solidification. So far there are several well-known mechanisms for interfacial amorphization in the solid state but no interfacial instability-driven amorphization/nanocrystallization during transition from liquid to solid state has ever been reported. The curvature of the interfacial area of the ordered Ni(Ti,Zr) phase is locally negative accompanying reverse atomic diffusion. This results in the frustration of the strong ordering tendency of the Ni(Ti,Zr) phase, and induces local amorphization/nanocrystallization.

MM 13.4 Tue 11:00 IFW B

Solidification and magnetic properties of Fe-Cr-Mo-Ga-P-C-B bulk metallic glasses — •Jürgen Eckert[1], Mihai Stoica[2,3], Nicolle Radtke[2], Stefan Roth[2], Ludwig Schultz[2], Jürgen Eckert[1], and Wei Hua Wang[4] — [1]Darmstadt University of Technology, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]IFW Dresden, PF 270016, D-01171 Dresden, Germany — [3]Present address : LTPCM-CNRS UA29, INP Grenoble 38402, France — [4]Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

Our work focused on $(Fe_{77.5-x-y-z}Cr_xMo_yGa_zP_{12}C_5B_{5.5}$ with (x,y,z) = (4,4,4), (4,4,2), (4,4,0) and (2,2,2)) alloys, which were cast into different geometries. The structure of the samples was checked by X-ray diffraction. Thermal stability studies and isothermal annealing were done in a differential scanning calorimeter (DSC). The fracture strength for the as-cast samples is around 3 GPa and the fracture strain reaches 2%. The Vickers hardness HV for the as-cast samples is about 885, and increases to 902 upon annealing. The fracture of this Fe-based BMG is not propagating along a well-defined direction and the fractured surface looks irregular. Instead of veins, the glassy alloy develops a high number of microcracks. The coercivity of as-cast samples is lower than 10 A/m, decreasing to 0.7 A/m after annealing. The saturation polarization at room temperature is around 0.8 T, increasing up to 1 T at 77 K. This work was funded by the National Science Foundation of China (Grants No. 50371098 and 50321101), the Chinesisch-Deutsches Zentrum für Wissenschaftsförderung (Grant No. GZ032/7) and the Deutsche Forschungsgemeinschaft (Grant Ec 111/12)

MM 13.5 Tue 11:45 IFW B

Effect of the S/L interface on the solidification of immiscible alloy — •Jie He[1], Jiuzhou Zhao[1], and Lorenz Ratke[2] — [1]Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, P R China — [2]Institute for Space Simulation, DLR, Cologne 51147, Germany

Directional solidification experiments have been carried out for Al-Bi based immiscible alloys at different solidification rates. The morphology of the solid/liquid (S/L) interface and the possible interaction modes between the droplets and the interface were discussed. A numerical model has been developed based on the population dynamic approach to calculate the formation of the microstructure under the common actions of the minority phase nucleation, growth, droplet motion ahead of the interface and the interaction between the interface and the droplets. Calculations have been carried out according to the practical solidification conditions. The effect of the interaction between the interface and the droplets has been discussed. The calculated results agree well with the experimental ones. This work will favor further understanding the solidification process of immiscible alloys.

MM 13.6 Tue 12:00 IFW B

Microstructure evolution in rapidly solidified immiscible alloys — •Frank Schmidt-Hohagen [1], Lorenz Ratke[1], and Jiuzhou Zhao[2] — [1]German Aerospace Center, Inst. of Space Simulation, Köln — [2]Inst. of Metal Research, Chinese Academy of Sci., Shenyang, China

When a hypermonotectic alloy is cooled from the single-phase liquid state into the miscibility gap, the components are no longer miscible and two liquid phases develop. Generally the liquid-liquid decomposition of an initially homogenous liquid begins with the nucleation of the liquid minority phase in the form of droplets, which grow by diffusion. Reaching the non-variant monotectic reaction temperature the matrix liquid decomposes into a solid and a second phase, being not distinguishable from the liquid minority phase that emerged in the miscibility gap. The size spectra of the drops of both processes merge the larger the cooling rate. Within a suitable interval of cooling rates they become, however, distinguishable and then the spectra stemming from the liquid-liquid decomposition gives unique access to the nucleation process inside the miscibility gap. Immiscible alloys like Al-Pb offer a great potential as for instance self-lubricating bearings in automotive applications, if a finely dispersed microstructure is achieved. This can be obtained under conditions of rapid cooling. In order to explore the potential of rapid solidification of immiscible alloys, investigations of the microstructure of different Al-Pb alloys were carried out, varying over a wide range of alloy-concentrations and cooling rates. The experimental results, obtained with the help of different methods, are compared with numerical simulations of the decomposition and the microstructure evolution process.

MM 13.7 Tue 12:15 IFW B

Rapid solidification of Cu-Co alloy — •Jiuzhou Zhao[1], Matthias Kolbe[2], Jianrong Gao[3], L. L. Gao[1], Lorenz Ratke[2], and Dieter M. Herlach[2] — [1]Institute of Metal Research, CAS, Shenyang 110016, China — [2]Institute of Space Simulation, German Aerospace Center DLR, D-51170 Cologne, Germany — [3]Key Lab of Electromagnetic Processing of Materials, Northeastern University, Shenyang 110004, China

A model is developed to describe the microstructure evolution in Cu-Co drops during cooling in the metastable miscibility gap in the liquid state. Calculations have been carried out according to the solidification experiments with $Cu_{84}Co_{16}$ alloy under drop tube conditions to the investigation of the kinetics of the liquid-liquid phase transformation in Cu-Co drops. It is demonstrated that the microstructure development is dominated by the common action of the nucleation and the diffusional growth of the minority phase droplets under the rapid solidification conditions. The calculated distribution of Co-precipitates and their average radius as a function of cooling rate are compared with the experimental results. The agreement is satisfactory.

MM 13.8 Tue 12:30 IFW B

Metal-like growth of silicon during rapid solidification — •Riping Liu[1], Q. Wang[1], Q. Jing[1], M. Z. Ma[1], Christian Panofen[2], and Dieter M. Herlach[2] — [1]Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, Hebei, P. R. China — [2]Institute of Space Simulation, German Aerospace Center DLR, D-51170 Koeln, Germany

In the theory of crystal growth, two idealized mechanisms, lateral growth and continuous growth, have been proposed. Systems with atomically rough or diffuse interfaces are thought to grow by the continuous growth mechanism. In this case, the solid-liquid interface is assumed to be rough on atomic scale so that the atoms can attach themselves uniformly on the interface. The grown crystals present non-faceted surface morphologies, as for metals. On the other hand, the solid-liquid interface may be atomically smooth except for the presence of atomic steps. Crystal growth in this case is lateral or edgewise. Atoms transferring from liquid to solid are first attached to the steps. The finally grown crystals often present faceted morphologies, as for silicon, germanium, and most of compounds.

Silicon is normally considered to grow in a faceted way. From our experiments on solidification of undercooled melt, however, growth of silicon at the beginning is continuous, just like that of metals. But with increasing of the crystal size or decreasing of the undercooling level, it will be transited to the faceted way.

MM 13.9 Tue 12:45 IFW B

Solidification of undercooled Si, Si-Co and Si-Ge melts — •Christian Panofen[1], Riping Liu[2], and Dieter M. Herlach[1] — [1]Institue of Space Simulation, German Aerospace Center (DLR), 51147 Köln, Germany — [2]Key Laboratory of Metastable Materials Science & Technology, Yanshan University, Qinhuangdao 066004, P. R. China

Pure Si, dilute Si-Co and Si-Ge melts were undercooled and solidified containerlessly by electromagnetic and electrostatic levitation techniques in a high purity environment. Large melt undercoolings of up to 330 K were achieved by this experiment procedure.

Crystallization of the undercooled melt was externally triggered by a nucleation stimulus needle at preselected undercooling and well defined position at the surface of the sample. In this way the velocity of the solidification front was measured as a function of undercooling by using a high speed CCD camera to record the propagation of the solid-liquid interface through the undercooled melt. High growth velocities of pure Si up to 16 m/s were determined.

The growth behavior was analyzed within current theories of crystal growth in undercooled melts. Special emphasis was placed to the transition from faceted planar to dendritic growth. The results of the growth measurements were correlated to microstructure formation upon undercooling prior to solidification.

This work is funded by the Sino-German Science Center, Beijing, DFG HE-1601/16

MM 13.10 Tue 13:00 IFW B

Undercooling and unidirectional solidification of Ni-Cu melts by electromagnetic levitation facility — •Qiang Wang[1], Riping Liu[1], Q. Jing[1], M. Z. Ma[1], Christian Panofen[2], and Dieter M. Herlach[2] — [1]Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, Hebei, P. R. China — [2]Institute of Space Simulation, German Aerospace Center DLR, D-51170 Koeln, Germany

Deep undercooling of metallic melt is a widely used method for investigation of nucleation and crystal growth during solidification. To obtain deep undercooling, electromagnetic levitation has been proved to be one of the most important techniques. A great deal of research has been given to nucleation, crystal growth, metastable phase formation (including metallic glass formation), thermal and physical properties of the undercooled melts, etc. Usually, the melt samples treated by this technique are spherical influenced by the gravity and the surface tension.

In this experiment, we report a new way to produce cylindrical undercooled melt samples with temperature gradients at different levels, and to investigate rapid unidirectional solidification of the undercooled melts. The cylindrical sample of Ni-Cu alloy, 5mm in diameter and 50 mm in height, was wrapped in dehydrated B_2O_3 flux in a quartz tube, and then heated by a gradient RF coil in an electromagnetic levitation facility. Treated by several cycles of heating and cooling, undercooling and directional solidification of the sample were obtained.

MM 14 Hydrogen in Metals I

Time: Tuesday 10:15–11:15 Room: IFW D

MM 14.1 Tue 10:15 IFW D

Modified Li-based alanate for hydrogen storage — •Stefania Doppiu, Ludwig Schultz, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

The development of new lightweight materials for hydrogen storage is an important requirement to use hydrogen as fuel for on-board application. Recently, alkali complex hydrides such as Li-alanates have attracted growing interest due to their high gravimetric and volumetric hydrogen densities. Efforts have been done to optimize the overall stability and, as a consequence, the hydriding temperature and the rehydriding pressure, by partial substitution of the alkali metal or the aluminum. In this study, LiAlH4 and LiAlH4 modified by adding MgH2 and TiCl3, subjected to mechanical milling under argon or hydrogen atmosphere, were investigated. Full structural characterization was performed by x-ray diffraction analysis using a full profile fitting procedure (Rietveld). The thermal stability was studied by high-pressure differential scanning calorimetry in a pressure range of 1-150 bar. Milling pure LiAlH4 induces

a partial decomposition of the hydride into Li3AlH6. DSC performed on the as-received and the milled samples shows a complex sequence of decomposition steps during heating. In the case of the samples doped with MgH2 and TiCl3, milling under argon induces almost complete decomposition of LiAlH4 into nanocrystalline LiH, MgH2, Al and H2. Further, it is demonstrated that milling under high hydrogen pressure (80 bar) allows to hinder to some extent the undesired decomposition reaction.

MM 14.2 Tue 10:30 IFW D

New hydride electrodes for Ni-MH batteries on basis of Mg-Ni-Y metastable alloys — •Bogdan Khorkounov, Annett Gebert , Christine Mickel, Margitta Uhlemann, and Ludwig Schultz — IFW Dresden, PF 27 01 16, Dresden, Germany

This work aims at characterizing of novel Mg-Ni-Y amorphous and nanocrystalline alloys with view to their possible application as new hydride electrode materials in Ni-MH batteries. On the example of Mg63Ni30Y7, the alloying conditions were optimised so that alloys with an amorphous or a nanocrystalline-amorphous microstructure were obtained. On basis of these alloy powders, hydride electrodes were fabricated and their electrode characteristics under battery operation conditions were investigated. The alloys with mixed nanocrystalline-amorphous microstructure prepared under use of a SPEX shaker mill and more considerable fraction of nanocrystalls reveal a higher electrochemical activity for hydrogen reduction at cathodic potentials and a higher maximum discharge capacity (247 mAh/g) than the alloys with predominantly amorphous microstructure (216 mAh/g) obtained when using a Retsch planetary ball mill at lowered temperatures. The positive role of increasing Y and Ni concentration in the alloy was observed. The influence of surface modification by coating of the alloy particles by graphite or nickel on the electrodes stability and reactivity was studied in detail.

MM 14.3 Tue 10:45 IFW D

Mechanism of hydrogen embrittlement in nickel, studied with in situ electrochemical nanoindentation — •Afrooz Barnoush and Horst Vehoff — Saarland University, Department of Materials Science, Bldg. D22. P.O. Box 151150, D-66041 Saarbruecken, Germany

The effect of hydrogen on the nucleation and multiplication of dislocations is examined on precisely oriented Ni (111) surfaces with a specifically designed nanoindentation set up for in-situ electrochemical experiments. With this set up, for the first time hydrogen/deformation interaction has been studied in-situ on a nano-scale under realistic conditions. The effect of the electrochemical potential on the indent load displacement curve, especially the unstable elastic plastic transition is studied in detail. Not only the surface films but also the local plasticity is influenced strongly by the potential. The experiments allowed to exclude surface from hydrogen effects. Clear evidence is provided that hydrogen atoms facilitate homogenous dislocation nucleation.

MM 14.4 Tue 11:00 IFW D

Local resolved hydrogen detection in technical alloys — •Christian Lenk, Matz Haaks, and Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nußalle 14-16 , D-53115 Bonn, Germany

The weldable aluminium alloy AA6013 used in aircraft construction shows during cyclic load in a corrosive medium an increased crack growth speed compared with deformation under normal atmosphere, as well as a slower annealing of point defects in the plastic zone. One assumes this behaviour is due to the uptake and diffusion of hydrogen during crack growth. This hypothesis has to be confirmed with an analytical detection of hydrogen in the plastic zone. For that purpose chips in the micrometer scale were cut from the sample in vacuum and in-situ heated under UHV conditions. The following increase of the partial pressure of hydrogen is recorded with a mass spectrometer. As a proof of principle, a sample made of a NiCu-alloy was loaded with a deuterium-concentration-structure. The distribution of the deuterium concentration was confirmed by the experiment.

MM 15 Hydrogen in Metals II

Time: Tuesday 11:45–12:45 Room: IFW D

MM 15.1 Tue 11:45 IFW D

Surface morphology changes and time dependency of hydride formation in thin epitaxial Nb-films — •Kai Nörthemann, Reiner Kirchheim, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The growth and arrangement of precipitates in thin epitaxial films is presented in this contribution, using the model system Niobium-Hydrogen.

With the surface sensitive scanning tunneling microscopy (STM) it is possible to distinguish between matrix and precipitates because of the different lattice parameter of niobium and niobium hydride. The STM measurements of thin epitaxial niobium films are taken during hydrogen loading, therefore the time dependency of the hydride formation and the orientation of the hydride can be examined. Two different types of hydride precipitates were found. Their appearance will be discussed. Their expansion is fitted to a Johnson-Mehl-Avrami kinetic. The stability of the α-phase and the hydride in the two phase field will be discussed.

This work is financially supported by the DFG via SFB 602.

MM 15.2 Tue 12:00 IFW D

Catalytic effect of oxides for decomposition of magnesium hydride explained by the gateway model. — •Andreas Borgschulte and Rüdiger Bormann — GKSS-Research Center, Geesthacht GmbH, WTP, building 59, Max-Planck-Straße 1, 21502 Geesthacht

The kinetics of the reversible reaction of hydrogen gas with magnesium forming MgH_2 is enhanced significantly by the addition of transition metals oxide catalysts and by using nanostructured powders. Hydrogen absorption and desorption properties of such systems were studied by high pressure differential scanning calorimetry (DSC) under hydrogen atmosphere, from which the heat of hydride formation and decomposition of magnesium hydride is revealed. We find an additional, slightly destabilized phase, which is formed within the first desorption. Its amount depends on the degree of nanostructuring and the used additive. The phase is attributed to destabilized magnesium hydride near grain boundaries. It is the intermediate step before the more stable, stoichiometric MgH_2-phase is formed. Thus the phase acts as a gateway for de-hydrogenation of MgH_2. The results correspond to neutron diffraction measurements, in which a $MgH_{x<<2}$ was found [1].

[1] H. Gijs Schimmel, Jacques Huot, Laurent C. Chapon, Frans D. Tichelaar, and Fokko M. Mulder, J. Am. Chem. Soc. **127**, 14348 (2005).

MM 15.3 Tue 12:15 IFW D

Optical characterisation of MBE grown neodymiumhydride films — •S. Weber, H. Schröter, and J. Schoenes — Institut für Physik der Kondensierten Materie, Mendelssohnstr. 3, D-38106 Braunschweig

Many rare earth metals have attracted attention because of their metal-insulator transition during hydrogen loading. Neodymium takes a special place among these as in addition to the opening of a large gap a transition to a ferromagnetic state has been reported.

Thin films of Nd have been grown onto CaF_2 and Si-substrates using the MBE technique. In order to prevent corrosion in ambient air and to allow hydrogenation of the samples a protective layer of palladium is mandatory. A Nb-bufferlayer is used to prevent interdiffusion between the Pd-layer and the Nd-film which strongly deteriorates the quality of the samples. Temperature dependend measurements on hydrogenated samples have been performed using a FT-IR-spectrometer in the energy range of 5meV to 1eV. The spectra show 5 phonon modes which can be assigned unambiguously to hydrogen vibrations by comparison with deuterium loaded samples. The transmission spectra of the samples which are multiple layer systems can be simulated using a thin film model. Subsequently, the optical properties of NdH_x can be determined. The modelling parameters indicate an expansion of the films by a factor of about 2

during hydrogenation which was confirmed by AFM measurements. Furthermore, the optical band gap was measured by UV/Vis-spectrometry.

MM 15.4 Tue 12:30 IFW D

Raman spectroscopy study of strong correlation effects in $YH_{3-\delta}$ — •A.-M Racu and J. Schoenes — Institut für Physik der Kondensierten Materie - TU Braunschweig Mendelssohnstrasse 3, 38106 Braunschweig

Temperature dependent Raman measurements on insulating $YH_{3-\delta}$ thin films have been performed from 4 K to 450 K. The most striking effect is the broadening by a factor of almost 6 between 4 and 300 K of a particular mode, which is assigned to a breathing vibration of the yttrium atoms. For higher temperatures, the line-width of this mode saturates, which is rather unusual for a phonon.

We developed a model which discusses the line broadening in terms of a coupling between this breathing mode and the electron excited from an octahedral H-vacancy into the 4d conduction band of Y. The data strongly support the correlated electron theory proposed by Ng *et al.* [1] for the metal-insulator transition in YH_x.

[1] K. K. Ng, F. C. Zhang, V. I. Anisimov, T. M. Rice, Phys. Rev. B **59**, 5398 (1999).

MM 16 Invited talk Lehmann

Time: Tuesday 14:00–14:30 Room: IFW A

Invited Talk MM 16.1 Tue 14:00 IFW A

Electron Holography - New Possibilities for Materials Characterization with (sub-)nanometer Resolution — •Michael Lehmann — Triebenberg Laboratory and Institute of Structure Physics (ISP), Dresden University, 01062 Dresden, Germany

The macroscopic properties of modern materials and nanostructured systems depend on their microscopic structure. Transmission Electron Microscopy (TEM) allows the characterization of these systems with atomic resolution at highest sensitivity. However, important structure details like e.g. electric potentials and magnetic fields are encoded in the phase of the electron wave not recorded by conventional TEM. This *phase contrast problem of imaging* is solved by electron holography, i.e. by recording an interference pattern ("electron hologram") in the TEM. By numerical reconstruction, the complete information is available in amplitude and phase. From the phase image, magnetic fields can be measured on a mesoscopic scale (10 .. 500 nm); electric potentials and ferroelectric polarization are also accessible at atomic resolution, where even single Au-atoms can be localized after numerical aberration correction.

MM 17 Symposium Severe Plastic Deformation IV

Time: Tuesday 14:45–17:30 Room: IFW A

Keynote Talk MM 17.1 Tue 14:45 IFW A

Creep properties of ultrafine-grained metals — •Wolfgang Blum — University of Erlangen-Nürnberg, Inst. f. Werkstoffwissenschaften LS1, Martensstr. 5, 91058 Erlangen, Germany

At elevated temperatures ultrafine-grained (ufg) materials produced by severe plastic deformation attain a relative maximum of deformation resistance short after yielding. The relative maximum of flow stress at constant strain rate corresponds to a relative minimum in the rate of creep at constant stress. It is observed not only in tension, but also in compression and consequently respresents a deformation characteristic which is independent of fracture through necking, but means that deformation occurs close to steady state conditions where the dislocation structure is in a state of dynamic equilibrium of generation and annihilation of dislocations. The relatively high strain rate sensitivity of the flow stress corresponds to a low stress exponent of the creep rate. It is a major reason for the good ductility of ufg metals and even leads to superplastic behaviour in cases where the ufg structure is stable enough for the necessary rise in deformation temperature. The special properties of ufg metals come into apparence as the fraction of high-angle boundaries in the deformation induced subgrain structure becomes significant. They are explained by modification of dislocation structure evolution through relatively easy annihilation of dislocations at high-angle grain boundaries and direct strain contributions through grain boundary sliding and diffusive flow.

MM 17.2 Tue 15:15 IFW A

ECAP of magnesium alloys — •Mikhail V. Popov[1], Yuri Estrin[1], Ralph J. Hellmig[1], Lazar L. Rokhlin[2], and Sergey V. Dobatkin[2,3] — [1]Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal, Agricolastr. 6, 38678 Clausthal–Zellerfeld — [2]Baikov Institute of Metallurgy and Materials Science, Leninsky pr. 49, 119991 Moscow, Russia — [3]Moscow State Institute of Steels and Alloys (Technological University), Leninsk pr. 4, 119049 Moscow, Russia

The magnesium alloy MA17 (Mg-Ce-Mn) exhibits a high strength at a reasonable ductility making this alloy well suitable for structural applications. To further improve the mechanical properties, ECAP experiments at elevated temperatures (250°C) were carried out. For example, tensile tests at room temperature on specimens that had underwent 6 ECAP passes (route B_C) revealed a significant increase in yield strength. To substitute the expensive rare earth elements, a Mg-Ca-Al alloy was investigated as well. Results of the investigation of the mechanical properties at different temperatures for both alloys are discussed and compared.

MM 17.3 Tue 15:30 IFW A

Effect of Equal Channel Angular Pressing on the Deformation Behaviour of Magnesium Alloy AZ31 under Uniaxial Compression — •Zuzana Zúberová[1], Yuri Estrin[1], Torbjørn T. Lamark[1], Miloš Janeček[2], Ralph J. Hellmig[1], and Markus G. Krieger[1] — [1]Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal, Agricolastr. 6, 38678 Clausthal–Zellerfeld — [2]Charles University, Faculty of Mathematics and Physics, Ke Karlovou 5, 12116 Prague 2, Czech Republic

The deformation behaviour of the magnesium alloy AZ31 under uniaxial compression was investigated using specimens produced by squeeze casting, hot rolling and hot rolling with subsequent equal channel angular pressing (ECAP). ECAP was performed up to 4 passes at 200°C following route B_C leading to a homogeneous fine–grained microstructure and improved mechanical properties. Results of compression tests under various testing conditions as well as microstructural investigations are presented and discussed.

MM 17.4 Tue 15:45 IFW A

Microstructural, mechanical and thermal properties of ultrafine-grained Cu with and without dispersed nanosized Al2O3 particles — •Florian Dalla Torre[1], Chris H.J Davies[2], Elena V. Pereloma[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland — [2]Victorian Centre for Advanced Materials Manufacturing and Department of Materials Engineering, Monash University, VIC, 3800, Australia

Pure Cu and Cu with 0.5 wt.% nanometer-sized Al2O3 particles were processed via equal channel angular extrusion (ECAE) up to 16 and 12 passes, respectively. Microstructural analysis of both materials indicates a strong change in texture, an increase in misorientation and a reduction in subgrain and grain size between the first and the fourth pass. With a higher number of passes a more equiaxed grain structure and decreasing cell-wall thickness evolves. After 16 passes several recrystallised grains, significantly larger than the surrounding grain size and with an abundance of Sigma 3 boundaries, were detected. The tensile tests performed show an increase in plastic strain and a reduction in strength after 4-8 passes. Additional compression tests were conducted to evaluate the work hardening and the strain-rate sensitivity (SSR) as a function of number of passes. The materials show elevated SSR and work-hardening

stages III, IV and V. An evaluation of the hardening contributions accounting for the Al2O3 particles indicates a linear additive behaviour in the Orowan hardening and Hall-Petch hardening for the grain-size range studied.

Keynote Talk

MM 17.5 Tue 16:30 IFW A

Thermal stability of ultrafine grained materials produced by severe plastic deformation — •Günter Gottstein, Xenia Molodova, and Myrjam Winning — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen, Germany

Equal-channel angular pressing (ECAP) has received considerable attention recently because it provides an easy means to produce an ultrafine grain size in bulk material for improved mechanical properties.

Despite much activity in this field, information on texture evolution during heat treatment is surprisingly sparse as compared to other aspects of ECAP. Comparatively little is known about the mechanisms of microstructural change during annealing. In Copper, a nonuniform coarsening leading to a duplex microstructure was reported by several authors and usually attributed to abnormal grain growth, but equally well it can be due to discontinuous recrystallization.

We investigated microstructure and texture evolution of Aluminium and Copper based materials after ECAP deformation and subsequent heat treatment. The deformed and annealed states were characterized by crystallographic texture analysis, EBSD measurements, microhardness tests and optical microscopy. Texture formation and microstructural changes were recorded and compared to other modes of large strain deformation. The annealing phenomena were analysed with respect to recrystallization and grain growth mechanisms. Theoretical concepts were developed and will be introduced to quantitatively account for the thermal stability of severely plastically deformed metallic materials.

MM 17.6 Tue 17:00 IFW A

Dilatometric studies on ECAP deformed Cu — •Kai Klement and Ferdinand Haider — University of Augsburg

By means of dilatometric measurements the excess volume of lattice defects in severely deformed Cu samples was investigated, in order to determine the type and concentration of these defects. Anisotropic behaviour and inhomogeneities where discovered.

High purity Cu (99.99%) was deformed by equal channel angular pressing for up to eight passes at room temperature, using 120° tooling, by either route A or B_C, generating high concentrations of non equilibrium defects. Annealing experiments with constant heat rate revealed shrinking of the samples in the order of 10^{-4} at temperatures between 180°C and 250°C, depending on the degree of deformation. The temperature characteristics of the annealing process did not provide any further information about different types of defects, showing only one sharp step in the dilatometer signal, which is in accordance with DSC, TEM and XRD investigations. Measurements along the three orthogonal directions of the die outlet channel showed significant differences in shrinking behaviour, indicating the annealing of anisotropic defect configurations like vacancy and dislocation agglomerates. In order to identify the nature of these defects, moleculardynamic simulations are planned, which provide the volumes of typical defect configurations.

MM 17.7 Tue 17:15 IFW A

Compaction of Amorphous and Partially Crystallised Al-Ni-La Alloys — •Jens Vierke, Markus Wollgarten, and John Banhart — Hahn-Meitner-Institute, Materials Dep., Glienicker Str. 100, D-14109 Berlin, Germany

Morphology, microstructure and crystallisation behaviour of Argon (Ar) and Helium (He) atomised $Al_{87}Ni_8La_5$ and $Al_{85}Ni_{10}La_5$ alloy powders were studied by scanning and transmission electron microscopy, X-ray diffraction (XRD) and differential scanning calorimetry. XRD measurements of He-atomised $Al_{85}Ni_{10}La_5$ powders show a complete X-ray-amorphous structure. Ar-atomised powders of the same alloy exhibit fcc-Aluminium crystals in an amorphous matrix. In the case of $Al_{87}Ni_8La_5$, the microstructure consists of an amorphous phase, fcc-Aluminium as well as intermetallic phases. DSC measurements reveal that the amorphous phase of all alloys is stable up to a temperature of about 170°C, applying a heating rate of 20 K/min. The powders were compacted by uniaxial pressing, direct extrusion and equal channel angular pressing. Different compaction temperatures were applied with regard to the conservation of the amorphous phase. First results of the study will be presented. The support of the Institute of Materials and Machine Mechanics of the Slovak Academy of Sciences is gratefully acknowledged.

MM 18 Materials Design

Time: Tuesday 14:45–16:00 Room: IFW B

MM 18.1 Tue 14:45 IFW B

Three-dimensional analysis of globular microstructures by means of phase sensitive Synchrotron Tomography — •Simon Zabler[1], Andreas Lohmüller[2], Alexander Rack[3], Astrid Haibel[1], Heinrich Riesemeier[4], Jürgen Goebbels[4], John Banhart[1], and Antonio Rueda[1] — [1]Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung — [2]Neue Materialien Fürth GmbH — [3]Forschungszentrum Karlsruhe - ANKA — [4]Bundesanstalt für Materialforschung und -prüfung Berlin

We investigate materials with globular microstructure as used in Thixocasting processes like A356, A357 and AZ91D alloys. Phase sensitive synchrotron tomography is the ideal non-destructive tool for the analysis of such materials. The effects of growth and coarsening are analysed as well as the dynamics of the semi solid melt.

The aim of our work is to use 3D image processing in order to reveal the correlation between the alloys microstructure and its rheological properties (e.g. viscosity) in the semi solid state. Because all the samples under test represent alloys that are built from neighbouring elements with similar densities (e.g. Aluminium and Silicon) standard absorption tomography lacks any visible contrast in the images. We apply phase contrast imaging yielding a contrast up to three orders of magnitude superior to absorption contrast rendering the microstructure of all the alloys under test visible. Tomography data is available in form of phase sensitive 3D images or holotomographic data sets when the tomographic reconstruction is combined with a direct phase retrieval algorithm.

MM 18.2 Tue 15:00 IFW B

Synchrotron Tomography on Complex Material Systems — •A. Rack[1], L. Helfen[1], I. Manke[2], S. Zabler[2], C. Knabe[3], H. Riesemeier[4], M. Stiller[3], J. Goebbels[4], T. Baumbach[1], and J. Banhart[2] — [1]Forschungszentrum Karlsruhe – ANKA — [2]Hahn-Meitner-Institut Berlin, Bereich Strukturforschung — [3]Charité Berlin — [4]Bundesanstalt für Materialforschung und -prüfung, Berlin

High resolution synchrotron-tomography investigations on metal foams, commercial batteries and novel rapidly resorbable bone substitutes (ceramics like Bioglass, Cerasorb) are reported. The measurements were performed with high spatial resolutions at the synchrotrons ESRF (ID19), BESSY (BAM*line*) and ANKA (TOPO-CT). The use of monochromatic radiation and the application of subsequent 3d image analysis [1] enables us to separate different material phases in the volume data sets, e.g. solid matrix and blowing agents' particles in metal foams or tissue and ceramics in a reshaping jawbone. This provides the basics for *ex situ* and *in situ* imaging on materials and devices. Firstly, the pore formation process in early stages (1% to 10% porosity) of aluminium foams could be studied *ex situ*. Secondly, the time and spatial dependence of a commercial batterie's zinc powder decay was quantified *in situ*. Finally, quantitative determination of the formation and structural changes of the bony tissue in a given defect plus the biodegradation of the bone substitute materials within animal and human biopsies 3, 4 and 6 months after implantation were performed *in vitro*.

[1] J. Ohser and F. Mücklich, *Statistical Analysis of Microstructures in Materials Science*, John Wiley & Sons, 2000

MM 18.3 Tue 15:15 IFW B

Beating the Miscibility Barrier Between Magnesium and Iron Group Metals (Fe, Ni, Co) by High-Pressure Alloying — •Leonid Dubrovinsky[1], Natalia Dubrovinskaia[2], Igor A. Abrikosov[3], and Levente Vitos[4] — [1]Bayerisches Geoinstitut, Universität Bayreuth, Germany — [2]Physikalisches Institut, Universität Bayreuth, Germany — [3]Department of Physics and Measurement Technology, Linköpings University, Sweden — [4]Department of Materials Science and Engineering, Royal Institute of Technology, Sweden

It is now generally recognized that all metals and compounds show some solubility in the solid or liquid state, but the extend of solid solubility is different in different cases. Fe and Mg are almost immiscible at ambient pressure. Though two close chemical analogues of iron, namely nickel and cobalt, form intermetallic compounds with magnesium, solubility of Mg in these metals is also negligibly low. The low solubility of Mg in Fe is in complete agreement with well-known Hume-Rothery rule for metallic alloys. However, compressibility of Mg is much higher than that of Fe, and therefore the difference in atomic sizes between these two elements decreases dramatically with pressure. Based on the predictions of ab initio theoretical calculations, we demonstrate in series of experiments in a multianvil apparatus and in electrically- and laser-heated diamond anvil cells, that high pressure promotes solubility of magnesium in iron and at megabar pressure range more than 10 at% of Mg can dissolve in Fe, and then quenched to ambient conditions. Up to 4 at% of Mg could be dissolving in Ni or Co at 20 GPa and 2200 K.

MM 18.4 Tue 15:30 IFW B

Synthesis and properties of new materials in the B-C system — •Natalia Dubrovinskaia[1,2], Georg Eska[1], Grigorii A. Sheshin [1,3], Leonid Dubrovinsky[2], and Hans F. Braun[1] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany — [3]B. Verkin Institute for Low Temperature Physics and Engineering, 61103 Kharkov, Ukraine

Synthesis of a series of bulk samples of B-doped diamonds was realized in a wide spectrum of pressures and temperatures (up to 20 GPa and 2700 K) using a 5000 tonne multianvil press. The properties of the samples were characterized using X-ray diffraction, SEM, TEM, and microprobe analysis. Electrical resistance of the samples was measured at the temperature range between 300 K and 10 mK. It was found that the samples exhibit semiconducting an superconducting behavior at different temperature intervals. A bulk sample (˜7.5 mm3) of heavily boron-doped diamond containing 2.6(0.6) at.% B was synthesized by means of direct reaction between boron carbide and graphite. Electrical resistance measurements revealed a transition to superconducting state at 2.4 K to 1.4 K. Sharpening of the temperature interval of the transition to superconducting state in magnetic field suggests that superconductivity in our samples may arise from filaments of zero-resistant material. Crystallographic aspects in explanation of the observed electrical properties will be discussed.

MM 18.5 Tue 15:45 IFW B

The evolution of the structure of liquid aluminium foams: comparison between in-situ X-ray observations and numerical calculations. — •Oliver Brunke and Stefan Odenbach — TU Dresden, Professur für Magnetofluiddynamik, 01062 Dresden

Drainage is one of the driving forces for the temporal instability of liquid metal foams. For usual aqueous foams this phenomenon is very well examined and understood on both, the experimental as well the theoretical side. The situation is different for metallic foams. Due to their opaque nature, the observation of drainage is just possible by either measuring the density distribution of solidified samples ex-situ, or by x-ray or neutron radioscopy. We will report on the drainage behaviour of Al foams grown by a powder-metallurgical production route. The changes of the structure during the ageing of the foam have been observed in-situ by means of a tabletop x-ray radioscopy system. This method allows us to get direct information about the temporal density redistribution and therefore the drainage behaviour of liquid metallic foams. A direct comparison of the experimental data to numerical results obtained by solving the foam drainage equation shows that this theory, which has proved to be successful for the theoretical description of aqueous foams, can in principle also be used to model the material redistribution in metallic foams.

MM 19 Electronic Properties I

Time: Tuesday 16:30–17:45 Room: IFW B

MM 19.1 Tue 16:30 IFW B

Correlation-induced double-plasmon excitations in simple metals studied by inelastic x-ray scattering — •C. Sternemann[1], S. Huotari[2], G. Vankó[2], M. Volmer[1], H. Sternemann[1], G. Monaco[2], A. Gusarov[3,4], H. Lustfeld[3], K. Sturm[3], M. Tolan[1], and W. Schülke[1] — [1]Institute of Physics / DELTA, University of Dortmund, D-44221 Dortmund, Germany — [2]European Synchrotron Radiation Facility, BP 220,*F-38043 Grenoble Cedex, France — [3]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [4]SCK · CEN, Belgium Nuclear Research Centre,*Boeretang 200, B-2400 Mol, Belgium

Peaklike structures in the high energy-loss tail of the dynamic structure factor of simple metals were predicted by many-body perturbation theory of the homogeneous electron gas beyond the random-phase approximation [1]. Such structures were experimentally observed in the dynamic structure factor of Aluminium and, based on a comparison with the calculations, were attributed to intrinsic double-plasmon excitations because of the distinct momentum transfer dependence of their energy position and intensity [2]. A systematic inelastic x-ray scattering study of this kind of excitations for different materials as a function of electron density was accomplished recently at beamline ID16 of the European Synchrotron Radiation Facility. The measured spectra of the intrinsic plasmon-plasmon excitations will be discussed and compared with corresponding calculations.

[1] K. Sturm and A. Gusarov, Phys. Rev. B **62**, 16474, (2000).
[2] C. Sternemann *et al.*, Phys. Rev. Lett. **95**, 157401, (2005).

MM 19.2 Tue 16:45 IFW B

Cold-atom systems as solid-state simulators: the issue of trapping — •Chris Hooley[1] and Jorge Quintanilla[2] — [1]School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, U.K. — [2]ISIS facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, U.K.

Since the achievement of Bose-Einstein condensation in cold trapped gases in 1995, much attention has been devoted to experiments on such systems. Some of this work has involved the imposition of laser standing waves (so-called 'optical lattices') on the atom gas. It has been proposed that such set-ups could be used as simulators — or, more accurately, analogue computers — of the solid state, with the atoms playing the role of electrons and the laser standing wave playing the role of the periodic ionic potential. Immanuel Bloch poetically called these "artificial crystals of light".

In this talk, we critically assess this proposal, concentrating in particular on one important difference between the atom-gas system and the solid state: in the solid state, electrons are confined by hard-wall boundaries, whereas in the atom-gas, they are more usually trapped by a smooth (often harmonic) effective potential. We demonstrate that this can make a qualitative difference to the behaviour of such systems, and explore how the 'simulator' proposal needs to be modified accordingly. We compare our results with recent experimental and numerical work.

MM 19.3 Tue 17:00 IFW B

Electron-phonon coupling reflecting dynamic charge inhomogeneity in copper-oxide superconductors — •D. Reznik[1], L. Pintschovious[1], M. Ito[2], S. Iikubo[2], M. Sato[2], H. Goka[3], M. Fujita[3], K. Yamada[3], G. Gu[4], and J.M. Tranquada[4] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe, Germany — [2]Department of Physics, Division of Materials Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan — [3]Institute for Material Research, Tohoku University, Katahira, Aoba-ku, Sendai, 980-8577, Japan — [4]Physics Department, Brookhaven National Laboratory, Upton, New York 11973

The attempt to understand cuprate superconductors is complicated by the presence of multiple strong interactions. While many believe that antiferromagnetism is important for the superconductivity, there has been resurgent interest in electron-lattice coupling. The conventional superconductor MgB2 has a very strong electron-lattice coupling predicted by standard theory. We show that there is a similarly strong anomaly in the Cu-O bond-stretching phonon in cuprate superconductors however, this behavior is completely absent in conventional calculations. Instead, the anomaly is strongest in compounds that exhibit static stripe order. It occurs at a wave vector corresponding to the charge order. The results suggest that this giant electron-phonon anomaly, which is absent in undoped and over-doped non-superconductors, is associated with charge inhomogeneity. It follows that electron-phonon coupling may be important to understanding superconductivity although its contribution to the mechanism is likely indirect.

MM 19.4 Tue 17:15 IFW B

Effect of Mn doping on the specific heat of the high Tc superconductor YBaCuO — •Ashok Rao[1], Radhe Shyam[1], Anirban Das[1], Y. F. Lin[2], K.M. Sivakumar[2], Y. -K Kuo[2], Bhasker Gahtori[3], and S K Agarwal[3] — [1]Sikkim Manipal Institute of Technology, Majitar,Rangpo, Sikkim-737132,India — [2]Department of Physics, National Dong-Hwa University, Hualien 974, Taiwan — [3]National Physical Laboratory, K.S. Krishnan Marg, New Delhi-1100012, India.

There have been several efforts to get new super conducting materials while seeking to explain the transport mechanism in ceramic high temperature superconductors [1].Several investigators have carried out the substitution effects in the high Tc superconductors which has helped in understanding the mechanism of superconductivity and to improve the magnetic properties, like flux pinning etc.We present first reports of the investigations of specific heat on Mn-doped compounds Y1Ba2 (Cu1-xMnx)3Oy (0 <x < 2%). The specific heat of the samples was determined using high-resolution ac calorimeter. It is observed that the transition temperature of Mn doped samples of YBaCuO samples do not change appreciably.Jump in specific heat was observed for samples with low concentration of Mn, however for concentrations above 1%, small change in slope is observed. It may be mentioned that replacing 0.5% Cu by Mn has little effect on the transition temperature; however, the jump decreases by a factor of 3.This clearly demonstrates that these constituents are being incorporated into the superconductors as a whole and not in the form of a local cluster. References 1.Rao A 2004 J. Phys. Condens. Matter 16 1439

MM 19.5 Tue 17:30 IFW B

Structural and Electronic properties of the Layered $Na_{0.46}CoO_2$ — •Dimitri Argyriou[1], L.C. Chapon[2], C. Milne[1], O. Prokhnenko[1], and P.G. Radaelli[2] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, Berlin D-14109, Germany — [2]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK

The onset of antiferromagnetic ordering coupled to a sharp rise in the resistivity of $Na_{0.5}CoO_2$ has recently been taken as evidence of charge ordering in this half doped cobaltate[1]. We have used neutron powder diffraction to investigate the lattice response to this charge and magnetic ordering using high resolution powder diffraction from 2 till 600K. Our sample is a little off the ideal composition x=0.46, but shows the identical transitions at T_{co}=52K and at 87K, as other single crystal sample of nominal x=0.5 composition. We find that the orthorhombic structure of $Na_{0.46}CoO_2$ (Pnmm) is stable from 460K to 2K, even below the charge ordering transition at 50K. At room temperature we can clearly identify two Co sites which are distinguishable from their octahedral distortions. One site, labeled Co(1) is at the center of a CoO_6 octahedron that shows an octahedral distortion 5 times larger than the octahedron centered in the Co(2) site. The average bondlength for both Co sites is essentially the same, 1.890Å, suggesting the same bond-valence. With lowering temperatures below T_{co}, we find no anomalies in Co-O bondlengths or octahedral distortion parameters, suggesting that the sharp increase in the resistivity at 50K may arise from an effect other than charge ordering. [1] M.L. Foo, et al. Phys. Rev. Lett. 92, 247001 (2004).

MM 20 Amorphous and Liquid Materials I

Time: Tuesday 14:45–16:00 Room: IFW D

MM 20.1 Tue 14:45 IFW D

Soft-Particle-Reinforced Bulk Metallic Glass Composites with High Ductility — •Marco E. Siegrist and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, Swiss Federal Institute of Technology (ETH) Zürich, CH-8903 Zürich, Switzerland

We introduced graphite particles into an amorphous $Zr_{52.5}Cu_{17.9}Al_{10}Ni_{14.6}Ti_5$ (Vit 105) matrix with the aim of increasing plasticity and improving the wear and friction properties of monolithic metallic glass. The graphite particle size was varied from 25-75 microns and the reinforcement content from 5-30 vol%. By adjusting the processing parameters part of the graphite can be transformed into ZrC, which allows a systematic change in mechanical properties. This contribution describes the thermophysical and mechanical properties of these graphite/ZrC Bulk Metallic Glass matrix composites. The crystallization sequence of the matrix was studied using differential scanning calorimetry, and the amorphous structure was confirmed by x-ray diffraction. The effect of varying the particle size and carbide content on composite hardness, fracture strength and ductility was investigated. We found that graphite causes a decrease in hardness, whereas carbide formation leads to an increase in hardness compared to the monolithic matrix material. The best mechanical properties were observed with large particles at low volume fractions of graphite, where 18.5% plastic deformation combined with a fracture strength of 1.85 GPa was achieved. The effect of particle reinforcement on fracture behavior was studied using high-resolution scanning electron microscopy.

MM 20.2 Tue 15:00 IFW D

Is $Cu_{47}Ti_{33}Zr_{11}Ni_8Si_1$ a bulk glass former ? — •Shankar Venkataraman[1], Mihai Stoica[2], Sergio Scudino[1], Ki Buem Kim[1], Ludwig Schultz[3], and Jürgen Eckert[1,3] — [1]FG Physikalische Metallkunde, FB 11, Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany — [2]Institut National Polytechnique de Grenoble, ENSEEG, LTPCM, 1130 rue de la Piscine, PO Box 75, 38402 St.Martin d'Hères campus, Grenoble, France — [3]Institut für Metallische Werkstoffe, Leibniz-Institut für Festkörper-und Werkstoffforschung, Helmholtzstraße 20, D- 01069 Dresden, Germany

The microstructures of $Cu_{47}Ti_{33}Zr_{11}Ni_8Si_1$ ribbons and rods synthesized by melt spinning and copper mold casting have been investigated using transmission electron microscopy (TEM) as well as high-resolution TEM (HRTEM). Though a fully amorphous microstructure is observed for the as-spun ribbons, a fine nanocrystalline microstructure is observed for the rods suggesting that the bulk glass forming-ability of this alloy has been previously overestimated. This work attempts to address the reasons for the lack of a fully glassy phase in the bulk $Cu_{47}Ti_{33}Zr_{11}Ni_8Si_1$ alloy.The present study shall also show that the selection of a proper sample preaparation method is also crucial in observing an artifact free microstructure under the TEM. This work was supported by the German Research Foundation (Grant no. Ec 111/12) as well as by the European Union within the framework of the Research Training Network on "ductile bulk metallic glass composites" (MRTN-CT-2003-504692).

MM 20.3 Tue 15:15 IFW D

The Origin Of Glass Forming Ability in Zr-Ti-Ni-Cu-Be Bulk Glasses — •S. Mechler, M.-P. Macht, and N. Wanderka — Hahn-Meitner Institut-Berlin, Glienicker Str. 100, 14109 Berlin

$Zr_{46.8}Ti_{8.2}Ni_{10}Cu_{7.5}Be_{27.5}$(V4) is one of the best metallic glass formers known so far. This glass exhibits an extended supercooled liquid region. At temperatures above the glass transition it can form a quasicrystalline phase. The quasicrystals are found to be mainly depleted in Be and enriched in Ti. A series of alloys based on V4 composition with variation of Be content (from 0 to 35 at.%) were produced in order to investigate the influence of the Be on the glass forming ability (GFA). The Be-free glass shows only a narrow temperature region between glass transition and crystallization. After heat treatment around the glass temperature it shows a polymorphous transition from the amorphous to the quasicrystallline state. Higher Be contents result in better GFA. The GFA has its maximum for the alloys with Be contents between 25 at.% and 27.5 at.%. During annealing of these alloys the formation of the quasicrystalline phase is retarded. Upon heating in DSC the crystallization is shifted to higher temperatures, leading to the observed large temperature range between glass transition and crystallization of V4 glass. Investigations of the short range order in the glasses with different Be content indicated correlation between Icoshedral Short Range Order (ISRO) and Be content, with a highest degree of ISRO in the Be-free alloy. It is concluded that the ISRO is the key parameter in understanding the bulk glass forming ability and the extended stability of the supercooled liquid in the Zr-Ti-Ni-Cu-Be system.

MM 20.4 Tue 15:30 IFW D

Glass forming ability and thermal behavior of Ni-based alloys — •Konrad Eymann, Uta Kühn, Helmut Hermann, Norbert Mattern, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The Ni-based alloys Ni-Zr-Al-Y [1], Ni-Nb-Ti-Zr-Co-Cu [2], Ni-Nb-Sn [3], and Ni-Cu-Ti-Zr-Al [4] were evaluated concerning their glass forming ability (GFA) by preparing ribbons and bulk specimens in form of cylindrical rods with diameters of 2 or 3 mm. The samples were prepared by melt spinning technique as well as by copper mold casting. The microstructure of the ribbons and rods were characterized using XRD measurements and TEM. The thermal behavior was measured by DSC. For example the glass transition temperature was used for the calculation of the parameter gamma [5] to evaluate the Ni-alloy with the best theoretical GFA. The gamma-parameter was compared to the actual microstructure of the bulk samples. The alloy with the highest GFA was found to be Ni-Cu-Ti-Zr-Al. To enhance the GFA of this alloy the composition was modified by adding further elements. The elements were chosen by computer simulations using the Bernal's model of simple liquids generalized for multicomponent metallic systems, which finally lead to a liquid with optimized density.

[1] Yi, S. et al., Mater. Lett. 48, 258 (2001). [2] Zhang, T. et al., Mater. Trans. 43, 4, 708 (2002). [3] Choi-Yim, H. et al., Appl. Phys. Lett. 82, 7, 1030 (2003). [4] Xu, D. et al., Acta Mater. 52, 3493 (2004). [5] Lu, Z.P. et al., Acta Mater. 50, 3501-3512 (2002).

MM 20.5 Tue 15:45 IFW D

Microstructure controlled magnetic properties of the Zr53Co23,5Al23,5 bulk metallic glasses — •Ahmed Shariq[1], Talaat Al-Kassab[1], Reiner Kirchheim[1], Dmitrij Bogdanov[2], Konrad Samwer[2], Qiang Jianbing[3], and Chuang Dong[4] — [1]Institut für Materialphysik, Friedrich Hund platz 1, D 37077, Göttingen, Germany — [2]I. Physikalisches Institut, Friedrich Hund platz 1, D 37077, Göttingen, Germany — [3]Department of Materials Engineering, Dalian University of Technology, Dalian 116024, China — [4]State Key Laboratory of Materials Modification, Dalian University of technology, Dalian 116024, China

The unique set of properties offered by the amorphous alloys triggered intensive microstructural investigations in the last few years. The new amorphous alloys have much wider supercooled liquid region defined as the difference between crystallisation and glass transition temperatures and require relatively slower cooling rates. Zr53Co23,5Al23,5 has already been reported as a good glass forming alloy. In the present contribution, the magnetic properties of the bulk metallic glass of the above said system are shown. The bulk sample shows very soft ferromagnetic properties. The crystallization in this system occurs in two steps. With the introduction of the crystalline phase the magnetic properties vary considerably and the bulk sample also shows some magnetic anisotropy. The kinetics of the formation of these crystalline phases as a function of temperature and subsequent effect on the magnetic properties will be discussed.

MM 21 Amorphous and Liquid Materials II

Time: Tuesday 16:30–17:45 Room: IFW D

MM 21.1 Tue 16:30 IFW D

DeGennes slowing down in a liquid metal revisited: A neutron spin echo study — •Franz Demmel[1], Peter Fouquet[2], Wolfgang Haeussler[3], and Christoph Morkel[3] — [1]ISIS Facility — [2]ILL Grenoble — [3]TU Muenchen

The decay of density fluctuations shows a slowing down at the structure factor maximum in liquids, which is well known as deGennes narrowing in the frequency domain. Molecular simulations for the liquid metal Rubidium and mode coupling theory has suggested that the relaxation process has to be described with two terms in the memory function [1]. We have probed these predictions by inelastic neutron scattering using the spin echo technique to measure the dynamics directly in the time domain. The liquid alkali metal Rubidium was measured near the melting point with the spin echo instrument IN11C at the ILL, Grenoble. The resulting intermediate scattering function is in remarkable quantitative agreement with predicted values from the mode coupling calculations and the molecular dynamics simulations. The question will be discussed whether this slow decay is related to the solidification process. [1] U. Balucani and R. Vallauri (1989) Phys. Rev. A 40 2796

MM 21.2 Tue 16:45 IFW D

Inelastic Neutron Scattering on AlNi melts — •Sebastian Stüber, Suresh Mavila Chathoth, and Andreas Meyer — Physik Department E13, TU München

We report on inelastic neutron scattering (INS) measurements on Al_4Ni melts, comparing an alloy with natural Ni isotopic composition to a ^{58}Ni enriched sample. The experiments were performed at the new time-of-flight instrument of the neutron source FRM-II in Garching, yielding an exceptionally good signal-to-background ratio.

AlNi melts exhibit an intermediate range order (IRO), associated with a strong non-linear behaviour of the Ni self-diffusion coefficients as a function of composition [1]. Isotopic comparison enables a closer look on intermediate correlations, as ^{58}Ni scatters only coherent, whereas Ni in natural abundance is a strong incoherent scatterer. The amplitude as well as the time scale of diffusive atomic motion exhibit a strong dependence on coherent, respectively incoherent contributions to scattering, and secondly, their oscillations are in phase with the static structure factor. This data set allows a detailed investigation of the diffusion mechanism in AlNi melts. The experimental results are compared with Molecular Dynamics computer simulations.
[1] S.K. Das, J. Horbach, M.M. Koza, S. Mavila Chathoth, A. Meyer, Appl. Phys. Lett. **86**, 011918 (2005)

MM 21.3 Tue 17:00 IFW D

Short-range Order in Undercooled Ti-Fe-Si-O Melts — •Oliver Heinen, Dirk Holland-Moritz, and Dieter M. Herlach — DLR, Inst. für Raumsimulation, D-51170 Köln

Comparing the energy of different types of monoatomic clusters and assuming radial symmetric Mie type interaction potentials, the icosahedron truns out to be the most stable configuration of all clusters with 13 atoms. Basing on this finding Frank proposed an icosahedral short-range order (SRO) prevailing in metallic liquids. This hypothesis has been approved by a number of experimental and theoretical examinations. The assumption of radial symmetric interaction potenials is justified for purely metallic systems. In this work we present investigations of the SRO of liquids containing metallic as well as covalent bonding atoms. For the investigation the Ti-Fe-Si-O system was chosen since this system is supposed to have strong covalent Ti-O bonds in the solid as well as in the liquid state. The liquids were containerlessly processed and in-

situ investigated using the combination of the electromagnetic levitation technique together with energy dispersive diffraction of synchrotron radion at the European Synchrotron Radiation Facility as well as neutron diffraction at the Institute Laue-Langevin. This work was financially supported by DFG under contract No. Ho1942/4 and by ESRF and ILL.

MM 21.4 Tue 17:15 IFW D

The oscillation spectrum of two-phase liquid drops — •Leonie Kraus[1], Karol Debinski[2], Rudolf Schmitz[2], and Ivan Egry[1] — [1]Institut für Raumsimulation, DLR Köln — [2]Institut für Theoretische Physik, RWTH Aachen

The interfacial tension between two immiscible liquids is of basic and technical interest, especially concerning melts of multicomponent metallic alloys. In principle, it may be calculated from the oscillation spectrum of a two-phase droplet. For a force free, spherical droplet, two frequencies are expected which can be clearly assigned to the surface oscillations and the interface oscillations respectively. This assumption is approximately fulfilled for electromagnetically levitated droplets under microgravity conditions. A corresponding experiment was performed within a parabolic flight campaign in 2005. The alloy Cu40Ni30Ag30 was examined, which has a stable miscibility gap in the liquid range.

In levitation experiments on Earth, the gravitational force and the levitation force break the spherical symmetry of the droplet. So the external forces need to be considered and the corresponding theory should be extended. In general, for the lowest translation and oscillation modes, one gets a 16-dimensional equation of motion, which may be approximatively diagonalized.

In this talk, both the experimental results from the parabolic flight and the theory for aspherical two-phase drops are introduced and discussed.

MM 21.5 Tue 17:30 IFW D

Structure and transport properties of amorphous Ag-Sn Alloys — •D. Hauschild, S. Neubert, P. Haeussler, I. Kaban, and W. Hoyer — Chemnitz University of Technology, Institut of Physic, 09107 Chemnitz, Germany

Within the last years binary amorphous alloys of metal-metal and metal-semiconductor type were investigated resulting in a model of global resonances between the electronic system and the forming static structure [1].

Two of us (I K and W H) have measured the liquid state by means of X-ray diffraction. It was shown that the liquid state contains clusters of well defined composition and is micro-inhomogeneous. The variation of the overall composition results in a variation of their volume fraction, whereas the composition of the individual clusters stays constant. By decreasing the temperature the size of the clusters is increasing. Three of us (S N, D H and P H) have measured the amorphous state by means of electron diffraction in transmission. Here we compare a-Ag-Sn with l-Ag-Sn as well as with the corresponding states of Au-Sn and Cu-Sn. The results were discussed in the Hume-Rothery-Model with a possible enhancement by hypridization.

The amorphous alloys were prepared in situ at T = 4K in a HV-cryostate. Immediately after the evaporation and at various annealing steps, up to the crystalline state, we measured the static structure and the resistivity.

[1] P. Haeussler, Collective dynamics of nonlinear and disordered systems, Springer (2004)

MM 22 Electronic Properties II

Time: Wednesday 14:00–15:30 Room: IFW A

MM 22.1 Wed 14:00 IFW A

Real-space methods in Density Functional Theory — •Ralf Meyer — Theoretische Tieftemperaturphysik, Universität Duisburg-Essen, Campus Duisburg, D-47048 Duisburg, Germany

Density functional theory (DFT) has proven to be a reliable and accurate tool for the *ab-initio* calculation of materials properties. The most popular approach to the solution of the DFT equations is probably the plane-wave method. While a plane-wave basis is very efficient for dense periodic systems like crystalline solids, it is less suitable for the description of non-periodic systems like clusters. Moreover, the necessity to perform Fourier-transforms hampers the efficiency of the plane-wave method on massively parallel computers. These problems are avoided by real-space approaches like the finite-element or finite difference method that directly discretize the DFT equations in real space. In this presentation, calculations of metallic nanoclusters using a newly developed real-space code are shown and compared with corresponding results obtained with the plane-wave method.

MM 22.2 Wed 14:15 IFW A

The fundamental gap in reduced-density-matrix-functional theory — •N. Helbig[1], N.N. Lathiotakis[1], M. Albrecht[2], and E. K. U. Gross[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Theoretical Chemistry FB 08, University of Siegen, 57068 Siegen

We present a novel method for calculating the fundamental gap. To this end, reduced-density-matrix-functional theory is generalized to fractional particle number. For each fixed particle number, M, the total energy is minimized with respect to the natural orbitals and their occupation numbers. This leads to a function, $E^M_{\rm tot}$, whose derivative with respect to the particle number has a discontinuity identical to the gap. In contrast to density functional theory, the energy minimum is generally not a stationary point of the total-energy functional. Numerical results are presented for alkali atoms, for small molecules and ionic periodic systems.

[1] N. Helbig, N.N. Lathiotakis, M. Albrecht, E.K.U. Gross, cond-mat/0504436

MM 22.3 Wed 14:30 IFW A

Reduced-density-matrix-functional theory for the homogeneous electron gas — •N. N. Lathiotakis, N. Helbig, and E. K. U. Gross — Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Reduced-density-matrix-functional theory (RDMFT) is one possible way to treat electron correlation beyond density-functional theory. One of the drawbacks of the first generation RDMFT functionals is their failure to reproduce the correletion energy of the spin-unpolarized homogeneous electron gas (HEG). Recently, new RDMFT functionals were introduced which considerably improve the results for atoms and molecules. We apply these functionals to the HEG and show that they also improve dramatically the results obtained for the HEG: On one hand, they give correlation energies closer to the exact ones and, in contrast to the first-generation functionals, they properly yield a finite jump of the HEG momentum distribution.

Furthermore, we generalize the second-generation functionals in such a way that they reproduce the correlation energy of the HEG exactly over the whole range of electron densities. We discuss ways to apply the resulting functionals to both finite and inhomogeneous periodic systems.

MM 22.4 Wed 14:45 IFW A

The intrinsic defect structure of $Al_{1-x}B_2$ – an ab initio electronic structure study — •Katrin Koch, Yuri Grin, and Helge Rosner — MPI CPfS Dresden

Ab initio calculation of phase diagrams is still in its very early stages. For an outset towards new developments, we have chosen the simple hexagonal system AlB_2, which is nevertheless very interesting due to its close relation to the surprising superconductor MgB_2. Up to now, the synthesis of stoichiometric AlB_2 has been impossible: grown in aluminium flux, a composition between $Al_{0.9}B_2$ (from x-ray refinement) and $Al_{0.85}B_2$ (from mass density measurements) has been found [1]. Here, we present band structure calculations within the local density approximation to investigate the structural stability in the phase equilibrium $AlB_2 \Longleftrightarrow Al_{1-x}B_2 + x{\cdot}Al$. The defects are treated using the coherent potential approximation (CPA). Taking into account the full lattice relaxation depending on x, we find a stable energy minimum for the composition $Al_{0.85}B_2$. This is in excellent agreement with the experimental findings and explains the nonstoichiometric composition of present AlB_2 samples. The influence of the defects on the electronic properties will be discussed.

[1] U.Burkhardt *et al.* Journal of Solid State Chemistry **177**, 389, (2004)

MM 22.5 Wed 15:00 IFW A

The highly distorted hcp lattices of Zinc and Cadmium: Comparison of different ab-initio approaches — •Beate Paulus[1], Krzysztof Rosciszewski[2], Priya Sony[3], Ulrich Wedig[4], and Martin Jansen[4] — [1]MPI for the Physics of complex Systems, Dresden, Germany — [2]Institute of Physics, Jagellonian University, Krakow, Poland — [3]Institute of Technology, Mumbai, India — [4]MPI for Solid State Research, Stuttgart, Germany

Among the metallic elements crystallizing in a hexagonal closed packed structure, Zn and Cd are unusual because of the significant increase of the c/a ratio. Attempts to explain this distortion theoretically suffer from the fact that the calculated properties vary significantly with the method used. In order to investigate the peculiarities and the reliability of the different methods, ground-state properties like cohesive energy, the lattice constants and the elastic constants were calculated for Zn and Cd using the Hartree-Fock method, various density functionals and hybrid methods. In addition calculations were performed for Mg as a reference system with the ideal hcp structure. The dependence of the results on the computational methods and parameters gives further insight into the bonding mechanisms leading to the distortions in Zn and Cd and helps to judge the reliability of computed electron density maps to interpret experimental results.

MM 22.6 Wed 15:15 IFW A

Lifshitz-transitions in Osmium under pressure — •Daniela Koudela, Klaus Koepernik, Ulrike Nitzsche, and Manuel Richter — IFW Dresden

The search for Lifshitz-transitions [1] is a recent subject of interest. Occelli et al. claimed, that they found evidence for a Lifshitz-transition in Osmium [2]. To explore this hypothesis from the theoretical side, we did very accurate first principle calculations applying the DFT-based bandstructure code FPLO [3]. From the resulting bandstructure, Fermi surfaces, and total energies we conclude, that Osmium undergoes three Lifshitz-transitions in the pressure range between 0 GPa and 150 GPa, which should be invisible in the elastic properties.

[1] I.M. Lifshitz, Zh. Eksp. Teor. Fiz. 38, 1569 [Sov. Phys. JETP 11, 1130 (1960)].

[2] F. Occelli, D.L. Farber, J. Badro, C.M. Aracne, D.M. Teter, M. Hanfland, B. Canny and B. Couzinet, Phys. Rev. Lett. 93, 095502 (2004).

[3] K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999); www.fplo.de.

MM 23 Mechanical Properties I

Time: Wednesday 14:00–15:15 Room: IFW B

MM 23.1 Wed 14:00 IFW B

Deformation of laminated niobium and alumina: constraints from the interfaces — •Yonghe Liu[1,2] and Dieter Brunner[1] — [1]Max-Planck-Institut für Metallforschung, 70569 Stuttgart, Germany — [2]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The forming of thin metal sheets is highly constrained by interfaces between workpiece and dies. Constraints are usually treated as friction in a form of stiction, or coulomb friction depending upon lubrication. Our study of the deformation behavior of thin niobium sheets focus on the effects of constraints from interfaces. Polycrystalline niobium and sapphire joints were prepared by diffusion bonding in ultra high vacuum chamber to simulate the stiction, while the coulomb friction was simulated by stacking the niobium/sapphire pieces, or niobium/niobium pieces. We applied an optical full field strain mapping method to determine the strains on the side faces of the metal layers in in-situ deformations. In the case of stiction, the detected strain patterns are coupled with strain localization at interfaces and along the maximum shear directions. Once friction changes from stiction to coulomb friction through interface debonding, the strain localization at interface disappears. A ductile fracture model considering stress triaxiality was employed to understand the results. The results obtained by strain mapping can be directly compared with that obtained by finite element method.

MM 23.2 Wed 14:15 IFW B

Fatigue of highly strengthended Cu-Ag alloys — •J. Freudenberger[1], H.-J. Klauss[1], K. Heinze[1,2], A. Gaganov[1], M. Schaper[2], and L. Schultz[1,2] — [1]IFW Dresden, Institute for Metallic Materials, P.O.-Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institute of Material Science, D-01062 Dresden, Germany

The fatigue behaviour of high strength Cu-Ag conductor materials which have undergone thermal treatments and subsequentially progressive strain hardening by repetitive cold drawing is reported. When a maximum load of 1 GPa and a minimum-to-maximum stress ratio of $R = 0.1$ is applied, the investigated materials show a similar behaviour and a fatigue lifetime in the range of $5 \ldots 9 \times 10^3$ cycles to failure is observed. The fatigue lifetime of all investigated materials is sufficient with respect to the intended application, which the materials are developed for, i.e. conductors for pulsed high field magnets.

MM 23.3 Wed 14:30 IFW B

Friction and adhesion of selected bearing materials in vacuum — •Mikhail Kosinsky[1,2], Yonghe Liu[1], Wolfram Hild[1], and Juergen A. Schaefer[1] — [1]Technische Universität Ilmenau, Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Postfach 100565, 98684 Ilmenau, Germany — [2]Bauman Moscow State Technical University, MT-11, BMSTU, 2nd Baumanskaya 5, Moscow, 105005, Russia

There is a strong interaction between the contact surfaces of bearings in vacuum. It may lead to high adhesion and high friction that can deteriorate the performance of positioning systems transported by bearings. We characterize the friction and adhesion of selected pairs of bearing materials including steel, copper, gold, sapphire and Si_3N_4 in high vacuum. A driving unit based on piezoelements were built in a vacuum (10^{-8} - 10^{-6} Torr) chamber, which can be refilled with various atmospheres (O_2, N_2). The load prescribed by the driving unit was applied to a glass cantilever through which a sphere was in contact with a specimen. We obtained the normal load and friction force by measuring the deflection of the cantilever in normal and lateral direction and multiplying the spring constants. A laser interferometer mounted outside of the vacuum chamber was employed to measure the deflection. The gas composition was monitored by an in-situ mass spectroscopy. The results were discussed with respect to the changes of normal load, velocity and gas composition.

MM 23.4 Wed 14:45 IFW B

Investigation of crack formation in single-crystal sapphire due to combined normal and lateral forces — •Maksim Karniychuk[1], Thomas Chudoba[2], Volker Linss[2], and Frank Richter[1] — [1]Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany — [2]ASMEC Advanced Surface Mechanics GmbH, Bautzner Landstr. 45, 01454 Radeberg, Germany

One difficulty in contact mechanics is the detection of crack formation and the evaluation of the critical tensile stresses responsible for this effect. Nanoindentation is a non-destructive method for in situ detection of mechanical failures for instance by the observation of pop-in events in normal force-displacement curves. However, a direct observation of indentation induced pop-in events for many materials such as single-crystal sapphire is often very difficult. Another problem is that there exist ambiguous failure reasons without application of additional methods for the investigation of the failure.

The failure formation in single-crystal sapphire was detected in situ during combined normal and lateral force-displacement measurements by using a new Lateral Force Unit together with a commercial UMIS-2000 nanoindenter. Further analysis allows to conclude that crack opening is the first failure after pure elastic deformation. Thus, the knowledge of the critical lateral and normal forces can be used for the calculation of the critical tensile stress for crack formation with the help of a theoretical model for elastic deformation. The critical tensile stress value was estimated 9.5-10.5GPa.

MM 23.5 Wed 15:00 IFW B

Initiation of microcracks with predefined slip planes and directions to investigate the interaction with micro-structural barriers — •Michael Marx, Wolfgang Schäf, and Horst Vehoff — Universität des Saarlandes, Werkstoffwissenschaft und Methodik, Geb. D23, 66041 Saarbrücken

It is well known that the propagation of microstructurally short cracks can be reduced as result of the interaction with microstructure elements like grain- and phase boundaries. This effect is exploited in materials like composites and multiphase materials with defined phase and boundary conditions to get an improved toughness and fatigue resistance. Further improvement can be expected from grain boundary engineering. Therefore it is necessary to investigate the interaction mechanisms between cracks and boundaries systematically on a microscopic scale. To do this a reproducible method to initiate artificial microcracks with predicted conditions like crack length and distance from the crack tip to the boundary is needed. It will be shown that with a Focused Ion Beam (FIB) such artificial microcracks can not only be initiated but even the direction of the propagation can be predefined. This is possible due to a combination of a complete crystallographic specimen characterization by electron back scatter diffraction (EBSD) and the locally precise adjustable ion beam. So cracks can be initiated directly on the preferred slip system. As a first result the interaction of microcracks with different grain boundaries in a directionally solidified nickel based superalloy will be presented.

MM 24 Quasicrystals

Time: Wednesday 14:00–15:15 Room: IFW D

MM 24.1 Wed 14:00 IFW D

Formation of quasicrystals and complex periodic intermetallics in the Al-Pd-Ru and Al-Pd-Rh alloy systems — •Benjamin Grushko[1], Dmytro Pavlyuchkov[1,2], and Bartosz Przepiórzyński[1,3] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]I.N. Frantsevich Institute for Problems of Materials Science, 03680 Kiev 142, Ukraine — [3]Institute of Materials Science, Silesian University, 12 Bankowa, 40007 Katowice, Poland

This work continues the study of formation of complex intermetallics, including quasicrystals, in ternary Al-Pd-TM systems. The Al-Pd-Ru system is related to extensively studied Al-Pd-Fe [1, and Al-Pd-Rh to Al-Pd-Co [2]. We confirmed the thermal stability of the icosahedral (I) phase. The ternary extension of the Al-Pd Epsilon-phases is comparable to that in Al-Pd-Co. Three ternary cubic phases isostructural to C, C1 and C2 in Al-Pd-Fe were revealed. No stable quasicrystals were revealed in Al-Pd-Rh. The Al-Pd and Al-Rh Epsilon-phases form a continuous range. Also C-Al5Rh2 exhibited significant solubility of Pd. Two ternary phases structurally related to C-Al5Rh2 phase were revealed: cubic C2, isostructural to that in Al-Pd-TM (TM=Fe,Co,Ru) and hexagonal C3. The latter has a wide compositional range along about constant Al. [1] S. Balanetskyy, B. Grushko, T.Ya. Velikanova and K. Urban, J. Alloys Comp. 376, 158 (2004). [2] M. Yurechko, B. Grushko, T. Velikanova and K. Urban, J. Alloys Comp. 337, 172 (2002).

MM 24.2 Wed 14:15 IFW D

Molecular dynamics simulation of diffusion processes in decagonal quasicrystals — •Stephen Hocker, Franz Gähler, and Peter Brommer — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Diffusion in decagonal Al-Ni-Co and Al-Cu-Co quasicrystals is investigated by molecular dynamics simulations using newly developed EAM potentials. The potentials are determined with the force matching method: For a selection of small reference configurations, the cohesion energies, stresses, and forces on individual atoms are calculated by ab-inito methods, and the parametrized potentials are adjusted to optimally reproduce these data. One difficulty with these aluminium-rich ternary alloys is that short distances between transition metals are rare in realistic reference structures, so that there is not enough data to determine the short-range part of the transition metal potential accurately. The diffusion properties, however, depend sensitively also on these parts of the potential. Nevertheless, for a number of important diffusion processes the energy barriers determined by molecular statics simulations agree well with the activation enthalpies determined by ab-initio simulations and experimental data.

MM 24.3 Wed 14:30 IFW D

Planar binary dipolar colloidal quasicrystals — •Johannes Roth and Ulrich Koschella — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

The stability of planar binary decagonal quasicrystals interacting by dipolar potentials has been studied recently [1] with the help of computer simulations. Here we present new results from the search for possible decagonal and dodecagonal ground states. We discovered a path linking the quasicrystal structures with the best crystalline configurations. Although this proves that the quasicrystals cannot be the ground state in general we can argue that the quasicrystal structures have an advantage if the energy of grain boundaries between different phases and structural relaxations are taken into account. The results are confirmed by Monte-Carlo simulations.
[1] F. Scheffler, P. Maass, J. Roth, and H. Stark, European Physical Journal B **42**, 85 (2004)

MM 24.4 Wed 14:45 IFW D

Structure factor of the harmonic Fibonacci chain — •Steffen Sonntag, Michael Engel, Hansjörg Lipp, and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

In quasicrystals peculiar dynamic modes, the phasons, are existing in addition to the usual phonons. However, experimentally little is known about their precise nature. In order to investigate the interplay between phasons and phonons on an elementary level we resort to various one-dimensional model systems and study them with a special molecular dynamics code. Our main observables of the dynamics are the coherent and the incoherent dynamical structure factor. In a first talk we present simulation results for harmonic chains, (i.e. chains without phason flips), especially the harmonic Fibonacci chain. The structure factor consists of one-phonon and multi-phonon branches arranged periodically or quasiperiodically and is resolved in great detail by our algorithm. Comparison is made to analytical calculations which can be performed for certain approximations. The examination of the harmonic Fibonacci chain is prerequisite for separating phonon and phason dynamics in a chain with flippable atoms.

MM 24.5 Wed 15:00 IFW D

Structure factor of the dynamic Fibonacci chain — •Michael Engel, Steffen Sonntag, Hansjörg Lipp, and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

We have constructed an anharmonic chain, denoted "dynamic Fibonacci chain", where neighbouring atoms interact by double-well potentials. Thus they are able to perform both harmonic motions and phason flips where short and long atomic separations are exchanged. Molecular dynamics simulations show that the difference between the coherent and incoherent structure factors of the dynamic and the harmonic Fibonacci chain is in general tiny and has the form of a characteristic broadening of the phonon branches. We ascribe it to the phasons flips. The temperature dependence of the broadening is discussed. Attempts are made to filter out the flip dynamics by suppressing the harmonic motion. If a bias is introduced in the well depth, broadened optic phonon bands split off. In direct space we observe correlated phason flips propagating with phonon excitations.

MM 25 Poster Session

Time: Wednesday 15:30–17:30 Room: P4

MM 25.1 Wed 15:30 P4

IMPROVED PLANAR HOMOGENEITY OF MULTICRYSTALLINE SOLAR SILICON — •Andrey Sarikov, Vladimir Litovchenko, Anatoly Evtukh, and Vitaly Kostylyov — V. Lashkarev Institute of Semiconductor Physics NASU, 45 Nauki avenue, Kiev 03028, Ukraine

In this work, the influence of the gettering treatment by the combined getter of Al deposited on Si with developed surface on the distribution of diffusion length of minority charge carriers in multicrystalline silicon has been investigated. For the calculation of the parameters of diffusion length distribution, a new method has been proposed based on the mathematical treatment of experimentally measured integrated spectra of surface photovoltage measured by capacitor method (capacitor photovoltage).

The investigation carried out has demonstrated that the gettering treatments of multicrystalline Si samples lead to the increase of the homogeneity of the diffusion length of minority charge carriers, together with the increase of its average value. The distributions of the diffusion length in multicrystalline silicon can be well described by the normal distributions.

The proposed method allows resource-saving calculations of the parameters of the distributions of minority carrier diffusion length in inhomogeneous materials based on the analysis of integrated spectral dependences of capacitor photovoltage.

MM 25.2 Wed 15:30 P4

Computational optimization of non-crystalline multicomponent metallic alloys with respect to density — •Helmut Hermann[1], Antje Elsner[1], Kristin Lochmann[2], and Dietrich Stoyan[2] — [1]IFW Dresden, P.O.Box 27 01 16, D-01171 Dresden — [2]Freiberg University of Mining and Technology, Institute of Stochastics, Agricolastr. 1, D-09596 Freiberg

The generalized Bernal's model for simple liquids is used as an approach to the structure of liquid and glassy metallic alloys with multiple components. The input parameters of the computer simulations are size distribution and composition of components. The atoms are approximated by hard spheres with the corresponding metallic radii. For each parameter set the maximum density of the system is searched. Additionally, size distribution and composition are varied in order to find systems with particularly high density. The results are discussed in terms of the so-called atomic size distribution plot introduced recently to characterize multicomponent bulk metallic glasses.

MM 25.3 Wed 15:30 P4

Calculation of the Excess Volume of an Edge Dislocation by MD-Simulations — •Bernd Eberhard[1,2], Rolf Anders[2], and Ferdinand Haider[2] — [1]OSRAM GmbH, Mittelstetter Weg 2, 86830 Schwabmünchen — [2]Universität Augsburg, Institut für Physik

Edge as well as screw dislocations should not change the density of metallic systems within linear theory of elasticity, as dilatoric and compressive contributions to the density should be balanced. Taking second order displacements into account, this cancellation is not at all perfect, so that a net contribution of dislocations to the density could be expected. In present work, this effect of nonlinearity is reviewed with selected examples.

We prepared an fcc-lattice with edge dislocations using linear elasticity theory. This was then relaxed in an MD-simulation with variable periodic boundary conditions and the resulting volume per atom was compared to a perfect fcc-lattice. In addition to the average volume the spatial distribution of the excess volume was determined by constructing Voronoi polyhedra around all atoms.

Likewise an *ab initio* derived EAM interaction scheme for tungsten is used to derive the equilibrium state of a single edge dislocation with emphasis on special boundary conditions which take care of the far reaching displacement fields of dislocations. Also, the *Peierls stress of the first kind* was derived with proper strains applied to the cell.

MM 25.4 Wed 15:30 P4

Mechanical and Electric Properties of a Nanocable (5,5)C-NT at (17,0)BN-NT — •A. N. Enyashin[1,2], A.L. Ivanovskii[2], S. Gemming[1], and G. Seifert[1] — [1]Physikalische Chemie und Elektrochemie, Technische Universität, D-01062 Dresden. — [2]Institute of Solid State Chemistry, Ekaterinburg, Russia.

Atomistic simulations are performed to investigate the structural, mechanical and electronic properties of a coaxial C/BN nanocable composed of (5,5) C and (17,0) BN nanotubes under axial elongation, torsional and buckling deformations using quantum-chemical MD simulations in comparison with "free"components. Our results show that in the case of the elongation the elastic properties of the nanocable are determined by the carbon tube, and the fracture toughness by the BN tube. During a bending or a buckling of the nanocable a collapse of the BN wall is obtained later than in the case of "free"BN tube. In the process of the rupture a formation of carbon as well as -C-B-N- atomic chains is obtained. An analysis of the electronic structure shows that during the deformations the C/BN cable retains the basic electronic characteristics (metallic-like for the inner carbon nanotube and dielectric for the outer BN tube).

MM 25.5 Wed 15:30 P4

Elastic properties of the fine-grained materials produced by severe plastic deformation — •Przemyslaw Witczak, Zbigniew Witczak, Jolanta Borysiuk, and Ryszard Jemielniak — Institute of High Pressure Physics, Polish Academy of Sciences, Sokolowska 29, 01-142 Warszawa, Poland

The effect of the microstructure on elastic properties of severely deformed materials has been investigated. The hydrostatic extrusion was used to avoid microcracking in the materials being deformed. The pure copper and the dispersion-strengthen aluminium alloy were deformed at room temperature while the NiAl intermetallic compound was subjected to the hot hydrostatic extrusion. The total true strains of 4.2-6.5 were applied. Finally, the fine-grained materials were obtained with the average grain sizes in the range of 100-200 nm. The microstructure and elastic properties of the material were controlled at each stage of the deformation process. To take into account the developing texture in the material its full tensor of elasticity was measured using a resonant ultrasound spectroscopy (RUS) method. To describe the evolution of elastic properties with deformation the bulk modulus as the quantity independent of the texture and the equivalent elastic moduli of the isotropic material were calculated at each state of the process. The dependence of elastic properties on the equivalent true strain and the grain size of the material were obtained. As a final result of the refinement of the microstructure of the investigated materials to the grain size of 100-200 nm the reduction of their bulk moduli by 10-20 % was noticed. These results are discussed comparing them with the theoretical predictions.

MM 25.6 Wed 15:30 P4

Effect of Grinding Deformation on the Reheating Behavior of Steels — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

In the production of machine elements, after soft forming and heat treating processes hard surface finishing represents the final manufacturing step. Besides dimensional shaping, its main goal is the fabrication of functional areas with low roughness for good wear resistance. Additionally, crack-inhibiting compressive residual stresses are formed near the surface. During grinding of hardened steel, a narrow edge zone of about 0.01 mm in thickness experiences strong plastic deformation. Mechanical residual stresses up to 600 MPa in compression are built up. Although the dislocation density rises, the martensite {211} line broadening decreases by around 0.2° because of the formation of more stable defect structures like multipoles. Recently, post-machining thermal treatment of such steel parts below the tempering temperature was proposed to extend service lifetime of bearings or cogwheels [1]. It is shown for martensitic and banitic hardening that the pronounced reduction in XRD half width corroborates this recommendation. A model is established, which explains the effect by dislocational segregation of carbon and carbide dissolution. [1] J. Gegner: German Patent No. DE 102 09 264 B4 (2005)

MM 25.7 Wed 15:30 P4

Experimental Residual Stress Analysis of Hertzian Loaded Machine Parts — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

X-ray diffraction measurement represents an established testing tool for material response or residual life and failure analysis of machine elements that are highly loaded under Hertzian-contact fatigue conditions. The modified industrial-suited technique is described in detail and its application illustrated considering rolling bearings as example. Apart from the residual stress depth profiles, which could simpler be determined by the mechanical hole-drilling method, the martensite {211} line broadening characterizes material aging of hardened steels. Under rolling contact, the loaded volume in the edge zone sustains continuous constitutional changes, such as microstructure transformation (e.g. retained austenite decay) or carbide dissolution, caused by energy dissipation. By means of the X-ray diffraction technique, alterations of residual stresses and line broadening can be detected. For quantitative evaluation of these measured distance curves, calibration data, which permit comparison with the statistical parameters of the Weibull failure frequency distribution in the form of the L10 life equivalent, is available for ball and roller bearings.

MM 25.8 Wed 15:30 P4

Near- and Sub-Surface Fatigue of Rolling Bearings — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Material response of hardened steel to rolling contact starts with strain strengthening in the plastically deformed edge zone and the build-up of compressive residual stresses in the short shakedown period. The following steady-state stage controls a certain part of bearing lifetime, the duration of which depends on the loading conditions. The depth profiles of the equivalent stresses that are defined by the applied Hertzian pressure determine the positions of maximum residual stress (v. Mises) and material aging (orthogonal shear stress). In the final instability stage, steel softening occurs and is accompanied by decreasing XRD half width: in the classical Voskamp sub-surface rolling contact fatigue mode, high residual stresses can be built up, the magnitude of which correlates to the external load. On the other hand, for instance in case of boundary lubrication with metal-metal contact, the Nierlich (near-) surface failure mechanism is characterized by diminishing stress levels. In order to investigate this practically most important damage mode in more detail, X-ray diffraction based material response analysis of gear roller bearings stemming from rig tests is performed.

MM 25.9 Wed 15:30 P4

Investigation of micro-cracks and micro-cavities in rocks by means of tomography — •S. Zabler[1], K. Thermann[2], B. Kremmin[2], A. Rack[3], I. Manke[1], N. Kardjilov[1], and A. Haibel[1] — [1]Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung — [2]TU Berlin — [3]Forschungszentrum Karlsruhe - ANKA

The investigation of the microstructure of hard rock as greywacke, limestone or basalt is of special interest for basic research in applied geosciences. Hard rocks are composed of minerals, pores and micro-cracks containing gas or fluids. Technical parameters as permeability, uniaxial compressive strength and deformability (Young modulus) depend on the particular combination of the three phases. First of all, the influence exerted by the cavities as well as the closed and opened micro-cracks on the technical relevant parameters is a subject of research. It is known that compressive deformation is accompanied by nucleation, growth and coalescence of many small fractures. To obtain quantitative information of the pattern of micro-cracks in the past many research projects were performed using geophysical as well as microscopic techniques. In this work high resolution synchrotron tomography and neutron tomography are used for analysis of micro-cracks, micro cavities and the chemical composition of limestone and greywacke and basalt. The rocks were measured before and after uniaxial compression. It was possible to determine where and how micro cracks are initiated.

MM 25.10 Wed 15:30 P4

Physical aspects complete butt runout measuring — •Maryna Aliakseyeva — Minsk

In the given work the improved instrument for measuring complete butt runout is offered. The main features of the offered construction are parts broad range measuring possibility, small overall dimensions, simplicity in operation and high received end measures accuracy. This work concerns the physical aspects of measuring process. The offered construction can find broad applying in the field of metrology and quality control.

MM 25.11 Wed 15:30 P4

Advanced high strength and ductile Fe-based materials — •Katarzyna Werniewicz[1], Uta Kühn[1], Norbert Mattern[1], Birgit Bartusch[1], Ludwig Schultz[1], and Tadeusz Kulik[2] — [1]IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany — [2]Faculty of Materials Science and Engineering, Warsaw University of Technology, Wołoska 141, 02-507 Warsaw, Poland

We report about phase formation and mechanical behavior of copper mold cast Fe-Cr-Mo-Ga alloys. The rod-shaped samples with a diameter of 3 mm were prepared by centrifugal casting technique using different crucible materials. Interestingly, the samples prepared under different conditions show significant different microstructures and mechanical properties. It was found that one of the samples consists of a ductile bcc α-Fe phase embedded in a fcc Fe_3Ga. In order to characterize the mechanical properties of our alloy, Vickers hardness and room temperature compression tests were performed. The measured hardness of the α-Fe phase is about two times smaller (4.48 GPa) than the hardness of Fe_3Ga (8.08 GPa). The combination of the ductile and high strength phase leads to a material with high fracture strength (3 GPa) connected with excellent ductility (15%). This mechanical behavior has never been observed before for any Fe-based crystalline as well as bulk glassy alloys. We assume that these unique mechanical characteristics result from the formation of the specific two-phase structure, which occurs during the casting considering certain parameters.

MM 25.12 Wed 15:30 P4

The influence of doping with Ni on viscosity of liquid Al — •Andriy Yakymovych, Stepan Mudry, Vasyl Sklyarchuk, and Volodymyr Halchak — Physics of Metals Department, Ivan Franko Lviv National University,Kyrylo I Mephodiy Str. 8, 79005, Lviv, Ukraine

The addition of Ni to aluminium allows to improve its physical-chemical properties, which are important for practical use. It is interesting to clarify how change the main properties of Al in liquid state upon doping. On that, reason the viscosity of Al-Ni molten alloys with 2.5, 5, 7.5 at.% of Ni has been studied in this work by means of oscillating crucible method. Analyzing the available data on viscosity of Al and Al-based alloys one can conclude that there is a discrepancy between them.

Temperature dependence of viscosity coefficient for melts of various Al content shows Arrhenius like shape. With addition of Ni-atoms to aluminium the viscosity coefficient increases. The experimental data were compared with ones calculated for hard sphere model.

It is shown that chemical atomic ordering which is more pronounced for higher content of Ni may be the main reason of observed viscosity and activation energy change. We suggest that due to preferred interaction of Al and Ni atoms associates are responsible for the viscosity changes of neareutectic molten alloys. The content of Al and Ni in such chemically ordered structural units can vary in some wide range. This range is supposed to be significantly wider than homogeneity range for solid AlNi compound.

MM 25.13 Wed 15:30 P4

Tomographic atom probe (TAP) study of the chemical ordering in bulk amorphous alloys — •A. Shariq[1], T. Al-Kassab[1], R. Kirchheim[1], D.J. Safarik[2], and R.B. Schwarz[2] — [1]Institut für Materialphysik, Friedrich Hund Platz 1, D-37077, Göttingen, Germany — [2]Los Alamos National Laboratory, MST Division, Structural Property relation group, Los Alamos, NM 87545, USA

Amorphous alloys are characterized by the absence of atomic long range order and reveal only topological and sometimes chemical short range order. The wider supercooled liquid region in new amorphous alloys allows to explore the kinetics and thermodynamics in this region. In this study Pd based amorphous alloys are investigated using the TAP. Atomic scale chemical ordering in such alloys put great demands on the characterizing techniques. The 3D-tomographic atom probe (TAP) is proved to be currently the best experimental tool to gain information on chemical heterogeneities at the atomic scale. A new algorithm has been developed, which enables to extract information from the TAP data. The reconstructed volume has been used to elucidate the atomic distance between neighbouring atoms. Pd40,5Cu40,5P19 bulk amorphous alloy are produced as 2 mm diameter rod with the length of almost 46mm. The chemical ordering parameters elucidated by this algorithm for this Pd based amorphous alloys are discussed in this contribution.

MM 25.14 Wed 15:30 P4

Modeling of dendritic crystal growth in undercooled Ni-Zr melts — •Peter Galenko[1], Dieter Herlach[1], Denis Danilov[2], and Britta Nestler[2] — [1]German Aerospace Center, Institute of Space Simulation, Cologne, Germany — [2]University of Applied Sciences, Karlsruhe, Germany

Growth of dendritic crystals in undercooled Ni-Zr samples is studied by experimental, analytical and numerical methods. Experimental results provided by electo-magnetic levitation technique are compared with predictions of a sharp-interface model and of a diffuse-interface model. Using the sharp-interface model, kinetics of dendritic growth has been evaluated in the whole range of measured undercooling and of growth velocity of Ni-Zr dendrites. For the undercoolings up to 100 K the results of 2D isothermal and non-isothermal phase-field simulations are compared with the corresponding sharp-interface predictions. A form of modeled dendrites is compared with parabolic dendritic tip analytically found in the sharp-interface model. This work was performed with support from DFG under the projects Nos. He 1601/13 and Ne 822/2.

MM 25.15 Wed 15:30 P4

Controlling of structure formation in crystal growth — •Marco Fell and Jörg Bilgram — Laboratorium für Festkörperphysik, ETH, 8093 Zürich

Instabilities of the solid-liquid interface of xenon dendrites growing from pure melt give rise to the formation of side branches at arbitrary locations in the first some tip radii behind the tip. Side branches show a characteristic spacing, depending on undercooling, but the development on opposite sides of the dendrite is uncorrelated which, together with the coarsening effect, leads to a 'statistical symmetry' of dendritic crystals. We control the branching of a single crystal in our experiments by two kinds of external perturbation: i) A sole short-time heating pulse initiates synchronously side branches in all growth directions. Statistical processes govern their further development as the system relaxes to the steady-state growth some seconds after the pulse. ii) Melting the crystal by stabilizing the temperature of the melt slightly above melting temperature for some minutes leads to a reduction of interface curvature. Then a sharp temperature drop restarts the growth and new side branches are initiated symmetrically in all growth directions. They seem to interact over a macroscopic distance of more than 50 tip radii (1 mm) across the dendrite as they perform higher order branchings simultaneously.

A dendrite tip reacts upon the temperature drop by showing a hysteresis behavior in its radius. The branching as the result of unstable interfaces can be controlled by specific heating. The instability of spherical as well as flat solid-liquid interfaces are used to obtain a highly symmetric crystal in a controlled manner.

MM 25.16 Wed 15:30 P4

Characterization of Instabilities of 3D Xenon Crystals — •Oliver Wittwer and Jörg Bilgram — Laboratorium für Festkörperphysik, ETH, CH 8093 Zürich, Switzerland

The formation of complex structures like dendrites and seaweed is an example of structure formation at conditions far from equilibrium. We use xenon as a model substance in our experiments to study the growth of three dimensional crystals.

Instabilities of the solid-liquid interface are responsible for the formation of sidebranches as well as for tip splitting and the formation of multiple tips. The formation of doublons and multiple tips can be initiated in our experiments by changing the temperature distribution around the dendrite tip [1].

We report on transitions from dendrites to doublons, triplons and quadruplons. A symmetry classification of these structures has been developed. We have found a new type of doublon with different symmety. Examples and a characterization of such transitions will be presented.

[1] I. Stalder and J. H. Bilgram, Europhys. Lett. **56**, 829 (2001)

MM 25.17 Wed 15:30 P4

Dendritic solidification of metallic melts with ceramic particles — •Matthias Kolbe[1], Thomas Lierfeld[1,2], Phanikumar Gandham[1,3], Thomas Schenk[4,5], Gunther Eggeler[2], and Dieter M. Herlach[1] — [1]Institute for Space Simulation, DLR, Cologne, Germany — [2]Institute of Materials, Ruhr-University Bochum, Germany — [3]Department of Metallurgical and Materials Engineering, IITM, Chennai, India — [4]Experiments Division (ID19), ESRF, Grenoble, France — [5]Laboratoire de Physique des Matériaux, ÉdM de Nancy, France

The interaction of a dendritic solid/liquid interface with ceramic particles ($Ni_{98}Ta_2$ + Ta_2O_5) has been investigated by undercooling experiments at different levels of convection: (i) in a terrestrial electromagnetic levitation facility (EML) and (ii) in TEMPUS, a facility for containerless processing, under low gravity conditions during parabolic flights. Entrapment of particles in ground experiments and engulfment of a significant fraction of submicron particles under low gravity conditions are attributed to the lower level of convection in the latter experiments and to morphological features of dendritic solidification. Directional solidification of $Al_{90}Cu_{10}$ with alumina particles has been observed in-situ by X-ray radiography at ESRF. Tip splitting of Al-rich dendrites and evolution of cauliflower morphology has been observed. No evidence has been found for an influence of the alumina particles on dendrite growth.

MM 25.18 Wed 15:30 P4

Ion implantation of halogens: a promising technique for enhancing the high-temperature oxidation resistance of TiAl alloys — •Rossen Yankov[1], Alexander Donchev[2], Michael Schütze [2], and Edgar Richter[1] — [1]Institute of Ion Beam Physics and Materials Research, Forschungszentrum Rossendorf, 01314 Dresden — [2]Karl-Winnacker-Institut der DECHEMA, 60486 Frankfurt/Main

Gamma-TiAl alloys (γ-TiAl) are of great interest for advanced automobile, aerospace and power generation applications due to their light weight and high strength. However, excessive oxidation occurring in these materials at temperatures above 700°C has to date hindered their widespread use. Accordingly, in the present study, high-temperature oxidation behavior of γ-TiAl has been examined with consideration of the role of some halogens (Cl and F) in providing practically useful oxidation protection. Samples of technical γ-TiAl alloys have been treated by either beamline ion implantation or plasma immersion ion implantation (PIII) using various precursor gases. The degree of oxidation protection has been evaluated by testing ion implanted samples under conditions of isothermal and thermocyclic oxidation at 900°C. Optimized ion implantation processing has been found to produce marked improvement in the oxidation behavior of γ-TiAl. On the basis of the results obtained, a commercially viable process for enhancing the high-temperature oxidation resistance of γ-TiAl alloys using PIII of halogens is being developed.

MM 25.19 Wed 15:30 P4

Electron Holographic Materials Analysis at Atomic Resolution — •Martin Linck, Hannes Lichte, and Michael Lehmann — Institute for Structure Physics, Technische Universität Dresden, Dresden, Germany

Electron holography is a promising method to contribute also to the question "Which atoms are where?": The phase shift phi of the electron wave by an atom is related to the atomic number Z. Therefore, measuring the phase shift from a holographic phase image at atomic resolution in principle allows determining the atomic number. For quantitative evaluation, the atomic phase shift was determined by means of simulations, which are presently refined by means of DFT-calculations [1]. It turns out that - in addition to a coarse increase as phi proportional to Z^0.6 - the phase dependence is also strongly influenced by the electron configuration of the atoms, by thickness effects of the specimen, and by dynamical electron diffraction. Consequently, the inversion as Z(phi) is mostly not straightforward. Nevertheless, we succeeded in distinguishing atomic columns in binary materials, e.g. of Ga(Z=31) and As (Z=33) in (110)-oriented GaAs, showing the high potential of the method.

[1] Axel Rother et al., this conference

MM 25.20 Wed 15:30 P4

Stability and Electronic Properties of Inorganic Fullerenes from Quantum Chemical Simulations — •A. N. Enyashin, S. Gemming, and G. Seifert — Physikalische Chemie und Elektrochemie, Technische Universität, D-01062 Dresden.

The perspective applications of inorganic hollow nanoparticles as elements of nanodevices and lubricants require their profound theoretical investigations. In this work the structure models of the molybdenum sulfide fullerenes (nanooctahedra) both of stoichiometric and nonstoichiometric composition were proposed. Using the Density Functional Tight-Binding method (DFTB) it was shown for the first time that the "ideal"MoS_2 single-walled nano-octahedra with sizes at least less than 1700 atoms exhibit a high instability. The most stable skeletons of these sizes are provided by fullerenes with nonstoichiometric composition. Based on the DFTB estimations we would expect a stability of

the MoS_2 multi-layered fullerenes composed of more than 12000 atoms. In contrast to the semi-conducting nature of bulk or nanotubular MoS_2 allotropes a metallic-like character of electronic states is predicted for all molybdenum sulfide nanoparticles.

MM 25.21 Wed 15:30 P4

EBSD-study in a scanning electron microscope for the characterisation of metals with ultrafine microstructure — •M. Hockauf[1], M. Hietschold[2], L. Krüger[1], L. W. Meyer[1], and S. Schulze[2] — [1]Technische Universität Chemnitz, Professur Werkstoffe des Maschinenbaus — [2]Technische Universität Chemnitz, Professur Analytik an Festkörperoberflächen

In recent years the treatment of light metal materials like Mg, Al, Ti and their alloys by severe plastic deformation (SPD) attracts increasing attention as innovative way to achieve ultra fine microstructures. This causes unique properties of such materials as compared with conventional ones. Electron Back Scattering Diffraction (EBSD) in the SEM is a sophisticated technique to obtain detailed microstructure information. It closes the gap between light microscopy and TEM providing crystallographic data from large areas and allowing statistics of grain orientations and boundaries. On the other hand EBSD reaches high spatial resolution and allows correlation to macroscopic properties like fatigue-, corrosion-, strength-, deformation- and fracture behaviour. We studied light metals with ultra fine grained microstructures, as produced by equal channel angular pressing (ECAP). We demonstrate the significant change of the Aluminium alloy AA6063-T6 by SPD treatment: Starting from 100 um grain size with a high fraction of high-angle grain boundaries we end up with approximately 500 nm grain size and a high fraction of low-angle boundaries. This leads to a remarkable enhancement of strength and high cycle fatigue life (HCF). Further treatment however strengthens the material while limiting the HCF.

MM 25.22 Wed 15:30 P4

Preparation of porous membranes for the synthesis of nano- and micro-functional materials — •Giray Kartopu, Andre Piorra, Claus-Henning Solterbeck, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences, Kiel, Germany

Nanoparticles of functional materials of the form of nano-wires and -tubules have recently attracted wide interest. There are many chemical routes existing for their synthesis. One of the most promising techniques involves the so-called "template synthesis"[1,2], developed in the last decade, and employ a porous membrane (made of, e.g., alumina, polymer, etc.) as shape-protector and a suitable deposition technique for pore-filling, such as electrodeposition, sol-gel, CVD, etc. The choice of the to-be-produced material determines what sort of template and synthesis methods must be used. It is possible to control many properties of the final products: length, composition, shape (wire or tube), diameter, inter-distance, density, and so on.

In this work, it was aimed to prepare porous templates with controllable pore sizes and to fabricate metal and ceramic nanowires using them. By anodization of high-purity *Al* foils and p-type, low-resistivity Si wafers, self-standing, 10-100 μm thick templates with 1-2 μm and 20-100 nm pores, respectively, were obtained. Initial results of nano- and micro-wire deposition, such as solution-deposited TiO_2 nanowires (dia. $\sim$ 50 nm) will also be presented.

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[2] T. Wade, and J. E. Wegrove, Eur. Phys. J. Appl. Phys. 29, 3 (2005)

MM 25.23 Wed 15:30 P4

Microstructural investigation of Zr73.5Nb9Cu7Ni1Al9.5 nanostructure-dendrite composites produced by different casting techniques — •K. B. Kim[1], J. Das[1,2], W. Löser[2], M. H. Lee[3], D. H. Kim[4], S. K. Roy[5], and J. Eckert[1,2] — [1]FG Physikalische Metallkunde, FB 11 Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany — [3]Materials and Engineering Physics Program, Ames Laboratory, Iowa State University, Ames IA 50011, USA — [4]Center for Noncrystalline Materials, Department of Metallurgical Engineering, Yonsei University, 134 Schinchon-dong, Seodaemun-ku, Seoul, 120-749, Korea — [5]Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Kharagpur-721302, India

Zr73.5Nb9Cu7Ni1Al9.5 nanostructure-dendrite composites were fabricated using two different casting techniques: centrifugal casting and arc-melting. The microstructures of the centrifugally-cast and the arc-melted samples are overall homogeneous, consisting of micrometer-scale dendrites that are homogeneously distributed in a nanostructured matrix. The comparison of the microstructures of these two alloys reveals that the formation of nano-scale twins and a disordered ω-phase in the β-Zr dendrites only happens in the centrifugally-cast sample. The differences in the phases and the microstructures between the differently prepared samples significantly influence the corresponding mechanical properties of the specimens.

MM 25.24 Wed 15:30 P4

Thermal characterization of micro-structured NiTi samples by 3ω scanning thermal microscopy (SThM) — •Jürgen Gibkes[1], Mihai Chirtoc[2], Jean-Staphan Antoniow[2], Rolf Wernhardt[1], and Josef Pelzl[1] — [1]Inst. f. Experimentalphysik, Ruhr-Iuniversität Bochum, 44801 Bochum, Germany — [2]LTP, UTAP, Université de Reims, BP 1039, 51687 Reims Cedex 2, France

SThMs with thermal resistance probes offer a means to measure the local thermal conductivity by modulated local heating of the sample at the probe position and detecting the response of the probe at the frequency 3ω. The capability of the technique has been thoroughly investigated on homogenous samples by different research groups. In this contribution we report on recent results from a microstructured NiTi sample. The shape memory (SM) alloy NiTi has found a variety of important applications in industry and medicine. With decreasing sizes of the SM devices new techniques for structuring and shaping have to be employed. To prepare structures in the nano- and micrometer scale the focused ion beam offers a promising tool. However regions which have been treated with the ion beams may be distorted and their properties may deviate considerably from that of the untreated areas. Apart from the thermal transport parameters the changes of the phase transformation temperature would have a considerable undesired impact on the performance of the shape memory micro device. Scanning near field techniques are most suited to study these changes on nanoscale. This work is supported by the SFB 459

MM 25.25 Wed 15:30 P4

Advanced Materials Analysis using the Field Ion Image Tomography — •Alexander Heinrich, Catharina Wille, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The newly developed Field Ion Image Tomography is an excellent method which combines atomic resolution with a comparably large analysis volume in the order of 200nmx200nmx200nm. Due to the absence of cyclic stress with respect to the field assisted evaporation sequence of surface atoms during a Tomographic Atom Probe (TAP) analysis, specimen stability is improved and analysis of brittle materials is possible. The authors will introduce this new technique and give recent examples which demonstrate the capability of Field Ion Image Tomography. In particular, unique results on the thermal stability of nanocrystalline materials with respect to grain size and orientation and on the decomposition of CuCo, showing a long-scale arrangement of precipitates in phase decomposition due to the influence of elastic strain, will be introduced.

MM 25.26 Wed 15:30 P4

Extended Common Neighbour Analysis for results of molecular simulations of binary atomic systems — •Norbert Lümmen and Thomas Kraska — Physical Chemistry, University of Cologne, Luxemburger Str. 116, D-50939 Köln, Germany

Structural information extracted from atomic configurations obtained by molecular simulations are usually analysed by the pair correlation function. It describes the probability to find an atom at a certain distance from a reference atom. By comparison with pair correlation functions of perfectly ordered crystal structures one can determine the structure of the given system. Difficulties arise when several crystal structures are present within the same system and partly ordered/disordered binary systems are investigated.

The Common Neighbour Analysis (CNA) is a simple and powerful method for determining the amount of different crystal structures from molecular simulation configurations. For each atom within a configuration, the structural environment can be determined by a geometric analysis of the arrangement of its nearest neighbours. Up to now this method has been applied to monatomic systems. Here we describe an extension

of this method towards binary atomic systems. For four face centred binary structures the new extended signatures are presented. These are the $L1_0$ (AuCu), $L1_1$ (CuPt), $L2_0$ (Cu_3Au), and $L6_0$ ($CuTi_3$) structures. The bulk structure as well as the 100-, 110-, and 111-surface structures are included in the analysis.

MM 25.27 Wed 15:30 P4

Liquid-Liquid Interfacial Tension in Ternary Al-Bi-Cu Alloys — •Ivan Kaban and Walter Hoyer — Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany

Al-based monotectic alloys are considered as potential candidates for advanced bearings in car engines. Therefore a large number of various experimental investigations have been carried out in order to become proficient in casting of these alloys. However surprisingly it is, there exist virtually no experimental data on the physical property playing a crucial role in the demixing and solidification processes - liquid-liquid interfacial tension.

In this work we study the phase separation phenomenon in the ternary Al-Bi-Cu system, which is characterized by a very large miscibility region in the liquid state. The temperatures of the monotectic reactions, density difference of the coexisting phases and liquid-liquid interfacial tension in the ternary alloys $Al_{100-x}Cu_xBi_{65.5}$ (wt.%) are determined in wide temperature and composition ranges. The method is based on the experimental measurement of the force exerted on a stamp detached to the liquid-liquid interface and determination of the meniscus volume, on the one hand, and the theoretical calculation of the shape of meniscus and its volume as a function of the contact line, on the other hand.

It is established that the interfacial tension gradually increases when Al is substituted by Cu in the ternary $Al_{100-x}Cu_xBi_{65.5}$ alloys. The temperature dependences of the interfacial tension for the studied alloys show a behaviour similar to that in the binary Al-Bi monotectic system.

MM 25.28 Wed 15:30 P4

Ferroic multilayers with highly mobile interface charges — •Sibylle Gemming and Gotthard Seifert — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden

The multilayered system SrTiO3(001)|LaAlO3(001) was investigated by density-functional band-structure calculations. The system contains two interface terminations with differing physical properties. For SrO(001)|AlO2 (I) the interface spacing amounts to 190 pm, for TiO2(001)|LaO (II) the spacing is reduced to 186 pm. A model system with equal amounts of both terminations, is electronically neutral with an indirect band gap of about 2 eV and a direct one of 2.5 eV at the local-density level. Model systems with only termination I exhibit holes, localised in the O-based valence band; for systems with pure termination II the additional electrons occupy a Ti-based conduction band with stronger dispersion. Projections of the electron density show that both types of charge carrier are confined to the heterophase boundary region, and that the valence band holes are spatially more strongly localised than the additional conduction band electrons. Due to the complex strain state the dielectric properties of the system exhibit a pronounced asymmetry, which is enhanced by the presence of the interfaces.

MM 25.29 Wed 15:30 P4

Adhesion between NiTi shape memory alloy and thermoplastic polymers — •Klaus Neuking, Stephane Youcheu Kemtchou, Anwar Abu-Zarifa, and Gunther Eggeler — Ruhr-Universität Bochum, Werkstoffwissenschaft

NiTi has a particular technical importance due to its good shape memory properties. To increase the engineering potential, the combination with polymers is particularly interesting. One method to improve the poor bonding between metal and polymer is to deposit a thin interlayer which acts as a coupling agent between the two components. In this study the influence of silanisation on the adhesion to polyamid 6 and thermoplastic polyurethane has been investigated. The NiTi-surface was characterised with XPS and AFM to identify the oxide types and the morphology. The coated material was investigated with FT-IR spectroscopy and spectroscopic ellipsometry. Additionally pull-out tests were made to show the effect of the silanisation on the adhesion.

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MM 25.30 Wed 15:30 P4

Grain boundary and triple junction excess energy in nanocrystalline Gadolinium — •Stella Oldenbürger and Rainer Birringer — Universität des Saarlandes, FR 7.3 Technische Physik, Geb.D2.3, D-66123 Saarbrücken

Nanostructured materials are commonly used to investigate the influence of grain boundaries on macroscopic properties of polycrystalline materials. In a recent study on the grain size dependence of the lattice parameters of nanocrystalline Gadolinium it was found that, in addition to the grain boundary stress, a contribution of stress due to triple junctions had to be taken into account at grain sizes smaller than 10 nm. This result indicates that nanostructured Gadolinium is a candidate material to investigate the nature and behaviour of triple junctions. The aim of the present study is to determine the excess energy of the grain boundaries and triple junctions in nanocrystalline Gadolinium prepared by inert gas condensation. The excess energies of the samples are obtained by a sequence of isothermal calorimetric measurements at increasing temperatures. After each heating step, the average grain size is determined by X-ray diffraction. The contributions of the grain boundaries and the triple junctions to the excess energy are separated by a scaling analysis.

MM 25.31 Wed 15:30 P4

Very Cold Neutrons Reflection from surface of various materials — •Andrey Udovenko[1], Sergey Kuznetsov[1], Yurii Lapushkin[1], Anatolii Shelagin[2], Vitalii Grinev[3], Nataliya Kovaleva[3], and Liudmila Novokshonova[3] — [1]Lebedev Physics Institute, Moscow, Russian Federation — [2]Moscow Physics Technical Institute, Moscow, Russian Federation — [3]Semenov Chemical Physics Institute, Moscow, Russian Federation

Very cold neutron scattering and reflection were used to study the nano structure and the surface roughness of various materials. The dependence of the reflectivity coefficient vs. neutron wavelength for thermo pressed beryllium was obtained. The dimensions and concentrations of pores inside the sample, and the surface roughness were determined simultaneously. The average size and concentration of pores are in good agreement with the date obtained earlier by VCN transition method. The structural properties of Deuterated Polyethylene (DPE) covering grown on Si single-crystal surface activated previously by catalyst were studied by this technique. In particular, it was shown that the structure of the DPE layer near the Si substrate is more ordered than usual semi crystalline structure on the top of the DPE layer. This information can be of use for the development of the polymer composites with high polymer density around the filler particles. The results obtained are consistent with the observations made by optical and electron microscopy that suggests about the applicability of VCN reflectometry to the structural studies of the wide class of materials.

MM 25.32 Wed 15:30 P4

The influence of elastic strain on the early stages of decomposition in CuCo alloys — •Alexander Heinrich, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The early stages of nucleation in CuCo alloys with low supersaturation have always been of great interest to materials science as they are ideal model systems for phase separation. The authors would like to discuss results obtained with the Tomographic Atom Probe (TAP) and the Field Ion Image Tomography on the early stages of decomposition, annealed for times from one minute to one week at temperatures ranging from 703K to 853K. By means of a newly developed algorithm the determination of a radial distribution function is possible. Hence, it enables to detect initially small deviations from the homogeneous state and characterize clusters and precipitates with respect to size, morphology, number density and composition in all stages of nucleation. In addition, it was possible to quantify the formation of chains of precipitates owing to the influence of elastic strain. The results provide some new aspects to the decomposition path especially in the CuCo-system and will be discussed in terms of the linear elasticity theory.

MM 25.33 Wed 15:30 P4

Shape Memory Mechanism and Microstructural Analysis of Martensitic Transitions in Copper Based Alloys — •Osman Adiguzel — Firat University Department of Physics, 23169 Elazig/Turkey

The copper-based alloys can also exhibit the shape memory effect within a certain range of compositions. These alloys have bcc-type disordered structure at high temperatures and undergo the martensitic transition on cooling. In the case of reversible memory effect, forward and reverse transformations occur in the characteristic temperature intervals. Shape memory is related to the elastic behaviour of these materials depending on the temperature in the characteristic temperature ranges. If these alloys are deformed in martensitic condition, they keep the deformed shape, when the stress is removed, and furthermore, the deformation disappears and the material spontaneously returns to the original phase on heating over the austenite finish temperature. These alloys are also called thermoelastic materials due to this behaviour. Martensitic transformations occur by two or more lattice invariant shears on a {110}-type plane of austenite matrix which is basal plane or stacking plane of martensite. Martensite phase has the unusual layered structures which consist of an array of close-packed planes with complicated stacking sequences called as 3R, 9R or 18R martensites depending on the stacking sequences on {110}-type planes of the ordered lattice. Key Words: Shape memory effect, martensite, layered structures

MM 25.34 Wed 15:30 P4

Drift and fluctuation of M_S during thermal cycling of $Ni_{63}Al_{37}$ — •Leonard Müller, Benno Ludwig, and Uwe Klemradt — II. Physikalisches Institut, RWTH Aachen University

Measurement of time dependent phenomena in athermal martensite were conducted in a dedicated temperature chamber with an excellent temperature stability of ±4 mK over at least 63 hours. The phase transformation was observed in-situ by laserlight reflection and optical imaging.

The M_S temperature of an athermal martensite is classically considered to be a constant for each material system after some training. Results are presented that clearly show a trend in M_S and in addition a strong fluctuation of $\Delta M_S = \pm 4\,\mathrm{K}$ around this trend occuring during 125 thermal cycles. The reverse transformation shows the same behaviour. Statistical data analysis shows a non-normal distribution of M_S. Evidently, the thermal history is an important factor which can influence M_S and incubation times as well. Optical imaging shows microfractures in the sample that open in the martensitic phase, which probably affect the observed changes of M_S.

MM 25.35 Wed 15:30 P4

Preparation and optical characterisation of yttrium hydride films grown by pulsed laser deposition — •Helge Schröter and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig Mendelssohnstraße 3, 38106 Braunschweig

It is well known that rare earth metals e.g. yttrium, show a metal isolator transition, if they are exposed to a hydrogen atmosphere. In order to understand the mechanism of the metal isolator transition, we make investigations of layers with different concentrations of hydrogen in yttrium. The layers were manufactured by pulsed laser deposition in a hydrogen atmosphere. By variation of the hydrogen pressure thereby, it is possible to grow layers with different hydrogen concentrations. The change of the optical properties of the samples connected with the metal isolator transition, was examined by transmission spectroscopy and spectroscopic ellipsometry in the energy range between 1 eV and 30 eV. The ellipsometry measurements from 4 eV to 30 eV take place at the VUV/XUV ellipsometer at the BESSY II. To determine the surface finish of the layers, like quantity and dimension of droplets, AFM images of the layer surface were taken.

MM 25.36 Wed 15:30 P4

Hydrogen sorption properties of MgH2 prepared by high pressure reactive milling — •J. Zulkarnain, M. Herrich, B. Gebel, S. Doppiu, O. Gutfleisch, and L. Schultz — IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

Magnesium is considered as one of potential hydrogen storage materials because of its high capacity and low cost. However, high work temperature, slow raction kinetics and hard activation process limit the practical application of Mg-based hydrides. Recently, the reactive ball milling was successfully introduced to prepare hydrogen storage materials. In this work, MgH2 catalyzed with Ni nanoparticle was synthesized by high pressure reactive milling (HPRM) under hydrogen up to 100 bar. The hydrogen sorption properties were investigated using intelligent gravimetric analysis (IGA), phase identification and microstructure of the milled powders were examined using X-ray diffraction and scanning electron microscopy, respectively. Interesting to note that milling process could be reduced up to 2 hours which absorbed hydrogen about 5.3 wt% within 10 minutes. The results will be discussed in details.

MM 25.37 Wed 15:30 P4

Core hole effects in the O K absorption edge spectra of MgO, Al2O3 and ZnO — •T. Haupricht[1], R. Sutarto[1], H. Ott[1], H. Wu[1], H. -H Hsieh[2], H. -J Lin[3], C. T. Chen[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Chung Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan — [3]National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30077, Taiwan

One of the main challenges in theoretical solid state physics is to calculate accurately the response of a system to an external perturbation. This not a trivial task, not even for materials considered to be simple: band-insulators. Recently, several sophisticated methods have been developed to calculate the soft x-ray absorption spectra [1]. To test the accuracy of such calculation is also not trivial because not much reliable experimental data is available. For this we set out to do O K x-ray absorption measurement on standard materials like MgO, Al_2O_3 and ZnO. To obtain reliable data, i.e. not distorted by saturation effects, we have collected the spectra in the total electron yield mode, thereby taking also care that charging effects are neutralized. These experimental spectra are compared to the results of various theoretical approaches.
[1] Eric. L Shirley, Phys. Rev. B 80 (1998) 794

MM 25.38 Wed 15:30 P4

Effective Electron Mass of SrTiO3 based Thermoelectric Nano-Materials — •Wilfried Wunderlich — Nagoya Institute of Technology and Nagoya University, JST-CREST, Japan

The effective mass of electrons was calculated from the curvature of the electronic bands by ab-initio using Vasp- and Wien2k-code, which are based of the density-functional theory. The effective mass measured by the Hall effect in Nb-doped SrTiO3 single crystals showed comparable, but slightly larger values, which can be explained by interaction effects with phonons, polarons or other electrons. The understanding of these phenomena can be utilized in the improvement of thermoelectric materials based on layered composite materials, where the electrons travel nearly ballistic through a nano-wire like in a two-dimensional electron gas, while phonons are absorbed in the surrounding material. The natural superlattice of the Ruddlesden-Popper phases (SrTiO3)n-(SrO)m combines the semiconducting behavior of SrTiO3 with the low thermal conductivity of SrO and is a promising thermoelectric material.

MM 25.39 Wed 15:30 P4

Band-gap variation and structural phase transition in $Zn_{1-x}Mg_xO$ — •I.V. Maznichenko[1], M. Bouhassoune[2], A. Ernst[2], J. Henk[2], P. Bruno[2], M. Däne[1], D. Ködderitzsch[1], I. Mertig[1], W. Hergert[1], Z. Szotek[3], and W.M. Temmerman[3] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [3]Daresbury Laboratory, United Kingdom

Oxides are highly interesting materials with a huge potential for future applications. MgO is a well known spacer material in tunnel junctions whereas ZnO has a considerably smaller band gap and is applied for opto-electronic devices. The combination of both in the binary alloy $Zn_{1-x}Mg_xO$ exhibits extraordinary properties as a function of concentration x. First of all, $Zn_{1-x}Mg_xO$ undergoes a structural phase transition from the wurtzite structure of ZnO to the rock-salt structure of MgO at x=0.4. Second, the band gap of the alloy changes from 3.4 eV for x=0 to 7.2 eV for x=1. First-principle studies of the band gap as a function of concentration and the phase diagram based on total energy calculations of the alloy $Zn_{1-x}Mg_xO$ are reported. Full charge density-functional calculations in local-density approximation (DFT-LDA) were performed within the framework of the Korringa-Kohn-Rostoker method. The substitutional disorder was treated within the coherent potential approximation (CPA). For the Zn-3d levels we used the local self-interaction correction (SIC). The presented first-principle calculations are in good agreement with experimental results and demonstrate that a proper description of oxide semiconductors requires a treatment beyond LDA.

MM 25.40 Wed 15:30 P4

Investigation on structure and magnetic properties of La1-xSrxMnO3 — •Haifeng Li, Yixi Su, Jörg Persson , Paul Meuffels, Jens Walter, Rolf Skowronek, and Thomas Brückel — Institute for Solid State Research, Research Center Jülich, D-52425 Jülich, Germany

Transition metal oxides (TMO) have attracted strong attention since the interesting phase diagrams and unusual properties are expected depending on the interplay of lattice, spin, charge and orbital degrees of freedom. It has been realized the physical properties and the ground states of TMO are very sensitive to the synthesis conditions. In this poster, we report the optimization of powder preparation and single crystal growth of La1-xSrxMnO3. Structural and magnetic properties of air sintered, Ar and O2 annealed La7/8Sr1/8Mn1-γO3+δ have been systematically studied by neutron and X-ray powder diffraction and SQUID. [1] The possibilities of Mn deficiency after annealings and the sources of excess oxygen are studied. The correlation between both decreases of mean Mn-O and La (Sr)-O bond lengths and the increase of oxygen indicates excess oxygen is a superficies of cation vacancies. The ZFC magnetization of Ar annealed sample shows signatures of the reported structural transitions. The decrease of Tc after annealings is due to decrease of total strength of magnetic interaction, increase of magnetization coefficient B of spin wave, decrease of numbers of nearest magnetic neighbors and discontinuously increase of actual percentage of Mn site vacancies. The trace of Mn2+ is detected by XPS, indicating the possible existence of ligand hole states at oxygen. [1] H. F. Li, et al. (submitted)

MM 25.41 Wed 15:30 P4

Rauchgasseitige Hochtemperaturkorrosion von Wärmetauscherrohren in Kraftwerken — •Barbara Waldmann[1], Bernhard Stöcker[2], Ferdinand Haider[2], Siegfried Horn[1], Jahn Kehrle[2], and Julia Wagner[2] — [1]Universität Augsburg Lehrstuhl für Experimentalphysik II — [2]Universität Augsburg Lehrstuhl für Experimentalphysik I

Die Korrosion von Stählen an den Überhitzerrohren in Kraftwerken ist nach wie vor nicht in allen Einzelheiten verstanden. Speziell in Müllverbrennungsanlagen ist vor allem die rauchgasseitige Korrosion ein Problem von erheblicher technischer und wirtschaftlicher Bedeutung. Mit Hilfe einer Korrosionssonde wurden elektrochemische Messungen durchgeführt, die es ermöglichten die Korrosion online zu beobachten und mit Anlagenparametern zu korrelieren. Zusätzlich wurden nach den Messungen die Messelektroden offline im Labor (REM, Waage) untersucht um einen Zusammenhang von Korrosionsmechanismus und Messsignal zu untersuchen und die Korrosionsrate quantitativ zu bestimmen. Die mit der Sonde gefundenen Korrosionsraten stimmen gut mit den in der Anlage festgestellten überein. Desweiteren wurde die chemische Zusammensetzung des gebildeten Korrosionsproduktes und des Belags per EDX Analyse bestimmt, wobei sich eine Übereinstimmung mit der auf Überhitzerrohren aus der Anlage gefundenen Schichstruktur ergab. Außerderm wurden zur Entwicklung eines Korrosionsmodells Transportversuche im Labor durchgeführt.

MM 25.42 Wed 15:30 P4

Smart materials - copper based shape memory alloys a combined x-ray/ellipsometry study — •Yaroslav Filipov, Vasyl Staschuk, and Sergiy Bokoch — Taras Shevchenko Kiev National University, 6 Glushkova Prosp., Kiev 03127, Ukraine

The behavior of some materials which are often called smart materials is related to the structural changes in microscopic scale. One particular class of such materials is the shape-memory alloys (SMA) which exhibit a peculiar property called shape memory effect (SME). The origin of these phenomena lies in the fact that the material changes its internal crystalline structure with changing temperature. Metastable beta-phases of copper-based ternary alloys exhibit this peculiar property and transform from the ordered structures to the long period layered structures martensitically on cooling. Martensitic transformations in shape memory alloys occur by two lattice invariant shears in either of two opposite directions on a 110 plane of parent phase called basal plane of martensite. These planes are subjected to the hexagonal distortion with martensite formation on which atom sizes have important effect. In this work reported results of optical investigation by ellipsometry measurement and structure investigation by x-ray study of copper based SMA with estimated compound Cu83Al16Mn0,7Fe0,3. Finally it should be noted that the reported examinations results provides a useful platform for further advances.

MM 25.43 Wed 15:30 P4

Quasiperiodic structuresconstructed by projection in two stages — •Shelomo I Ben-Abraham[1] and Alexander Quandt[2] — [1]Department of Physics, Ben-Gurion University, IL-84105 Beer-Sheba, Israel — [2]Institut für Physik, Ernst-Moritz-Arndt Universität, D-17489 Greifswald, Germany

We study intermediate structures in which the periodic and quasiperiodic directions are intrinsically connected. One way to do so is by projecting a periodic structure in D(>3) dimensions into three-dimensional space in such a way that the second projection be quasiperiodic in a plane. We have achieved this earlier in the octagonal case [1] and partly in the dodecagonal case [2]. Here we briefly review these and present an improved dodecagonal version. We also present a new look at the pentagonal, or rather decagonal, case. In the octagonal case we cut and project first the four-dimensional simple cubic lattice Z4 into R3 and then into a suitable irrational R2. In the dodecagonal case we start with the root lattice D4 (in the earlier version it was Z6). For the pentagonal/decagonal case we have two variants: (1) In the *straightforward* version we start with the five-dimensional simple cubic lattice Z5, project it into an irrational R3 and then onto an R2. (2) In the *minimal* version we project the root lattice A4 (the checkerboard lattice) into an irrational R3 and then into an R2.

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MM 25.44 Wed 15:30 P4

Material modifications induced by swift heavy ions in NbTi superconducting wires — •Aleksandra Gruzdeva[1], Jürgen Eckert[2], Hartmut Fuess[1], Reinhard Neumann[3], Christina Trautmann[4], and Gertrud Walter[3] — [1]Darmstadt University of Technology, Materials Science, Structure Research, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]Darmstadt University of Technology, Materials Science, Physical Metallurgy, Petersenstr. 23, D-64287 Darmstadt, Germany — [3]Gesellschaft für Schwerionenforschung (GSI), Planckstr. 1, D-64129 Darmstadt, Germany — [4]

The Facility for Antiproton and Ion Research (FAIR) planned at GSI will be equipped with superconducting magnets. Due to the high beam intensities and related beam losses, radiation damage on the superconducting NbTi alloy used in the magnet coils has to be considered. We report first experimental results of NbTi multifilament wires and NbTi foil after irradiation with swift heavy ions. The wires were irradiated with U (2.6 GeV) ions and additionally NbTi foil was exposed to U (2.6 GeV) and Sm (1.7 GeV) ions at room temperature. The fluences were in the range between 10^{10} and $5 \bullet 10^{12}$ion/cm. The critical parameters of NbTi can be improved by precipitates of nanocristallites of the allotropic hexagonal close-packed α-Ti phase, which are responsible for flux pinning. Therefore, the value of critical current is related to the volume fraction and to the morphology of the α-Ti precipitates. The samples were analysed by x-ray diffraction and transmission electron microscopy. The filament samples show $< 110 >$ and foil samples (100)[$\bar{1}$10] texture. As a function of ion fluence, the amount of the α-Ti phase is considerably reduced. The texture diminishes equally under the same experimental conditions.

MM 25.45 Wed 15:30 P4

Casted or Hammered? Debye-Scherrer on an Ancient Cannon — •Matz Haaks[1], Ingo Müller[1], Hermann Franz[2], Stephan V. Roth[2], and Andreas Schoeps[2] — [1]Helmholtz- Institut für Strahlen und Kernphysik, Gruppe Maier, Nu*allee 14-16, 53115 Bonn — [2]DESY/HASYLAB, Notkestr.85, 22603 Hamburg

We present a solution achieved by physical methods on a discussion between historians about the authenticity of an iron alloy artefact. It was doubtful if an ancient cannon (baton à feu) from the Secq des Tournelles (Ferronnerie) museum at Rouen, France was originally wrought by a blacksmith in the 15th century or a reproduction cast in the 18th or 19th century. Due to the rareness of this cannon a non-destructive testing method is required to distinguish between the methods of manufacturing: casting or hammering. Contrary to casting, hammering introduces dislocation into the microstructure of the material, which can be detected non-destructively by X-ray diffraction. Because of the minimal wall thickness of 10 mm, we performed a Debye-Scherrer experiment at the hard X-ray beam-line at PETRA II at the DESY/HASYLAB, Hamburg using an X-ray energy of 106 keV. A comparison of the re-

flex broadening between the cannon and a reference sample of cast iron proofed the originality of the canon.

MM 26 Invited Talk Virk

Time: Thursday 09:30–10:00 Room: IFW A

Invited Talk MM 26.1 Thu 09:30 IFW A

Ion Tracks in Solids: An Overview of Technological Applications — •Hardev Singh Virk — 360, Sector 71, SAS Nagar, 160071, India

Heavy ion irradiation of solid materials has become an interesting field of basic and applied research during the last few decades. Ion tracks in solids have been used in material modification. Our laboratory has been engaged in the study of heavy ion tracks in insulators (mineral crystals, polymers and glasses) since 1980 using ion beams from UNILAC (GSI, Darmstadt), Synchrocyclotron (JINR, Dubna) and Pelletron (NSC, New Delhi). Ion beams from Li to U with fluences ranging from a single ion to 1014 ions/cm2 were used for material modification.

Polymers have been used in our laboratory for fabrication of ion track filters/membranes and investigation of optical and electrical response after heavy ion irradiation. The morphology of heavy ion latent tracks was revealed by atomic force microscopy. Etching and annealing behaviour of ion tracks and fission fragments in insulators was studied in great detail and single activation energy model for radiation damage annealing was proposed. Ion track filters were used for purification of contaminated water, air and blood samples. Microstructures comprising dots, wires, cones and tubules were created using electrochemical cell and template growth technique. Ion tracks technology is a state of art technology with potential applications in many diverse fields.

MM 27 Diffusion I

Time: Thursday 10:15–11:15 Room: IFW B

MM 27.1 Thu 10:15 IFW B

Transient heterogeneity in long-range order kinetics with limited vacancy mobility — •David Reith[1], Wolfgang Püschl[1], Ferdinand Haider[2], and Wolfgang Pfeiler[1] — [1]Institut für Materialphysik, Universität Wien, Boltzmanng. 5, AT-1090 Vienna, Austria — [2]Institut für Physik, Universität Augsburg, Universitätsstrasse 1, D-86159 Augsburg, Germany

Limited availability and mobility of vacancies may imprint a heterogeneous character on phase transformations which are otherwise expected to be homogeneous. This effect was investigated by a MC residence time algorithm for disorder-order and order-order transitions in long-range ordered intermetallics of $L1_2$ and B2 structure. The calculation cell was subdivided into coarse graining cells and heterogeneity assessed by the mean square deviation of the local long-range order parameter. A transient increase of this measure over the statistical fluctuation for the respective annealing temperature was observed for the B2 structure, but not in the $L1_2$ case. This can be understood in view of the majority sublattice as an easy diffusion highway. The effect in B2 is even more pronounced when starting from a disordered state. For a homogenous character of the kinetics to be restored, an earlier intuitive criterion relied on the overlap of regions bounded by the mean quadratic random walk distances of neighboring vacancies. Whereas this condition is in fact met at a very early stage in the kinetics, true homogeneity is reached only when a significant fraction of lattice sites has been visited by a vacancy.

MM 27.2 Thu 10:30 IFW B

Ordering kinetics is affected when jump barrier heights depend on local environment — •Martin Leitner[1], Wolfgang Püschl[1], Ferdinand Haider[2], and Wolfgang Pfeiler[1] — [1]Institut für Materialphysik, Universität Wien, Boltzmanng. 5, AT-1090 Vienna, Austria — [2]Institut für Physik, Universität Augsburg, Universitätsstrasse 1, D-86159 Augsburg, Germany

Kinetics of order-order transformations in a $L1_2$ long-range ordered model crystal was investigated by Monte-Carlo simulation employing a residence-time algorithm. Atoms were supposed to jump into nearest-neighbor vacancies. In doing so, they have to pass through a rectangular window of atoms which are nearest neighbors to both the initial and the final positions. ab initio calculations of jump profiles [Mat. Res. Soc. Symp. Proc. 842, S5.28 (2005)] for Ni_3Al show that barrier heights are markedly influenced by the kind of atoms occupying this window as well as their relative position. These results were incorporated as a rule into the MC algorithm, with a parameter characterizing the influence of the window atoms. If this parameter is increased from zero, three regimes of kinetic behavior can be discerned: a regime of finite but small influence below a certain threshold, a critical region where behavior changes quickly and in a qualitative way, an asymptotic region where the kinetics is stable against a further increase. It is discussed under which conditions the usual assumption of constant barrier height made in the literature will have to be modified.

MM 27.3 Thu 10:45 IFW B

Nonisothermal Internal Oxidation of Iron in Palladium — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Incomplete isothermal-isobaric internal oxidation of dilute homogeneous alloys is a frequently used experimental technique to measure the diffusion coefficient of oxygen in the base metal. Adopting this method, however, derivation of the Arrhenius equation requires a series of anneals at different temperatures. In the present work, a recently introduced [1], simplified experimental procedure is applied to the binary Pd-Fe system: incomplete temperature-controlled isobaric internal oxidation. Mathematical evaluation of the time development of the subscale thickness, which follows from SEM micrographs of samples that are removed from the furnace at several durations of the air annealing, is performed by means of an iterative computer model [2]. In this realistic process simulation, the sought quantity, i.e. the diffusivity D_O of oxygen in palladium, is the fit parameter and found to be:

$$D_O = 0.532 \cdot \exp\left(-18728.27/T\right)$$

Here, D_O is expressed in cm^2/s and temperature T ranges from 1073 to 1473 K. This result is compared with literature references.

[1] J. Gegner: Komplexe Diffusionsprozesse in Metallen. expert-Verlag, Renningen (2006), p. 397-402

[2] J. Gegner: New Computer Model for Internal Oxidation. Proc. MMT-2004, p. 1/28-1/37

MM 27.4 Thu 11:00 IFW B

Self-diffusion in Amorphous Silicon Nitride — •Harald Schmidt[1], Mukul Gupta[2], and Michael Bruns[3] — [1]Fakultät für Natur- und Materialwissenschaften, TU Clausthal, Robert-Koch-Str. 42, D-38678 Clausthal-Zellerfeld, Germany — [2]Laboratory for Neutron Scattering, ETH Zürich & PSI, Villigen, CH-5232, Switzerland — [3]Institut für Instrumentelle Analytik, Forschungszentrum Karlsruhe GmbH, D-76021 Karlsruhe, Germany

Amorphous silicon nitride is a model system for a covalently bound amorphous solid with extremely low atomic mobilities where reasonable values of self-diffusivities are still lacking. We used neutron reflectometry on isotope enriched $Si_3^{14}N_4/Si_3^{15}N_4$ multilayers to determine nitrogen self-diffusivities ranging from 10^{-24} to 10^{-21} m^2/s between 950 and 1250 °C. Time dependent diffusivities observed at 1150 °C indicate the presence of structural relaxation. For long annealing times (relaxed state) the diffusivities follow an Arrhenius law with an activation enthalpy of 3.6 eV. Possible diffusion mechanisms are discussed and the results are compared to the Si and N diffusivities in polycrystalline silicon nitride as obtained by Secondary Ion Mass Spectrometry.

MM 28 Amorphous and Liquid Materials III

Time: Thursday 11:45–13:00 Room: IFW B

MM 28.1 Thu 11:45 IFW B

Phase separation in liquid and amorphous Ni-Nb-Y alloys — •Norbert Mattern[1], Uta Kuehn[1], Annett Gebert[1], Thomas Gemming[1], Andreas Schöps[2], and Ludwig Schultz[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Hasylab, Notkestr. 85, D-22603 Hamburg, Germany

Novel phase-separated Ni-Nb-Y amorphous alloys were prepared by rapid quenching from the melt. The microstructure of the as-quenched ribbons consists of two amorphous regions Nb-enriched and Y-enriched with a size distribution from micrometer dimensions down to several nanometers. The two-phase amorphous structure was proven by electron micropscopy, X-ray diffraction and differential scanning calorimetry data. Decomposition and structure formation take place in the melt prior to solidification. In situ synchrotron high temperature X-ray diffraction measurements exhibit clearly a two stage melting in agreement with DSC measurement. An assessment of the Ni-Nb-Y phase diagram (CALPHAD method) pointed out that the miscibility gap of the monotectic binary Nb-Y system extends into the ternary system up to about 70at% Ni. The microstructure as well as the thermal behavior of the two-phase amorphous alloys depend on the chemical composition of the rapidly quenched alloy. The two amorphous phases crystallize separately at different temperatures. The microstructure after crystallization from the amorphous state is completely different from that obtained by crystallization from the liquid.

MM 28.2 Thu 12:00 IFW B

Liquid phase separation in Cu-based alloys — •Matthias Kolbe[1], Jianrong Gao[2], Lorenz Ratke[1], and Dieter M. Herlach[1] — [1]Institute for Space Simulation, DLR, Cologne, Germany — [2]Key Lab of Electromagnetic Processing of Materials, Northeastern University, Shenyang 110004, China

Many Cu-based alloys as Cu-Cr, Cu-Co, Cu-Nb and Cu-Fe exhibit in the binary phase diagram a flat liquidus, which is often associated to metastable phase separation in the region of the undercooled melt: When the metastable miscibility gap is entered, the homogeneous alloy separates into a Cu-rich and a Cu-poor liquid. Due to undercooling, the melt solidifies rapidly and properties of the metastable liquids are frozen in the solidified microstructure. We studied metastable phase separation and phase growth by electromagnetic levitation (EML), drop tube experiments and splat cooling of metallic melts. In addition, samples have been processed and solidified in the TEMPUS facility during parabolic flights under low gravity conditions. Compared to processing in EML on ground, the fluid flow is reduced in TEMPUS by an order of magnitude. The solidified microstructures show the influence of the different convection levels in the liquid on phase growth. The results are discussed within current models of liquid phase growth.

MM 28.3 Thu 12:15 IFW B

Microstructure and thermal behavior of Ni-Nb-Y alloys with additions of Sn and B — •Uwe Siegel, Uta Kühn, Norbert Mattern, Annett Gebert, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Ni-Nb-Y alloys with additions of Sn and B were prepared by melt-spinning and copper mold casting technique to achieve different cooling rates. The microstructure of the samples were investigated by means of X-ray diffraction and SEM and the thermal behavior was analysed by DSC measurements. The $Ni_{58.5}Nb_{20.25}Y_{21.25}$ alloy is known for its two phase amorphous microstructure obtained by rapid quenching [1]. Lower cooling rates, e.g. copper mold casting of this alloy, lead to a fully crystalline structure. Additions of Sn and B usually increase the glass forming ability of the Ni-Nb alloy system [2]. Based on these results the two-amorphous phase alloy was modified with different Sn and/or B contents in order to increase the glass forming ability and, therefore, to obtain bulk samples with a two amorphous phase microstructure. However, for the specific alloy composition, witch also contains Y, the formation of solid solutions is favoured what results in the precipitation of different crystalline phases during the solidification process at lower cooling rates. In contrast, using the melt spinning technique, decomposition of the amorphous phase was also obtained for Ni-Nb-Y-Sn alloys.

[1] Mattern, N. Kühn, U., Gebert, A., Gemming, T., Zinkevitch, M., Wendrock, H., and Schultz, L., Scripta Mater. 53, 271 (2005). [2] Choi-Yim, H., Xu, D. H., and Johnson, W. L., Appl. Phys. Lett. 82(7), 1030 (2003)

MM 28.4 Thu 12:30 IFW B

Cooling rate controlled microstructure and magnetic properties of metastable $Fe_{20}Nd_{80}$ alloys — •Jürgen Eckert[1], Golden Kumar[2,3], Jürgen Eckert[1], Annett Gebert[2], Ludwig Schultz[2], and Albrecht Wiedenmann[4] — [1]Darmstadt University of Technology, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]IFW Dresden,PF 270016, D-01171 Dresden, Germany — [3]Present address: NIMS, 1-2-1 Sengen, Tsukuba 305-0047, Japan — [4]Hahn-Meitner Institut Berlin, Glienickerstr. 100, D-14109 Berlin, Germany

The microstructures and magnetic properties of as-cast and annealed $Fe_{20}Nd_{80}$(hypereutectic) alloys were studied. Depending on the cooling rate the $Fe_{20}Nd_{80}$ alloys solidify into various metastable eutectic-like structures, which present a wide range of coercivity values varying from 0.2 to 0.48 T measured at room temperature. The alloys cooled at rates faster than 50 K/s display fine eutectic-like regions of Nd + A_1 and are hard magnetic. Transmission electron microscopy (TEM) studies clearly show that the hard magnetic A_1 regions are microscopically inhomogeneous. The alloys cooled slower than 25 K/s show a discontinuous rod-type eutectic of Nd + $Fe_{17}Nd_2$ and, consequently, exhibit a soft magnetic behaviour. The correlations between the cooling rate, the microstructure, and the coercivity of the $Fe_{20}Nd_{80}$ alloys are discussed. This work was supported by the German Science Foundation (DFG) via the DFG priority program "Phasenumwandlungen in mehrkomponentigen Schmelzen" under grant Ec 111/11.

MM 28.5 Thu 12:45 IFW B

On the plasma resonance of binary amorphous Al-TM alloys — •Martin Stiehler, Uta Giegengack, Jose Barzola-Quiquia, Jan Rauchhaupt, Steffen Schulze, and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Amorphous phases are ideal systems for investigating the mechanisms of structure formation. During the last years we reported about measurements of structure, electrical resistivity, thermopower, Hall-effect and thermal stability of binary a-AlTM alloys with 3d TM elements. The results were interpreted in a hybridization enhanced Hume-Rothery model with a composition-dependent valency of the TM.

Here we report on a unique systematics in the plasma resonance data of binary a-AlTM alloys. Conveniently, plasma resonance signals are used to determine the electron density of materials. For amorphous semiconductors we could apply this method in excellent agreement to the free electron model by calculating the electron density using the valencies of the elements from the periodic table. In a-AlTM alloys with 3d TM, the situation is different. Here such a simple approach fails. But with the valency of Al from the periodic table, in all this systems the 3d TM, including Ni, Co, Fe, Mn, Cr, V, Ti, and even Ca, seem to exhibit the same valency over the complete concentration range with no respect to the above mentioned hybridization effects. This result may be explained in a refined hybridization model.

MM 29 Poster Session (SYNW)

Time: Thursday 10:00–11:00 Room: P4

MM 29.1 Thu 10:00 P4

Contacting low dimensional metallic nanostructures on silicon — •Jan Rönspies[1], Svend Vagt[1], Tammo Block[1], Volkmar Zielasek[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Abteilung Oberflächen, Universität Hannover, Appelstr.2, 30167 Hannover, Germany — [2]Institut für Angewandte und Physikalische Chemie, Universität Bremen, 28359 Bremen, Germnay

The reliable fabrication of electrical contacts to conducting nanostructures is still a challenging problem to be solved. In our experiment we produced nanowires by a lithographic process with electron-beam stimulated thermal desorption of oxygen (EBSTD) in UHV from an ultrathin SiO_2 layer deposited on $Si(557)$ and $Si(111)$ substrates. We formed nanowires with a diameter of $10nm$ and a length of several hundred nanometers with Pb/Si(557) and Ag/Si(111) as example of 1D and 2D systems. For electrical contacting these nanostructures, an ex-situ electron beam lithographic process was used to create $TiSi_2$ macro-contacts forming a gap of a few hundred nanometers. The contacts were evaporated as a multi-layer system of Si followed by a Ti-layer and a capping of Si on a $Si(557)$ substrate to avoid stress induced trenches at the transition between the contacts and the substrate. We studied these contacts by SEM, STM, and Auger analysis, and found that they are stable up to $1200K$, UHV compatible and exhibit metallic conductance. Further analysis focusses on this transition from the macroscopic to the mesoscopic structures.

MM 29.2 Thu 10:00 P4

Integration of nanowires into microstructures by thin film fracture — •Seid Jebril, Mady Elbahri, and Rainer Adelung — Christian Albrechts Universitaet kiel

Microstructured PMMA- silicon substrate show a foot step in the formation of well aligned cracks. These microstructures were done by conventional lithography. The cracks are formed as a result of thermal stress. The shape of the microstructure affects the strain and stress concentration and creates predetermined fracture points which later relax via cracks. The cracks that are formed in such a manner serve as a template for the formation of nanowires, which are fabricated by metal deposition and consecutive mask lift-off. We report that channels made by conventional lithography can have a great influence on the control of the alignments of nanowires. These alignments can be precisely controlled by tailoring the width of the channels. When the channel in the order of around 10 microns, a regular zigzag nanowire pattern was observed. For example 20 Platinum nanowires with a zigzag fashion and aligned by 45 degree were fabricated in channels of 10 micrometer width and a length of 200 micrometer. These nanowires were connected end to end across the length of the channel with contacts. By tailoring the channel width, it is possible to control the alignment of the wire pattern in a desired way.

MM 29.3 Thu 10:00 P4

Reaction pathways of a regular disintegration of nanowires by thermocapillarity — •Lars Röntzsch and Karl-Heinz Heinig — Foschungszentrum Rossendorf, Dresden

Surface free energy minimization leads to morphological changes of wires, e.g. disintegration into a droplet chains (Rayleigh instability). At the nano-scale, capillary effects are much more pronounced than in macroscopic systems due to the large surface-to-volume ratio. However, capillary-driven self-organization processes are subject to increasing fluctuations with decreasing dimensions, which mostly prevent the formation of regular structures with long-range order. In this contribution, we predict by means of kinetic Monte Carlo simulations a novel method to fabricate size-controlled chains of nanodroplets. Our prediction rests on the temperature dependence of surface tension - the origin of thermocapillarity. Uncompensated forces occur due to surface temperature gradients. A surface tension gradient triggers the biased migration of atoms from hot to cold regions by surface diffusion. A periodic temperature gradient along a nanowire might be achieved by a surface-plasmon-polariton wave. Thus, long-range regularity of nanodroplet chains, that form during a self-organized disintegration of nanowires, might be considerably improved.

MM 29.4 Thu 10:00 P4

Fabrication of metal nanowires and their hydrogen sorption — •Sönke Schmidt and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Nanowire arrays of different metals (Pd, Fe, Nb, V) were produced by small angle sputtering on facetted sapphire, using the self shadowing effect of the facets. Minimum wires widths of about 50 nm were achieved. The wire length is given by the length of the facet. However, in case of Pd, Nb and Fe, island growth was found on the facets backside. The behaviour of Niobium wires during the exposure to hydrogen was investigated with AFM, using Contact mode, Lateral Force Microsopy (LFM) and Force Spectroscopy (FS), as well as Non-Contact mode. Resistivity measurements on Palladium wires arrays during hydrogen loading were carried out. The influence of hydride formation on the resistivity of wires will be discussed.

MM 29.5 Thu 10:00 P4

Quantum size effects and phase transitions in bismuth nanowires — •R. Lovrincic[1], T. W. Cornelius[2], M. E. Toimil Molares[2], S. Karim[2], R. Neumann[2], A. Pucci[1], and G. Fahsold[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg — [2]Gesellschaft für Schwerionenforschung, Planckstr. 1, 64291 Darmstadt

We investigate the IR-optical properties of bismuth nanowires (Bi-NW). The wires were prepared at the GSI in Darmstadt by template directed growth of Bi in etched ion tracks [1] and then dispersed on silicon wafers for IR-spectroscopic measurements under UHV-conditions. When the wire diameter is in the same range as the de Broglie wavelength of the conduction electrons, quantum size effects (QSE) occur and the energy bands split into subbands. As the electrons in Bi have a Fermi wavelenght of 40nm, the energy change due to QSE in Bi-NW is measurable for relatively thick wires [2]. We report on a shift of an absorption edge that is proportional to 1/dˆ2 while varying the diameter from 300 to 40nm. This blueshift is attributed to an increasing direct band gap. In addition we studied the thermal stability of these NW. During heating up, a strong jump in IR-transmission occurred which can clearly be attributed to the semimetal-metal transition at the melting point of bismuth. While cooling down, this jump occurred at a 100K lower temperature which can be explained within nucleation theory.

References

[1] T. W. Cornelius et al., Nanotechnology 16 (2005), 246. [2]Y.-M Lin et al., Phys. Rev. B. 62 (2000), 4610

MM 29.6 Thu 10:00 P4

Resonant metal nanowire excitation in the infrared — •F. Neubrech[1], S. Karim[2], F. Kost[1], T. Kolb[1], R. Lovrincic[1], R. Neumann[2], A. Pucci[1], and G. Fahsold[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg — [2]Gesellschaft für Schwerionenforschung, Planckstr. 1, 64291 Darmstadt

We analyse IR spectroscopic properties of single metal nanowires (Cu, Au) and compare the experimental results with simulations of electromagnetic scattering by a perfectly conducting wire. The nanowires with diameters from 50 to 200 nm are prepared by electrochemical deposition in polymeric etched ion track membranes [1]. After dissolution of the membrane, the single wires are put on an IR transparent KBr substrate for spectroscopic measurements, the most of which are performed with the IR microscope at the synchrotron light source ANKA. Spectroscopic microscopy allows to investigate single nanowires of a well defined length, volume, and orientation. We measured the IR transmission in the range from 700 cm-1 to 7000 cm-1 on nanowires with different diameters and lengths. For few micrometer long nanowires we see antenna-like resonances that depend on size and shape of the wires are in good agreement with our calculations. [2]

Due to an antenna-like resonance the enhancement of the electromagnetic nearfield is expected. For an experimental proof, we evaporate a thin paraffin layer on and around the wire and analyse the enhancement of vibration lines.

[1] M.E. Toimil Molares et al., Nanotechnology 15 (2004), 201
[2] G. Fahsold et al., ANKA annual report (2004).

MM 30 Symposium Nano Wires (SYNW)

Time: Thursday 11:00–13:15 Room: IFW D

MM 30.1 Thu 11:00 IFW D

Formation and Properties of Anodic TiO2 Nanotubes — •Patrik Schmuki, Julia Kunze, Hiroaki Tsuchiya, and Jan Macak — Uni Erlangen, Dept Mat. Sci, WW4

We present the electrochemical fabrication of self-organized high aspect ratio titanium oxide nanotubes achieved by an optimized and controlled anodization of Ti in fluoride containing solutions. In general, the morphology and the structure of porous layers are affected strongly by the electrochemical parameters used. Under optimized conditions self-organized highly ordered nanotubes with a length of several micrometers are formed consisting of arrays with single tube diameter of approx. 100 nm and a tube interval of 150 nm. Titanium oxides is a highly functional material that has numerous interesting properties, for example, in solar energy conversion, catalysis of decomposition of organic compounds (self-cleaning), wettability and biocompatibility. Therefore the tubes provide a novel functional and nanoscopic TiO2 form for numerous applications.

MM 30.2 Thu 11:15 IFW D

Formation of cobalt disilicide nanowires and nanochains in silicon by direct FIB writing — •Chavkat Akhmadaliev, Lothar Bischoff, Berndt Schmidt, and Arndt Mücklich — Forschungszentrum Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O.Box 510119, 01314 Dresden

A Focused Ion Beam (FIB) equipped with a CoNd alloy liquid metal ion source was used for the formation of cobalt disilicide nanowires and nanochains by an ion beam synthesis process. Co ions at 60 keV were implanted into silicon (111) and (100) substrates at 400-450°C followed by a two-step annealing at 600°C and 1000°C. During the FIB patterning of the samples using a digital scanning system the dose, the pixel dwell time and the relaxation time between the irradiation cycles were varied. The FIB spot size was in the range of 40 nm. The formation of long, stable nanowires occurs along the favoured <110>-crystal direction. The misalignment of the FIB trace relative to this direction leads to a decay of the wire into shorter ones or to the formation of chains of single-crystalline nanoparticles. Nanowires of 20-80 nm diameter and lengths up to 50 microns were obtained. Imaging of nanostructures was done in-plane by SEM, AFM and TEM. Cross-sections through nanowires were prepared by conventional Ga FIB milling across the nanowire. Further efforts will be concentrated in a better control of the nanowires growth, in the characterization of the electrical properties and in the fabrication of nanodevices.

MM 30.3 Thu 11:30 IFW D

Simple water based hot plate syntheses for complex nanostructures like Nanotubes, Nanoneedles and Nanowires — •Mady Elbahri, Seid Jebril, Dadichi Paretkar, and Rainer Adelung — Christian Albrechts Universitaet kiel

1-D one dimensional nanostructure like nanowire , nanotube, nanorods, etc. have attracted significant attention due to their unique properties and hence find various applications1. Because such structures represent the gateway towards the world of nanoscale devices, numerous approaches have been developed. However, a huge interest for cost effective as well as rapid methods covering large areas with complex nanostructures still remains a challenge. We present a family of new water based non equilibrium syntheses of nanostructures on a hot plate. Within this approach, structures like the formation of carbon nanotubes, square millimeter large arrays of upstanding Na2CO3 nanowires with typical length of 20 micrometer but diameters below 100 nm or surface nanowires from ZnO nanorods was performed within. Reproducibility and properties will be critically discussed together with possible applications. [1] Y. Xia et al., Adv. Mater 15, 353, (2003)

MM 30.4 Thu 11:45 IFW D

Electrical characterization of nanowires with the LEEPS microscope — •Dirk Weber, Berthold Völkel, Andre Beyer, and Armin Gölzhäuser — Physik supramolekularer Systeme, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

We introduce the Low Energy Electron Point Source (LEEPS) microscope as a tool for the electrical characterization of nanowires. The LEEPS microscope is a transmission electron microscope with electron energies from 20eV to 200eV. These electrons are emitted by a field emission tip with a radius in the atomic range. Because the electrons have a high spatial coherence the resulting detector image is an interference pattern which includes the structural as well as electrical and magnetic information of the object. We will present an imaging study which compares LEEPS images of metallic, semiconducting and insulating nanowires. Certain features in the image are related to the conductivity of the wire, e.g. the brightness of the wire centre in comparison to the adjacent background. In addition we measured the conductance of single nanowires by using a metallic tip as a movable electrode and the sample support as its counterpart. Length dependant measurements allowed a distinction between the wire conductance and the contact resistance.

MM 30.5 Thu 12:00 IFW D

Electric Field Induced Low Temperature Oxidation of Tungsten Nanowires — •C. Nowak[1], G. Schmitz[2], and R. Kirchheim[1] — [1]Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen — [2]Institut für Materialphysik, Universität Münster, D-48149 Münster

A study on room temperature oxidation of tungsten nanowires is presented, utilizing the high electric field arising at the tip of a nanowire if a moderate voltage is applied to influence the oxidation process.

Experiments were performed at room temperature under ambient atmosphere, TEM was applied to investigate the nanowires afterwards. Above a critical field strength, oxide layer formation occurs and is observed to virtually terminate at a field dependent state, determined by a critical field strength of $1.14(2) \times 10^9\,\mathrm{V/m}$ at the oxide-gas interface. This allows the controlled formation of oxide layers up to several 10 nm thick in the high field region at the tip of the nanowires. Diffraction pattern analysis reveals that the oxide is vitreous or nanocrystalline with a grain size of several nanometers. Additionally considering the stoichiometry it is concluded that mainly WO_3 is formed. The observed electric field induced modification of the natural oxidation process is discussed within the scope of the Cabrera and Mott theory of low temperature oxidation, particularly focusing on the aspect of charge compensation at the oxide-gas interface.

MM 30.6 Thu 12:15 IFW D

Properties of simple metal nanowire devices fabricated by thin film fracture — •Rainer Adelung, Seid Jebril, Mady Elbahri, and Dadichi Paretkar — Christian Albrechts Universitaet Kiel

It turned out that a thin film fracture based method [1] is well suitable to integrate nanowires into microstructures [2]. Nanowires exhibit a pronounced sensitivity to a change of chemical surrounding [3,4]. This effect can be based on two different principles. If a nanowire contains nanogaps, molecules with an affinity to the nanowire material cover these gaps. Typically, the conductivity of such a host guest structure is increased as the filled gaps assist the hopping transport. Contrary, it was shown that very thin nanowires without gaps show a decrease of conductivity if exposed to molecules. This is explained with a reduction of conducting electrons by localization at the chemical bond between molecule and wire. The electrical properties of nanowire devices fabricated with the thin film fracture approach will be presented. Changes in conductivity after exposure to different chemical species will be discussed. Those will be related with the structure of the nanowires and the device geometry. [1] R. Adelung et al. Nat. mater., 3, 375, (2004). [2] Pat. Nr. PCT/DE 2005/001852, (2005). [3] F. Patolsky and C. M. Lieber, Materials today, April (2005). [4] T. Hassenkam et al. , Nano Lett. 4, 19 (2004).

MM 30.7 Thu 12:30 IFW D

Electrical Properties of Self-Assembled Iron Nano Chains — •Hanna Onneken[1], Tim Hülser[1,2], Hartmut Wiggers[2], and Axel Lorke[1] — [1]Institute of physics, University Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg, Germany — [2]Institute of combustion and gas dynamics, University Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg, Germany

We report on the electrical properties of self-assembled iron nanochains. Morphological, structural and magnetic investigations confirm the existence of chains up to 300μm lengths, consisting of iron nanoparticles with diameter of about 35nm. A surrounding iron oxide shell on the particles can be explained by a self-limited oxidation process in ambient atmosphere.

Single chains can be deposited on substrates for electrical characteri-

zation or consequently collected in a particle precipitator for subsequent processing. Impedance Spectroscopy (IS) on single chains reveals two contributions to the overall impedance. The first contribution, an ohmic resistance is originated by the iron core of each particle. The second results from the intergranular contact between adjacent particles with a capacitance between the conducting iron cores, surrounded by the shell. From the core contribution a specific resistance of $4.4x10^{-8}$ Ωm has been calculated; this value is of the same order as that of bulk iron. Agglomerated chains from the precipitator can be separated in ultrasonic baths using polar and nonpolar solvents and consequently contacted via electron beam lithography for IS analysis.

MM 30.8 Thu 12:45 IFW D

Electrical and Mechanical Characterization of Carbon/Metal Core/Shell Nanostructures and Pure Metallic Nanotubes — •Maik Eggers, Thorsten Staedler, and Xin Jiang — Institute of Materials Engineering, University of Siegen, Siegen, Germany

One-dimensional nanostructures have been objects of interest for quite a while now. Nevertheless, the direct assessment of their material properties is still afflicted with difficulties as their characteristic size causes various handling issues. Besides the electrical, magnetic, and optical behaviour, the mechanical properties of nanostructures are of special interest as these basically determine the possibility to use the structures in order to design mechanically stable devices. In this work carbon nitride nanobells (CNNBs) and carbon nitride fibers have been deposited by chemical vapour deposition (CVD) onto a silicon wafer. In a second step these structures have been electroplated with nickel, creating films of carbon/nickel core/shell structures. A series of samples with various nickel film thicknesses is available for electrical and mechanical testing. In a third step the carbon host structure is removed by hydrogen etching leaving behind pure nickel tubes. Both, individual carbon, carbon/nickel, and films/networks of these structures as well as single nickel tubes have been mechanically characterized by scanning nanoindentation and scanning probe microscopy. The complex results, which cover the mechanical response of the system on the nano- and micro-scale, will be correlated and discussed.

MM 30.9 Thu 13:00 IFW D

BEC magnetic field microscopy of polycrystalline Goldwires — •Simon Aigner[1], Leonardo Della Pietra[1], Ron Folman[2], and Jörg Schmiedmayer[1] — [1]Physikalisches Institut, Universität Heidelberg, Germany — [2]Ben Gurion University, Be'er Sheva, Israel

A Bose Einstein Condensate on an atom chip can be used to measure magnetic field deviations of the trapping potential to unprecedented accuracy [1]. From the measured magnetic field map one can reconstruct angular deviations from straight current flow down to better then 10^{-4}rad. We use this magnetic field microscope to characterize the electric current flow in precisely prepared nano fabricated test wires of thin poly-crystalline gold. The wires have different combinations of grain size (50nm and 140nm), thickness (0.25μm and 2μm) and width (5μm to 200μm), while the edges show a roughness between 10nm-40nm. From our measurements we hope to get a better understanding for the material parameters that lead to deviations in the current direction and the resulting fragmentation potentials in atom chip experiments. The test chip has been fabricated by the group of Ron Folman at Ben Gurion University. We want to acknowledge support by the DFG SCHM1599/2-2, EU:HPRN-CT-2002-00304 (FASTNet) and German-Israel Project DIP-F2.2.

[1] Wildermuth et al, Nature 435, 440 (26 May 2005)

MM 31 Symposium Materials Modelling I

Time: Thursday 10:15–13:00 Room: IFW A

Keynote Talk MM 31.1 Thu 10:15 IFW A

Metallic nanoparticles: Challenging objects for computer simulations — •Karsten Albe — TU Darmstadt, Fachbereich Material- und Geowissenschaften, Petersenstr. 23, D-64287 Darmstadt

Metallic nanoparticles play an important role in many functional devices and can also be used as building blocks for nanocrystalline materials. Because of their finite size they exhibit peculiar structural, thermodynamic and functional properties that are not fully understood and in many cases difficult to reconcile with perceptions established for bulk materials. At this point computer simulations can serve as a valuable tool for gaining a better unterstanding of particle structure and properties as well as processing conditions. Although continuum models that include particle size as additional variable are applicable in some instances, atomic scale models appear to be the more appropriate choice for computer simulations of such finite objects. Nanoparticles, however, typically consist of several thousands of atoms and therefore are computationally too demanding for nowadays quantum mechanical methods. In this talk I will briefly present strategies how efficient, yet reliable, hamiltonians can be derived from first principles, that make atomic scale modelling feasible. Then a number of results obtained from molecular dynamics simulations on nanoparticle formation in the gas phase and nanoparticle-surface interactions will discussed. Finally, I will show lattice Monte-Carlo simulations that help to gain insights into the thermodynamics and kinetics of binary nanoalloys.

MM 31.2 Thu 10:45 IFW A

A Multi-lattice kinetic Monte Carlo study on the activation enthalpies for the interface mobility and interphase boundary diffusion in a massive transformation in iron — •Cornelis Bos, Ferdinand Sommer, and Eric-Jan Mittemeijer — Max Planck Institute for Metals Research, Heisenbergstrasse 3, D-70569 Stuttgart

Multi-lattice kinetic Monte Carlo simulations of lateral growth of ferrite in a massive austenite to ferrite transformation in iron were performed with a variable jump specific activation energy taking the local surroundings of the jumping atoms into account. From the simulations the activation enthalpy for the interface mobility and the migration activation enthalpy for interphase boundary diffusion were determined. It is shown that, depending on the interface structure the interface migration activation enthalpy can be larger or smaller than the migration activation enthalpy for boundary diffusion.

MM 31.3 Thu 11:00 IFW A

Ordering and correlation of cluster orientations in $CaCd_6$ — •Peter Brommer[1], Franz Gähler[1], and Marek Mihalkovič[2] — [1]Unversität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart, Germany — [2]Slovak Academy of Sciences, Institute of Physics, 84511 Bratislava, Slovakia

Cadmium and Calcium form a wide variety of complex alloy phases up to an icosahedral quasicrystal. The 1/1 approximant, a bcc arrangement of multi-shelled clusters, shows an order-disorder transition at around 100 K, probably caused by reorientation of the innermost, tetrahedral shell. We use molecular dynamics and EAM potentials generated by force matching to study this transition. Firstly, we isolated the 48 optimal locations for the tetrahedron atoms, out of which four are occupied. We then determined the ground state of a single cluster. From experiment it is known that the tetrahedron orientation in neighbouring clusters is correlated. By developing an effective cluster bond Hamiltonian we can explain the ordering and correlation of the cluster orientations in $CaCd_6$.

Keynote Talk MM 31.4 Thu 11:45 IFW A

Atomic-scale modelling of austenitic stainless steel — •Hans L. Skriver — CAMP, Technical University of Denmark

We have determined the stability of a ternary alloy of Fe, Cr, and Ni in the austenitic γ-FeNi phase including interstitial nitrogen and carbon by a variety of computational methods and approximations: the full charge density Exact Muffin-tin Orbitals (EMTO) method for accurate determination of formation energies, the order-N Locally Self-consistent Green Function (LSGF) method for efficient treatment of large supercells with a single interstitial nitrogen atom, and the Linear Muffin-Tin Orbitals (LMTO) method in conjunction with the Coherent Potential Approximation (CPA) and the Generalized Perturbation Method (GPM) for the calculation of the effective cluster interactions used in Monte Carlo simulations.

We find that the stability of nitrogen and carbon in the octahedral sites depends mainly on the number of Cr atoms in the first coordination shell. The calculated relative solution energies of nitrogen in γ-FeNi as a function of the local octahedral configuration and the abundance of the

different octahedral configurations obtained in the Monte Carlo simulations as a function of temperature form the basis for a discussion of the experimental uptake curves for nitrogen in stainless steel.

Keynote Talk MM 31.5 Thu 12:15 IFW A

Bond-Order Potentials: Bridging the electronic-atomistic modeling hierarchies in materials science — •Ralf Drautz and David Pettifor — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Quantum mechanical ab-initio methods are restricted to small numbers of atoms. Classical interatomic potentials, such as Tersoff, embedded atom (EAM), or Finnis Sinclair (FS) can simulate large numbers of atoms but their empirical character can render them inaccurate. In this talk we outline the derivation of interatomic bond-order potentials (BOPs) for sp-valent systems and d-valent transition metals by two well defined approximations within density functional theory. The resulting BOPs include a systematic variation of the bond order with valence [1] and are therefore applicable to a wide range of sp-valent and non-magnetic d-valent multicomponent systems. We demonstrate that the BOPs contain the Tersoff and EAM/FS potentials at the lowest order of approximation. [1] Drautz et al., Phys. Rev. B 72, 144105 (2005).

MM 31.6 Thu 12:45 IFW A

Effective potentials and dynamic fracture: C15 $NbCr_2$ — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

As fracture is ultimately determined by the breaking of bonds, an understanding of the fundamental mechanisms is required on the atomic level. To study such processes we perform molecular dynamics simulations on the Friauf-Laves phase C15 $NbCr_2$. For the interatomic interactions we match effective potentials to ab-initio data for the compound. Potentials for the elemental metals from the literature are also used for comparison. Ab-initio and experimental data indicate that our potentials are reliable and outperform available potentials making predictions on crack propagation reasonable. Fracture behaviour for the different potentials is discussed.

MM 32 Invited Talk Chen (SYMM)

Time: Thursday 14:00–14:30 Room: IFW A

Invited Talk MM 32.1 Thu 14:00 IFW A

From First-Principles Calculations to Precipitate Microstructure Evolution in Alloys — •Long-Qing Chen — Department of Materials Science and Engineering, Penn State University, University Park, PA 16802, USA

Precipitation reaction is one of the most important processes utilized to strengthen various engineering alloys, and the control of precipitate microstructures is the key to achieve desired mechanical properties. Various computational models have been applied to studying the thermodynamics and kinetics of precipitation reactions at different length and time scales. Examples include first-principles calculations of structural and thermodynamic properties of precipitate phases, phenomenological modeling of thermodynamics and phase equilibria in alloys with precipitates, and mesoscale models for predicting precipitate microstructure evolution. This presentation will discuss a number of approaches of integrating these different models through information passing at different scales with the objective to understand the relationships among the chemistry, microstructure and properties of materials. Examples of predicting the precipitate microstructure evolution in Al- and Ni-alloys will be presented.

MM 33 Symposium Materials Modelling II

Time: Thursday 14:45–16:30 Room: IFW A

Keynote Talk MM 33.1 Thu 14:45 IFW A

The first coarse-graining step in alloy theory from the electronic to the atomic level: Transferable potentials and cluster-expansion method — •Manfred Fähnle[1], Ralf Drautz[1,2], Alessandro Diaz-Ortiz[1], Frank Lechermann[1,3], Reinhard Singer[1], and Helmut Dosch[1] — [1]MPI Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — [2]Department of Materials, University of Oxford, Oxford, OX1 3PH, UK — [3]Ecole Polytechnique, CPHT, Palaiseau, F-91128, France

For the comprehensive description of the properties of alloys and compounds a combination of theories on various scales is required. On the most fundamental scale, i.e., the electronic scale, the density functional electron theory is able to yield reliable information for single systems, but it cannot scan a very large variety of competing structures in order to determine the ground-state structures or the finite-temperature phase diagrams in multi-component systems. To do this, a first coarse-graining step from the electronic to the atomic scale is required. It is shown [1] that this can be achieved, in principle whithout loosing the accuracy of the ab-initio calculations, by means of transferable potentials and by the cluster-expansion method (CE). The recently developed methods to construct terminated but well-converged CEs are discussed, as well as extensions of the CE method to magnetic degrees of freedom. The power and the remaining limitations of the presently established versions of the CE method are demonstrated for a variety of technologically interesting systems.

[1] R. Drautz et al., J. Phys.: Cond. Matter **16**, 3843 (2004).

MM 33.2 Thu 15:15 IFW A

Efficient tools for the surface cluster expansion of binary alloy surfaces — •Ole Wieckhorst and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen, Germany

The combination of density functional theory (DFT) with concepts from statistical physics is applied to the segregation at binary alloy surfaces. The binary alloy problem is solved in the cluster expansion by mapping DFT-based formation enthalpies of a number of selected input structures onto a finite set of pair and multibody interactions corresponding to characteristic figures like triangles, tetrahedrons, etc. One critical point of this concept is the selection of an appropriate set of figures, especially when the surface comes into play, which can be solved by treating this selection problem with a genetic algorithm. The number of figures, that has to be selected can be reduced dramatically by properly choosing a reference energy, which can be viewed as an approximation to the surface formation energies. It will be shown how the mixed space cluster expansion can be used to incorporate additional relaxation effects at the surface into this reference energy, thus reducing the need for a large number of manybody figures to compensate for large relaxation energies. As an example, we studied antisite segregation [1,2]in the B2-CoAl(100) surface. (supported by DFG)

[1] V. Blum et al., Phys. Rev. Lett. **89**, 266102 (2002).
[2] O. Wieckhorst et al., Phys. Rev. Lett. **92**, 195503 (2004).

MM 33.3 Thu 15:30 IFW A

Ab initio **calculation of thermodynamic properties of metals: xc-related error bars and chemical trends** — •Blazej Grabowski, Tilmann Hickel, Sixten Boeck, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf

Phase diagrams are indispensable tools in predicting material evolution during its processing. Current approaches to obtain such phase diagrams (e.g. CALPHAD) are based on extra- and interpolation of experimental data. Experimental costs and unreachability of metastable phases needed for these methods necessitate *ab initio* calculations without experimental input.

The accuracy of density-functional based *ab initio* methods is, in principle, only limited by the exchange-correlation functional. We have therefore evaluated the accuracy of the most commonly used functionals (LDA, PBE-GGA) by calculating key thermodynamic properties for a

wide range of metallic materials (Fe, Al, Cu, Rh, Li, etc.). In particular, we have calculated the volume dependence of the free energy employing the quasiharmonic approximation. Great care was taken to ensure sufficient convergence with respect to supercell size, k-point sampling, and energy cutoff. Based on these results, we have derived thermodynamic quantities such as the thermal expansion coefficient and the temperature dependence of the free energy, which yield a direct insight into the quality of LDA and GGA for the various metals when compared to experimental data.

MM 33.4 Thu 15:45 IFW A

First Principles Calculations of the Elastic Constants of Fe-Pt Phases — •Nikolay Zotov and Alfred Ludwig — Forschungszentrum Caesar, Ludwig-Erhard-Allee 2, D-53175 Bonn

The electronic structure of the ordered and disordered Fe-Pt phases has been extensively studied during the last two decades by ab-initio methods due to their outstanding electronic and magnetic properties. For example, thin films containing the fct ordered FePt phase are promising candidates for high-density recording media. Their elastic properties have received less attention although the bulk modulus anomaly in FePt alloys is experimentally known since long time. We have carried out a first-principles study of all zero-pressure elastic constants for the ordered Fe-Pt alloys including pure bcc Fe and fcc Pt. The calculations were made using the VASP code implementation of the density functional theory in the generalized gradient approximation (GGA) with Perdew-Wang exchange correlation and projector augmented wave pseudopotentials. The integrations of the Brillouin zone were made on a mesh of 11x11x11 k-points. The calculated elastic constants for bcc Fe and fcc Pt are in good agreement with experimental data and previous calculations. Several trends in the predicted elastic constants are established as a function of the chemical composition. The bulk and shear modulus as well as c_{11}, c_{12} and c_{44} have a minimum for the Fe_3Pt phase and a maximum for the fct FePt phase. The calculated elastic constants obey all conditions for mechanic stability of the cubic and tetragonal phases but $c_{11} - c_{12}$ is close to zero for Fe_3Pt suggesting a shear instability at this composition.

MM 33.5 Thu 16:00 IFW A

Temperature dependent properties of Ni_2MnGa — •Tilmann Hickel, Blazej Grabowski, Oliver Marquardt, and Jörg Neugebauer — Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

The ferromagnetic shape memory compound Ni_2MnGa undergoes a martensitic phase transition at 200 K. For temperatures well above this value it has a cubic $L2_1$ structure, whereas below the transition temperature the structure is orthorhombic. The resulting deformations drive the shape-memory effect. In order to understand the microscopic processes connected to this phase transition, we have investigated its temperature dependence combining density functional theory in the generalized gradient approximation and thermodynamic concepts. For this purpose, phonon and magnon spectra have been determined. Employing the quasiharmonic approximation we have calculated free energy surfaces as function of key reaction coordinates (lattice constant, c/a-ratio). A detailed analysis of the temperature dependence of the surface minima and the low energy paths allowed to extract direct information regarding the thermodynamic stability of the different phases (austenite, martensite, pre-martensite) and activation barriers. The results are compared with recent experiments.

MM 33.6 Thu 16:15 IFW A

High-precision mixed-space cluster expansion for Cu-rich Cu-Pd alloys: Controlling the LPS group — •S. Bärthlein[1], G.L.W. Hart[2], A. Zunger[3], and S. Müller[1] — [1]Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Department of Physics and Astronomy, Northern Arizona University, Flagstaff, Arizona 86011-6010 — [3]National Renewable Energy Laboratory, Golden, Colorado 80401

A remarkable feature of Cu-Pd alloys is the existence of long-periodic superlattices (LPS) on the Cu-rich side of the phase diagram. Whereas earlier studies did not include necessary information about the diversity of important, but until then inaccessible formation enthalpies, we are able by combining DFT calculations with a mixed-space cluster expansion, genetic algorithms [1] and Monte Carlo to predict the phase stability from millions of possible candidates. Effective interactions were constructed, enabling us to predict and to study the realm of one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) LPS with 1D-LPS3 being the $T = 0$K ground state at $x_{Pd} = 0.25$. Furthermore, we investigate the so-called "$L1_2$" phase, which emerges as a domain-mixture between the LPS3 and a newly discovered low-temperature phase at $x_{Pd} = 0.125$. Examination of the systems short-range order reveals a continuous transition from the domain-mixture to the disordered solid solution. (Supported by DFG and NSF.)

[1] G.L.W. Hart et al., Nat. Mater. **4**, 391 (2005)

MM 34 Symposium Materials Modelling III

Time: Thursday 17:00–18:45 Room: IFW A

MM 34.1 Thu 17:00 IFW A

Material Modelling and Mathematical Simulation of Steel Carbonitriding — •Nicolas Bontems[1], Taláat Al-Kassab[1], Jürgen Gegner[2], Reiner Kirchheim[1], and Peter-J. Wilbrandt[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Carbonitriding of low-alloyed steels is performed in the austenitic region in gas mixtures offering high carbon and nitrogen potential at temperatures of about 850 °C. Inward diffusing nitrogen leads to a varying microstructure from the surface to the bulk. Such process is often applied to standard bearing steel 100Cr6. Since nitrogen increases the carbon activity, carbon will be released by carbide dissolution and chromium nitride precipitates will be formed. Carbon diffuses in the steel according to the activity gradient, which is acting as driving force. Two basic models have been developed to treat these two complex diffusion problems. The first model for nitrogen diffusion distinguishes atoms dissolved in the lattice and trapped in precipitates or at phase boundaries. The second model for carbon diffusion considers the varying gradient of the carbon activity. A numerical scheme enables the solution of Fick second laws. First results show the applicability of the models, which deliver a numerical evaluation of the variations of the carbon activity with the amount of nitrogen and support a special kinetic mechanism for nitrogen in-diffusion in presence of CrN precipitates.

MM 34.2 Thu 17:15 IFW A

A parallel 3D simulator for solidification microstructures with fluid flow — •Britta Nestler, Michael Selzer, and Frank Wendler — University of Applied Sciences Karlsruhe, Moltkestr. 30, 76133 Karlsruhe

The effect of fluid flow on three-dimensional crystal growth structures is studied by numerical simulations. It is a phenomenon with particular effects in three dimensions where solute is transported in the spatial domain and around the growing crystals. From experiments, it is well known that fluid flow dramatically alters the solidification structure during a casting process. The presence of flow admits the possibility of instabilities due to the flow itself, in addition to the well known morphological instabilities found in crystal growth. Hence, flow has an important influence on the process conditions and on the resulting material properties during the solidification from a melt. We first present a new model for an arbitrary number of phases with fluid flow, which is thermodynamically consistent. Then we introduce our parallel 3D simulator optimized for solving the coupled set of the phase-field model equations and the Navier-Stokes equations for fluid flow. The phase-field equations contain partial differential equations describing the transport of mass and heat and the corresponding temporal evolution of the phase states (order parameters) in the system. Examples of applying the simulator to the solidification of alloy microstructures under the influence of forced and convective flow are considered, and the interaction between diffusion and convection is discussed. In particular, we show simulation results of growing grains and of eutectic microstructures in a flow field.

MM 34.3 Thu 17:30 IFW A

Using the phase-field method to treat large scale grain growth problems — •Frank Wendler and Britta Nestler — University of Applied Sciences Karlsruhe, Moltkestr. 30, 76133 Karlsruhe

A multi-phase-field model formerly introduced allows the treatment of free boundary problems with complex interface morphologies, where the phase-fields (order parameters) define diffuse interfaces between adjacent phases. Anisotropy in surface energies and kinetic coefficients of the crystalline phases enable the modelling of polycrystals where each grain is represented by a different phase. In the talk special attention is given to grain structures and polycrystals, with applications in alloy solidification as well as geology. Correctly choosen thermophysical and numerical parameters for the binary Ni-Cu alloy system allow for quantitative simulations, initiated with a high number of differently oriented seed crystals growing into an undercooled melt. When starting from a domain wall, selection processes depending on undercooling and distribution of crystal orientations were found and compared for 2D and 3D simulations. Secondly, the seeds are randomly distributed in the simulation domain to mimic homogeneous nucleation. In each case after a complete solidification the resulting polycrystal shows characteristic morphologies, directed by selection processes and grain orientation relationships. Additionally, the influence of a convective melt flow is shown. As a final processing step, grain coarsening at increased temperature is simulated and characteristic relations for grain size and orientational evolution were found.

MM 34.4 Thu 17:45 IFW A

Three dimensional investigation of the texture and microstructure below a nanoindent in a Cu single crystal using 3D EBSD and crystal plasticity finite element simulations — •Nader Zaafarani[1], Dierk Raabe[1], RamNiwas Singh[2], Franz Roters[1], and Stefan Zaefferer[1] — [1]Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Deutschland — [2]Materials Science Division, Bhabha Atomic Research Centre, Mumbai-400085, India

This is a 3D study on the microstructure and texture below a conical nanoindent in a [111] Cu single crystal at a nanometer-scale resolution. The experiments are conducted by using a joint high-resolution field emission SEM-EBSD set-up coupled with serial sectioning in a focused ion beam (FIB) system in the form of a cross-beam 3D crystal orientation microscope (3D EBSD). The experiments (conducted in sets of subsequent (11-2) cross section planes) reveal a pronounced deformation-induced 3D patterning of the lattice rotations below the indent. In the cross section planes perpendicular to the (111) surface plane below the indenter tip the observed deformation-induced rotation pattern is characterized by an outer tangent zone with large absolute values of the rotations and an inner zone closer to the indenter axis with small rotations. The 3D crystal plasticity simulations compared with the experiments have predicted a similar pattern for the absolute orientation changes but they fail to predict the fine details of the rotation patterning with the frequent changes in sign observed in the experiment. Also the simulations over-emphasize the magnitude of the rotation field tangent to the indenter relative to that directly below the indenter tip.

MM 34.5 Thu 18:00 IFW A

Discrete Dislocation dynamics simulation: plasticity in μ meter sized pillars — •Daniel Weygand and Magali Poignat — IZBS, Kaiserstr. 12, University of Karlsruhe, 76133 Karlsruhe

The mechanical behaviour of monocrystalline μ-meter sized pillars is investigated using the three dimensional discrete dislocation dynamics methodology. The dependence of the plastic response of the pillars on the dislocation microstructure initially present and on the loading/boundary conditions is investigated. The analysis of the plasticity is performed in terms of the time evolution of individual dislocation densities on the different slip directions. These density evolutions are discussed in the context of the observed hardening. The study shows furthermore the influence of the grain orientation on the plastic flow. The simulation results are compared to the small strain regime of experimental stress strain curves obtained from compression experiments of such pillars.

MM 34.6 Thu 18:15 IFW A

A refined statistical strain hardening and recovery model — •Volker Mohles, Prasad Gurla, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-52056 Aachen, Germany

Statistical models of dislocation density evolution are a means to quickly predict flow stress curves of metal alloys. They involve a relatively large number of parameters to be adjusted, but they can be utilized for instance in Finite Element simulations of plastic deformation for their low calculation effort. One such model actually applied for this purpose is the 3-Internal-Variables-Model 3IVM. This model has been improved recently in several aspects, especially so in respect of recovery kinetics: climb and cross slip are both allowed for, and an additional recovery mechanism has been added which is proportional to the strain rate. With this recovery model, 3IVM can now be fitted quite well to flow curves of Al-polycrystals (almost pure) at various strain rates and temperatures T in the range $20°C < T < 450°C$ with a single set of parameters. In addition, for improved coverage of alloys, the strengthening effect of solutes has been revised such that thermally activated dislocation glide is regarded accurately.

MM 34.7 Thu 18:30 IFW A

A grain boundary mechanism for nonlocal constitutive laws in crystal plasticity finite element simulations — •Anxin Ma, Franz Roters, and Dierk Raabe — Max Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

When the simulation scale in crystal plasticity becomes small such as in studies focused on the grain boundary region, nonuniform plastic deformations occur commonly which can cause non ignorable orientation gradients for a bulk material point in an infinite small neighborhood, and furthermore a certain number of additional dislocations have to be introduced to preserve the lattice continuity. Furthermore if studies are focused on the grain boundary zone, interactions between mobile dislocations and grain or phase boundaries have to be introduced into constitutive models to reflect the constraint relation between a grain or phase boundary material point with its neighborhood. Based on experimental findings, a grain boundary constitutive mechanism is proposed to consider interactions between two abutting crystals. In this mechanism an additional energy barrier coming from slip transmissions at grain boundaries is added to the general activation energy of dislocation slips in the bulk crystal to capture the thermal activated penetration event in the grain boundary zone. The approach is based on a conservation law for the Burgers vector loop around the interface affected. Furthermore a special grain boundary finite element is introduced in numerical simulations of three bicrystals with small, middle and large angle flat grain boundaries. The hardening effect of grain boundaries, strain distribution and texture evolution of bicrystals are discused carefully.

MM 35 Growth

Time: Thursday 14:45–16:30 Room: IFW B

MM 35.1 Thu 14:45 IFW B

Investigation of the initial transient in directional solidification of a binary AlCu alloy — •Anne Drevermann, Nils Warnken, Laszlo Sturz, and Gerhard Zimmermann — ACCESS e.V., Intzestr. 5, 52072 Aachen

For the formation of microstructures the initial transient, i.e. the very beginning of solidification, is of major relevance. At this stage a complex interaction between the velocity of the solidification front, the concentration pile-up and the temperature gradient takes place. In this work these three main variables and their coupling are investigated in experiments and numerical simulations.

Directional solidification experiments are carried out thermosolutally stable in a Bridgman-Stockbarger furnace with cylindrical Al-1.3wt.%Cu samples. During solidification the solidification velocity and the temperature profile are measured insitu while the concentration profile is determined afterwards in the processed sample by SEM/EDX analysis.

Numerical simulations were performed according to the Coriell model and with the phase field method. The Coriell simulations consider thermal diffusion in the liquid and the solid and solutal diffusion in the liquid while the phase field simulations consider only solute diffusion. The calculated transient solidification velocities and concentration profiles are in good agreement with the experimental results.

MM 35.2 Thu 15:00 IFW B

Crystal growth in undercooled Ti-Al-Nb melts — •Dirk Holland-Moritz and Thomas Volkmann — DLR, Institut für Raumsimulation, D-51147 Köln, Germany

Investigations on the solidification behaviour of undercooled Ti-Al-Nb melts are presented. The liquids are undercooled by application of the electromagnetic levitation technique. Maximum levels of undercooling of up to 320 K are achieved. Crystal growth during solidification of the undercooled melts is observed using a high-speed video camera at frame rates of 30000 frames per second. At small undercoolings an irregular shape of the solidification front is found. At larger levels of undercooling the growth front is smooth, but exhibits a pronounced anisotropy. From the recorded video sequences the growth velocities are determined as a function of the undercooling.

This work was financially supported by the IMPRESS Integrated Project (Contract NMP3-CT-2004-500656) that is co-funded by the European Commission in the 6th Framework Programme, the European Space Agency and the Swiss Government.

MM 35.3 Thu 15:15 IFW B

Molecular dynamics simulation of the nucleation and growth of platinum clusters — •Norbert Lümmen and Thomas Kraska — Physical Chemistry, University Cologne, Luxemburger Str. 116, D-50939 Köln, Germany

The formation of platinum clusters in an inert gas aggregation source is investigated by molecular dynamics simulation. At the beginning of the simulation the platinum atoms are in a highly supersaturated vapour state embedded in the carrier gas argon acting as a heat bath. The interactions of the metal atoms are modelled by the commonly used embedded atom method. Once the simulations are started the metastable phase remains for some time until clusters are formed by homogenous nucleation.

The nucleation rates are calculated from the cluster size statistics. Using a correlation of the nucleation rates as function of the supersaturation and the nucleation theorems the critical cluster size as well as the excess energy of the critical clusters are estimated. Also the continuation of the growth process by coalescence is traced in the simulations. In this context it is shown that coalescence can be the cause for a structural transition of a cluster. Even, or rather especially small clusters, which are often at high temperature, can be responsible for such transition.

Further results on the extension of the methodology on the investigation of nano alloy formation of will be reported. This will include the simulation of the formation process itself and the structural analysis of the resulting clusters.

MM 35.4 Thu 15:30 IFW B

Grain growth of two-dimensional grain structures with surfaces: a vertex dynamics approach — •Daniel Weygand — IZBS, Kaiserstr. 12, University of Karlsruhe, 76133 Karlsruhe

The time evolution of a two dimensional grain structure in presence of surfaces, e.g. a fibre geometry, is investigated. The influence of surface grooving and inhomogeneous heat treatments on the final microstructure is modelled using an enhanced vertex dynamics simulation. It is shown that, starting from a populations obtained by normal grain growth, the microstructure evolves toward a bamboo structure with interesting properties, e.g. depending on grooving parameter, grains with an non-uniaxial shape factor in the range of 1 to 7 occur. The grain size distribution is broader and larger grains are able to keep their size advantage due to the presence of the surfaces.

MM 35.5 Thu 15:45 IFW B

Dendritic Solidification of undercooled Ni-based alloy melts — •Sven Reutzel[1,2], Peter K. Galenko[2], and Dieter M. Herlach[2] — [1]Ruhr-University, Institute of Experimental Physics IV, 44780 Bochum — [2]German Aerospace Center (DLR), Institute of Space Simulation, 51170 Cologne

Morphology and size of dendritic microstructures sensitively depend on the solidification conditions, in particular on the crystallisation dynamics of the melt. Depending on the velocity with which a dendrite propagates into the undercooled melt a great spectrum of non-equilibrium phenomena can occur. For instance, if the velocity comes of comparable order with the atomic diffusive speed (1 - 10 m/s) solute trapping leads to the formation of supersaturated solutions and disorder trapping in intermetallic alloys produces disordered superlattice structures with completely different mechanical properties as the ordered counterparts. Also, as investigated in the present work grain refined alloys are solidified from the undercooled melt.

For a quantitative description of non-equilibrium solidification processes the growth velocity of the propagating dendrites in undercooled Ni and selected Ni-based alloy melts is experimentally determined as a function of undercooling on electromagnetically levitated drops. High accuracy measurements are realised even at small growth/undercooling values by applying a high speed camera technique, which allows for direct observation of morphology and dynamics of the solidification front. The analysis will be important to investigate and understand the development of various microstructures in as solidified materials.

MM 35.6 Thu 16:00 IFW B

Suppression of eutectic precipitation in rapid solidification of a binary system — •Peter Galenko and Dieter Herlach — Intitut für Raumsimulation, DLR, 51170 Köln, Germany

Experimental results on rapid solidification for binary systems in a range of eutectic concentration are analysed. Conditions at which eutectic precipitation is suppressed are found. A model for rapid crystal growth in a binary system of eutectic composition is developed. Analytical solutions of the model allow to predict beginning solidification of supersaturated solid solution without eutectic precipitation. It occurs at a solidification velocity equal to solute diffusion speed in bulk liquid. Within this point, a solute diffusion-limited growth is finishing with an onset of diffusionless solidification of the supersaturated solid solution. In such a case, complete solute trapping proceeds and eutectic solidification does not occur. The work was supported by DFG under contract No. He 1601/13.

MM 35.7 Thu 16:15 IFW B

Three dimensional normal grain growth: mean-field theory and Monte Carlo Potts model simulation — •Dana Zöllner and Peter Streitenberger — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Materialphysik, PF 4120, D-39016 Magdeburg

Normal grain growth in three dimensions has been studied on the basis of large-scale 3D Monte Carlo Potts model simulations, which enabled an extensive statistical analysis of the growth kinetics and topological properties of the microstructure within the quasi-stationary self-similar coarsening regime. It is shown that three dimensional normal grain growth can adequately be described by an average scaled growth law, which is a quadratic function of the relative grain size. A generalized analytic mean-field theory based on this growth law yields a scaled grain size distribution function that is in excellent agreement with the simulation results. The problem of the existence of a sharp cut-off in the simulated microstructure is discussed.

MM 36 Amorphous and Liquid Materials IV

Time: Thursday 16:30–18:00 Room: IFW B

MM 36.1 Thu 16:30 IFW B

Heterogeneous dynamics in MD simulated constant-shear-rate deformations of amorphous $Ni_{50}Zr_{50}$ — •Kevin Brinkmann and Helmar Teichler — Institut für Materialphysik d. Univ. Göttingen, 37077 Göttingen

Molecular-dynamics simulations of viscoplastic deformation of amorphous $Ni_{50}Zr_{50}$ show — in agreement with experiments — a characteristic stress-strain curve with an elastic linear regime for small strains, a pronounced stress overshoot and a drop to a constant flow stress, the latter indicating the transition into the steady-state flow regime. From analyzing changes in the local topological short range order, it is found that at $T = 700$ K strains below the upper yield point induce moderate, spatially homogenous atomic rearrangements only. Most of them are reversible, accounting for (an)elastic contributions. The marked decrease in stress between upper and lower yield point is due to a growing number of local rearrangement centers in the Zr-matrix. These rearrangements appear spatially heterogenous in the simulation cell, gradually filling a plane of maximum shear stress and forming a (micro-)shear-band. The interior of the shear-band exhibit significantly altered properties compared to topologically unchanged regions indicating a structural change in the shear-band resembling rejuvenation. At $T = 1000$ K ($T_g = 1050$ K), stress localization, is depressed leading to a highly unorganized formation of the structurally altered regions, rapidly covering the whole sample.

MM 36.2 Thu 16:45 IFW B

Rheology of selected metallic glasses — •Andreas A. Kündig[1], Thomas Schweizer[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Swiss Federal Institute of Technology (ETH) Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland — [2]Polymer Physics, ETH Zürich, CH-8093 Zürich, Switzerland

Metallic glasses exhibit a superplastic forming regime at temperatures above the glass transition temperature (T_g) and below the crystallization temperature (T_x). The formability in this range is limited by the onset of crystallization, which typically causes the characteristic properties of metallic glasses to deteriorate. In this work, the direct rheological parameters of selected low-temperature metallic glasses (Cu-, Mg-, and Au-based) were measured in parallel plate geometry. Using this technique, absolute values for the elastic modulus and the loss modulus as a function of the temperature are obtained, allowing us to compare formability in the different systems. Additionally, strain-rate sensitivity, dynamic viscosity and the onset of crystallization were measured to determine optimum forming parameters. The results are discussed with respect to more easily accessible estimates based on thermal values, such as the extension of the undercooled liquid regime $\Delta T(= T_x - T_g)$ or, normalized to the liquidus temperature (T_l), the value $S = \Delta T/(T_l - T_g)$.

MM 36.3 Thu 17:00 IFW B

Microscopic processes during shear transformation of metallic glasses - a Molecular Dynamic study — •Mareike Zink, Konrad Samwer, and Stefan G. Mayr — 1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The atomic-scale processes which underlie shear transformation in the model glass, CuTi, were studied with classical Molecular Dynamic computer simulations. The formation of shear bands and dynamical heterogenities below the glass transition temperature could be investigated as well as the influence of boundary conditions. Microscopic results were compared with macroscopic behavior and elastic constants [1]. The shear rate dependence of the shear modulus for various temperatures relected time scales for alpha-relaxation and flow processes in the model glass.

Financially supported by the DFG - SFB 602.

[1] *W.L. Johnson and K. Samwer,*PRL 95, 195501 (2005)

MM 36.4 Thu 17:15 IFW B

Effect of mechanical deformation on the quasicrystallization of Zr-based metallic glasses — •Sergio Scudino[1], Hergen Breitzke[2], Klaus Lüders[2], Ludwig Schultz[3], and Jürgen Eckert[1] — [1]FB 11 Material- und Geowissenschaften, FG Physikalische Metallkunde, Technische Universität Darmstadt, Petersenstrasse 23, D-64287 Darmstadt, Germany — [2]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [3]IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany

The devitrification of melt-spun $Zr_{57}Ti_8Nb_{2.5}Cu_{13.9}Ni_{11.1}Al_{7.5}$ glassy ribbon is characterized by the formation of a metastable quasicrystalline phase during the first stage of the crystallization process. To investigate the effect of the mechanical deformation on the formation of quasicrystals, the glassy ribbon was submitted to ball milling. The mechanical treatment drastically affects both the thermal stability and the microstructure evolution upon heating. In particular, primary quasicrystal formation is progressively suppressed with increasing milling time. The results reveal that oxygen, which is introduced during milling, is responsible for the modified crystallization behavior by selectively reacting with zirconium. However, the suppression of quasicrystal formation can be reversed by an appropriate variation of the chemical composition. This indicates that quasicrystal formation from glassy precursors is governed by the chemical composition rather than by the occurrence of a special quenched-in short-range order. This work was supported by the German Science Foundation under grants Ec 111/10-1,2 and Lu 217/17-1.

MM 36.5 Thu 17:30 IFW B

Structure and electronic transport of a-$Cu_x(Mn_{50}Al_{50})_{100-x}$ — •Jan Rauchhaupt and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Amorphous phases are precursors of the cristalline state and hence interesting for investigating fundamental structure forming processes and the related evolvement of electronic transport.

In the last years we could show by many different classes of alloys (from e.g. metals, semiconductors, ionic glasses, to those containig transition metals) that the alloys organize themselves under the influence of a resonance interaction between two global systems, namely the electronic system of the valence electrons and the forming static structure. For TM-containing Al-alloys we discussed our results as a resonance interaction of the Al-p-electrons with the empty d-states of the TM via hybridisation. This model needs to be refined when a second transition metal comes in play.

The amorphous ternary alloys of Cu, Mn and Al were produced in situ at T=4 K in a HV-cryostate and were annealed up to the cristalline state. The static structure, by means of electron diffraction, the resistivity and the thermopower were measured as a function of temperature and composition.

MM 36.6 Thu 17:45 IFW B

Positron annihilation spectroscopy of glassy $Mg_{65}Cu_{25}Y_{10}$ ribbons — •Dirk I. Uhlenhaut[1], Alberto Castellero[1], Florian Dalla Torre[1], Carlos Palacio[2], Nikolay Djourelov[2], Danny Segers[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Swiss Federal Institute of Technology (ETH) Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland — [2]Department of Subatomic and radiation physics, Gent University, Proeftuinstraat 86, B-9000 Gent, Belgium

The well-known Mg-Cu-Y amorphous alloys become brittle during quenching or ageing. The ductile state is obtained at high quenching speeds, while a low copper content delays embrittlement during room-temperature ageing. Here we report on positron annihilation spectroscopy of amorphous ribbons from the $Mg_{65}Cu_{25}Y_{10}$ bulk glass-former, measuring positron lifetime, Doppler broadening and coincidence Doppler broadening as a function of the alloy's room temperature age. A decrease in positron lifetime and changes in the Doppler peak width, corresponding to a reduction of free volume, were seen during the time the embrittlement takes place at room temperature. Coincidence Doppler broadening spectroscopy revealed changes in the immediate environment of the free volume during annihilation. Analogies with calorimetric measurments and mechanical tests are discussed.

MM 37 Nanostructured Materials I

Time: Thursday 14:45–16:15 Room: IFW D

MM 37.1 Thu 14:45 IFW D

Early stages of Al/Cu thin-film reaction — •Constantin Buzau Ene[1], Guido Schmitz[2], Talaat Al-Kassab[1], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund Platz 1, D-37077, Göttingen, Germany — [2]Institut für Materialphysik, Westf. Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

Aluminium and Copper are important components of current day metallization of semi-conductor devices, so that their initial reaction is technologically important. Al/Cu/Al triple layers with approximately 10nm single layer thickness were deposited onto needle shaped W tips and analyzed in the early stages of interreaction by means of atom probe tomography (TAP). Owing to the outstanding sensitivity of the method, even minor chemical modifications on the nanometer scale can be detected. After thermal treatments we were able to recognize the formation of the Al_2Cu phase starting after 5 min annealing at 110°C and its parabolic growth as a dense layer to a maximum thickness of 6 nm after 80 min annealing at 110°C. As a particularity of the tip-shaped tungsten tips we observed a remarkable asymmetry in the growth rate of the new phases. The thickness of the reaction product close to the W substrate is approximately 1.5 times thicker than the other one close to the surface. We suggest that this asymmetry is induced by different vacancy annihilation mechanisms at the two Al/Cu interfaces.

MM 37.2 Thu 15:00 IFW D

Pressure temperature phase diagrams of pure and Ag-doped nanocrystalline TiO2 photocatalysts — •Manuela Stir — Institut für theoretische und angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569, Stuttgart

M.Stir1, R.Nicula2, H.-E.Schaefer1 1Universitaet Stuttgart, Institut für theoretische und angewandte Physik, Pfaffenwaldring 57, D-70569 Stuttgart, Germany 2Universitaet Rostock, Institute für Physik August-Bebel-Str. 55, D-18055 Rostock, Germany

An essential issue in the development and use of nano materials in modern applications is the ability to maintain ultrafine particle sizes within extended temperature pressure ranges. Nanocrystalline titanium dioxide (nc-TiO2) is known as an excellent semiconductor photocatalyst for environmental protection applications such as the decontamination of polluted waste water and air purification. The photocatalytic efficiency of nc-TiO2 depends on its crystal structure and surface morphology and may further be enhanced by adequate metal-doping and by achieving mesoporous surfaces. The use of semiconductor photocatalysts in supported form (pellets or thin-films) eliminates the need for air-bubbling of the contaminated liquid media (to counteract powder sedimentation) and for subsequent complex photocatalyst powder recycling procedures.

MM 37.3 Thu 15:15 IFW D

The role of dislocations during deformation of nanocrystalline metals — •Jürgen Markmann[1,2] and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, Postfach 3640, 76021 Karlsruhe — [2]Universität des Saarlandes, FR 7.3 Technische Physik, Postfach 151150, 66041 Saarbrücken

During deformation of nanocrystalline metals various deformation mechanisms can be activated. Depending on the applied strain rate and size of the grains grain boundary diffusion, i.e. Coble creep, grain boundary sliding, and even grain rotation contribute to the material transport. Despite the fact that standard dislocation sources of the Frank-Read type in the interior of nano grains cannot be activated before the material fails, it has been shown that dislocations are active in nanocrystalline metals. Here the microstructure of nanocrystalline palladium after a true strain of $\epsilon \approx 0.3$ to 0.7 deformed by cold rolling at strain rates $\dot{\epsilon}$ between $0.08\,s^{-1}$ and $0.3\,s^{-1}$ was investigated. With increasing strain rate the stacking fault density decreases while the number of twins notedly increases as shown by HRTEM images. The number of discovered lattice faults especially after deformation at higher strain rates implies dislocation motion as the main and dominant mechanism of deformation. This means that the number of dislocations is a function of the applied strain rate or stress rather than a function of the strain or total deformation of the material. Furthermore the possibilities of nucleation of dislocations from grain boundaries as proposed by theory and the nucleation of a complete dislocation loop inside the grain are shortly discussed.

MM 37.4 Thu 15:30 IFW D

Thermal Stability of a Nanocrystalline Cobalt-Phosphorous Alloy — •Catharina Wille[1], Taláat Al-Kassab[1], Reiner Kirchheim[1], Melina da Silva[2], and Uta Klement[2] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen — [2]Chalmers University of Technology, Department of Materials and Manufacturing Technology, SE-41296 Göteborg, Sweden

Nano-crystalline Co-2.3at%P layers with a thickness of 200 μm and an average grain size of 12 nm were prepared by means of the pulsed current electro-deposition. These specimens were investigated both in the as prepared state and after different heat treatments by utilizing different analysis techniques such as Field Ion Microscopy (FIM), Tomographic Atom Probe (TAP), Transmission Electron Microscopy (TEM), Differential Scanning Calorimetry (DSC), X-Ray Diffraction (XRD).

The results reveal a high P-segregation at the grain boundaries already in the as prepared state. Between 723 and 753K, the allotropic phase transformation (hcp-Co to fcc-Co) sets in and abnormal grain growth is observed. The onset of abnormal grain growth at 673K is accompanied by the precipitation of the CoP-phase, whereas the formation of the equilibrium Co_2P-phase is not detected. For most of the neighboring grain boundaries, the level of P was depleted insofar as no significant excess segregation was detected.

Between 723 and 743K normal grain growth occurs. Thus the thermal stability of this alloy can be mainly attributed to the reduction of grain-boundary energy by P-segregation.

MM 37.5 Thu 15:45 IFW D

Self deformation during dealloying of silver-gold alloys — •Smrutiranjan Parida[1], Dominik Kramer[1], and Joerg Weissmueller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologi, Karlsruhe — [2]Universität des Saarlandes, Fachrichtung Technische Physik, Saarbrücken

Dealloying or selective dissolution is an important route to prepare nanoporous metals and alloys. We present a study of the dealloying process in silver-gold alloys, which uses SEM, TEM and XRD investigations of the obtained porous metals and measurements of the lateral shrinkage of the sample during dealloying by insitu dilatometry. This shrinkage, which depends on the dissolution rate (hence on dealloying potential) and the composition of the alloy, has not been reported before. The volume of the sample reduces by up to 30% during dealloying, although our measurements show that the original crystal lattice of the alloy is conserved. This result can not be explained with the existing model or with elastic lattice strain or with lattice parameter differences. Therefore, we suggest plastic deformation to explain the observation, which is consistent with the high defect concentration in dealloyed structure as observed by TEM. Several possible mechanisms to nucleate the defects during dealloying are discussed.

MM 37.6 Thu 16:00 IFW D

Characterization of the Microstructure and Texture of Nanostructured Electrodeposited CoNi by use of Electron Backscatter Diffraction (EBSD) — •Alice Bastos, Stefan Zaefferer, and Dierk Raabe — Max-Planck-Institut für eisenforschung, Max-Planck-Strasse 1, D-40237 Duesseldorf

A Co-20at%Ni polycrystal produced by electrodeposition has been investigated in planar and cross sections using orientation microscopy in a high resolution scanning electron microscope and focused ion beam microscope. The local crystallographic texture, grain size, amount of phases, and grain boundary character were characterized by electron backscatter diffraction (EBSD). This technique appears to be ideal for accomplishing a detailed microstructure characterization, particularly regarding the crystallographic character of the boundaries, which plays a special role in such nanostructured materials. Exploring the limits of the spatial resolution of the EBSD we present a detailed study of the microstructure and facilitate in this way the understanding its complexity. Additionally a combination of EBSD technique with a serial section method using a focused ion beam microscope (3D-EBSD) was applied in order to study the boundary character throughout the thickness of

the electrodeposited sample. The crystallographic relationship between neighboring grains was investigated to gain access to the understanding of the microstructure evolution and local texture development in connection with the deposit growth.

MM 38 Nanostructured Materials II

Time: Thursday 16:30–18:00 Room: IFW D

MM 38.1 Thu 16:30 IFW D

Charge induced reversible magnetization in nanocrystalline transition metal alloys — •Sadhan Ghosh[1], Christian Lemier[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Technische Physik, Universität des Saarlandes, Saarbrücken

Ferromagnetism is fundamentally related to the electronic density of states. Therefore, it is interesting to study how far one can modify the magnetic order of solids by changing their electron density. While this is usually done by alloying, one can also change the charge density by inducing space-charge regions at the metal surfaces. This is particularly interesting in nanostructured materials, since the high surface to volume ratio maximizes the effect of the local property changes on the macroscopic scale [1]. Here we intend to explore possibility of changing the magnetic properties of transition metal alloys by using the concept of Helmholtz double layer space charging at the metal-electrolyte interface. Since charging also leads to volumetric strain in the nanoporous materials [2] the effect of resulting pressure on magnetism [3] has also been considered.

[1] Gleiter H., Weissmüller J., Wollersheim O., Würschum R. Acta mater. 49 (2001), 737. [2] Weissmüller, J., Viswanath, R.N., Kramer, D., Zimmer, P., Würschum, R., Gleiter, H. Science 300 (2003), 312. [3] Lemier C., Ghosh S., Weissmüller J., Viswanath R. N., MRS Symp. Proc. 876E R2.6 (2005)

MM 38.2 Thu 16:45 IFW D

Size Effect on the Néel Temperature of NiO nanoparticles — •X. M. Li, Z. Q. Guan, H. Wolf, and Th. Wichert — Technische Physik, Universität des Saarlandes, D-66041 Saarbrücken

Nanocrystalline NiO with different particle sizes has been prepared by electrochemical deposition followed by thermal treatment. The particle sizes ranged from 7 nm to 26 nm as determined by XRD and TEM. Using the method of perturbed $\gamma\gamma$-angular correlation (PAC), the antiferromagnetic order of nanocrystalline NiO as a function of temperature was studied for different particle sizes. The results show that the Néel temperature decreases with decreasing particle size. For the Néel temperature T_N as a function of the particle size d a relation of (T_N(bulk)-T_N(nano)) $\sim d^{-\lambda}$ has been obtained yielding for the exponent $\lambda = 3.45(1)$. A similar relation was obtained in nano-crystalline Gd for the Curie temperature as a function of the particle size by D. Michel [1]. The exponent $\lambda = 1.07$, however, is significantly smaller than that in the present case of nanocrystalline NiO.

supported by the Deutsch Forschungsgemeinschaft (SFB277).

[1] D. Michel, Thesis, Universität des Saarlandes, Saarbrücken, Germany(2005).

MM 38.3 Thu 17:00 IFW D

Nanoporous Metals Obtained by Dealloying and their Charge-dependent Strain — •Dominik Kramer[1], Smrutiranjan Parida[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Universität des Saarlandes, Fachrichtung Technische Physik, Saarbrücken

It has been suggested recently [1] to use nanostructured metals obtained by dealloying for actuator applications: Dealloying by the selective dissolution of the less noble component(s) of an alloy, is an important and convenient route to prepare nanoporous metal and alloy samples of arbitrary size and shape, and it ensures that all the pores are filled with electrolyte solution. Due to the dependence of the surface stress on the surface charge, it is possible to use nanostructured metals in an electrolyte as actuator materials, by using a counter electrode in the same electrolyte [1].

We present a study of the dealloying of silver-gold-platinum and palladium alloys, and a dilatometer investigation of the reversible strain of the resulting structures in various electrolytes. The strain measured is discussed as a function of potential, and of the structure size and composition of the different samples.

[1] D. Kramer, R. N. Viswanath, J. Weissmüller, Nano Lett. 4 (2004) 793

MM 38.4 Thu 17:15 IFW D

Ductile ultrafine eutectic in Ti-Fe-base alloys — •J. Das[1,2], K. B. Kim[1], F. Ettinghausen[1], W. Xu[1], W. Löser[2], and J. Eckert[1] — [1]FG Physikalische Metallkunde, FB 11 Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany

A Ti67.79Fe28.36Sn3.85 ternary alloy has been prepared through arc-melting and solidification at a cooling rate of 40-10 K/s. The as-prepared microstructure of the button-shape ingot exhibits a two phase ultrafine eutectic consisting of FeTi (Pm3m, B2) and beta-Ti (Im3m, A2) phases. The mechanical properties (maximum strength = 1939 MPa, strain to fracture = 13.5%) are considerably improved compared to the Ti70.5Fe29.5 binary eutectic alloy (maximum strength = 1733 MPa, strain to fracture = 3.4%). The improvement of the strength and plastic deformability is assessed in terms of a detailed investigation of the microstructure and fractographic studies. The presence of Sn is believed to boost the ease of slip transfer across the interface between the A2/B2 phases due a higher lattice mismatch between the structures. This work was funded by European Union within the framework of the Research Training Network on "ductile bulk metallic glass composites" (MRTN-CT-2003-504692) and by Alexander-von-Humboldt Foundation.

MM 38.5 Thu 17:30 IFW D

The influence of interfaces on the properties of nanostructured materials considering the different melting behaviour of Al-Pb composites — •Harald Rösner, Jörg Weissmüller, and Gerhard Wilde — Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, Institut für Nanotechnologie

Al-Pb composites composed of nanometre-sized Pb particles embedded in a polycrystalline Al matrix serve as a model system for size-dependent melting studies. Depending on the processing pathway, i.e. ball-milling or melt-spinning, the Pb nanoparticles either display a faceted morphology or are spheroidical with curved interfaces. The faceted and spheroidical particles were observed to melt at temperatures above and below the melting temperature of bulk Pb, respectively. However, the observed difference in melting behaviour cannot be explained purely by the different morphologies exhibited by the particles. Recent high-resolution TEM investigations showed that two types of misfit dislocations are present at the interfaces in both types of particles. Based on these results we present a new model that accounts for the different melting behaviour by considering the different mobility of atoms at curved and faceted Al-Pb interfaces.

MM 38.6 Thu 17:45 IFW D

Diffusion of oxygen in nanocrystalline $ZrO_2{\cdot}Y_2O_3$ — •Harald Drings, Anthony Madubuonu, Gregor Knöner, and Hans-Eckhardt Schaefer — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart, Germany

Zirconia-based materials are known to have oxygen transport properties which give rise to many applications, such as gas sensors or solid electrolytes for fuel cells. It has been recently shown that the oxygen diffusivity in the grain boundaries of nanocrystalline $ZrO_2{\cdot}Y_2O_3$ is strongly enhanced [1] compared to the volume diffusion. Due to the large amount of interfaces in nanocrystalline materials, this should significantly enhance the oxygen diffusion current. This could lower the operating temperature e.g. of solid oxide fuel cells (SOFC) and reduce material deterioration. The samples were prepared by gas phase synthesis of metallic nanoparticles that were oxidized, compacted and sintered to a fully dense oxide specimen. Here, we report on reducing the grain size in n-$ZrO_2{\cdot}Y_2O_3$ by Al doping in order to increase the diffusion current.

[1] G. Knöner et. al. , PNAS **100**, 3870 (2003)

MM 39 Invited Talk Molodov

Time: Friday 10:15–10:45 Room: IFW A

Invited Talk MM 39.1 Fri 10:15 IFW A

Effect of High Magnetic Field on Crystallographic Texture and Grain Microstructure Evolution in Non-Ferromagnetic Metals — •Dmitri A. Molodov — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University

The current research on grain boundary dynamics, texture and grain structure development in high magnetic fields will be reviewed. Grain boundary motion can be affected by a magnetic field, if the anisotropy of the magnetic susceptibility generates a gradient of the magnetic free energy density across the boundary. If a magnetic energy density gradient as a driving force is superimposed to a curvature driving force during grain growth, this biases the microstructure evolution with regard to grain size and crystallographic texture, as it is demonstrated on polycrystalline zinc and titanium. Analysis of individual orientation data reveals that the observed asymmetrical texture is to a large extent due to a difference in grain numbers of the individual texture components. A theoretical analysis of the grain growth kinetics in the presence of an external magnetic field reveals that magnetically affected grain growth may result in a skew distribution of grains in favour of those with a lower magnetic free energy density. The results of computer simulations of magnetically affected grain growth in 2-D polycrystals are in a good agreement with experimental findings and confirm theoretical predictions concerning the effect of magnetic field on grain topology during grain growth.

MM 40 Nanostructured Materials III

Time: Friday 11:00–12:00 Room: IFW D

MM 40.1 Fri 11:00 IFW D

Compaction of Amorphous and Partially Crystallised Al-Ni-La Alloys — •Jens Vierke, Markus Wollgarten, and John Banhart — Hahn-Meitner-Institute, Materials Dep., Glienicker Str. 100, D-14109 Berlin, Germany

Morphology, microstructure and crystallisation behaviour of Argon (Ar) and Helium (He) atomised $Al_{87}Ni_8La_5$ and $Al_{85}Ni_{10}La_5$ alloy powders were studied by scanning and transmission electron microscopy, X-ray diffraction (XRD) and differential scanning calorimetry. XRD measurements of He-atomised $Al_{85}Ni_{10}La_5$ powders show a complete X-ray-amorphous structure. Ar-atomised powders of the same alloy exhibit fcc-Aluminium crystals in an amorphous matrix. In the case of $Al_{87}Ni_8La_5$, the microstructure consists of an amorphous phase, fcc-Aluminium as well as intermetallic phases. DSC measurements reveal that the amorphous phase of all alloys is stable up to a temperature of about 170°C, applying a heating rate of 20 K/min. The powders were compacted by uniaxial pressing, direct extrusion and equal channel angular pressing. Different compaction temperatures were applied with regard to the conservation of the amorphous phase. First results of the study will be presented. The support of the Institute of Materials and Machine Mechanics of the Slovak Academy of Sciences is gratefully acknowledged.

MM 40.2 Fri 11:15 IFW D

Aerosol synthesis of magnetic iron oxide nanoparticles — •Markus Ames, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, FR 7.3 Technische Physik, Postfach 151150, 66041 Saarbrücken

The metal-organic compound $[Fe(O^tBu)_3]_2$ is used as precursor in CVD processes to deposit thin films of iron oxide on a substrate. Depending on substrate temperature, three different modifications were observed: Haematite ($\alpha - Fe_2O_3$), Maghemite ($\gamma - Fe_2O_3$) and Magnetite (Fe_3O_4). The purpose of the present study was to evaluate this particular precursor for aerosol synthesis of nanocrystalline iron oxide particles. The reaction temperature in a hot-wall reactor was varied between 300°C and 800°C. The produced materials were characterized by X-ray diffraction, magnetization measurements and transmission electron microscopy. At temperatures below 400°C the yield of material was too low to allow further examination. The X-ray diffraction analysis revealed that Haematite was not produced and only Maghemite or Magnetite was found at all temperatures. The latter phases could not be distinguished by XRD due to their similar diffraction patterns. From magnetization measurements a saturation magnetization between 40 and 50 emu/g was obtained.

MM 40.3 Fri 11:30 IFW D

Elastic Properties of nanocrystalline palladium — •Markus Thirion and Rainer Birringer — Universität des Saarlandes, FR 7.3 Technische Physik, Postfach 151150, 66041 Saarbrücken

We investigate the elastic properties of nanocrystalline palladium by means of velocity of sound measurements. The samples are prepared by inert-gas condensation and compaction and have grain sizes ranging from 10 to 25 nm. Due to an unavoidable residual porosity, the specimen densities lie in the range between 90 and 95% of the bulk density of coarse-grained palladium. From the velocities of longitudinal and transversal polarized ultrasonic waves, the elastic moduli (Young's, shear and bulk) can be determined. In the low porosity regime (<10%), we find a linear dependence of moduli versus porosity, allowing to extrapolate the moduli of the pore-free material state. The extrapolation reveals slightly enhanced effective moduli of the nanocrystalline palladium (pore-free), as compared to the coarse-grained reference material. This enhancement will be discussed in terms of a rule of mixture approach for a two-phase system made up of crystalline grains and grain boundaries.

MM 40.4 Fri 11:45 IFW D

Structure and conductance in metal nanosystems — •Tammo Block[1], Jan Rönspies[1], Svend Vagt[1], Volkmar Zielasek[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Universität Hannover — [2]Institut für Angewandte und Physikalische Chemie, Universität Bremen

Recently the Pb/Si(557) system has been demonstrated to exhibit a high quasi one-dimensional conductance along the Si(557) step direction on a macroscopic scale, associated with a metal-semiconductor phase transition [1]. Here we describe how to bring this system one step further, by using a lithographical method to perform measurements on only a few of these wires selected out of the 'wire array' of the Pb/Si(557) system. We employ electron-beam stimulated thermal desorption of oxygen (EBSTD) in UHV from ultrathin SiO_2 layers on a Si(557) surface to generate windows of clean Si in a SiO_2 mask, usually in the form of narrow (≤20nm) lines along the 557-step direction. Subsequent deposition of Pb and annealing to 640 K forms the 1D conducting system descibed above. TiSi contacts, produced previously ex-situ with conventional e-beam lithography, and the tip of a STM are used to connect these wires for conductivity measurements.The influence of various kinds of defects on electrical transport in the structures will be discussed.

[1] PRL 95 (2005) 176804

MM 41 Nanostructured Materials IV

Time: Friday 12:30–13:15 Room: IFW D

MM 41.1 Fri 12:30 IFW D

Electronic structure and properties of single-walled carbon nanotubes interacting with DNA bases — •Yong Kong and Huajian Gao — Max-Planck Institute for Metals Research, Heisenbergstr. 3, 70569 Stuttgart, Germany

Functionalization of carbon nanotubes (CNTs) has been extensively studied due to its potential in facilitating miniature electronic and optic devices for broad applications. Recently, Zheng et al. (Nature materials 2 (2003) 338; Science 302 (2003) 1545.) reported DNA-assisted dispersion and separation of CNTs. They found that bundled single-walled CNTs were effectively dispersed in water by their sonication in the presence of ssDNA and suggested ssDNA could bind to CNTs through π-stacking, resulting in helical wrap-ping to the surface. Very recently, CNT-based bio-nano-complex has been used to electrically detect protein and DNA (e.g. J. Am. Chem. Soc. 126 (2004) 3010.).

In order to advance the understanding of CNT-based bio-nano-system and further to predict/optimize the properties and performance of bio-CNT-complex based miniature devices, we conduct DFT-based ab initio calculations to investigate the interaction of DNA bases (A, T, C and G) with perfect and defective single-walled CNTs. DNA base-specific effects on electronic structure and electrical transport properties of single-walled CNTs with vacancy and stone-wales defects and with different chiralities are discussed on the basis of electronic structure and transport calculations. Our results suggests that the CNT-DNA base complex could be further exploited for applications such as DNA modulated molecular elec-tronics, molecular sensors and electronic DNA sequencing.

MM 41.2 Fri 12:45 IFW D

Analysis of phase contrast X-ray tomograms of nutshells: relating structure to properties — •Boris Breidenbach[1], Adrian Sheppard[2], Ulrike Wegst[3], and Klaus Mecke[1] — [1]Institut für theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — [2]Applied Mathematics, Australian National University, Canberra, Australia — [3]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Physical quantities of a porous materials, like elasticity and conductivity, depend on its chemical as well as structural properties. To examine the influence of structural properties only, chemically identical materials can be studied. Some biological materials, like wood and nutshells, mainly consist of cellulose, but the size and shape of fibers and pores is very different, as was found using various imaging techniques. Here we present the results of a study of nutshell properties using phase contrast X-ray tomography.

We determined the structure of six types of nutshells at a resolution of 0.3 μm to resolve the microscopic pore space. Parallel implementations of anisotropic diffusion and a region growing algorithm have been used to segment the data (typical size of 2000^3 voxels). Subsequently, we calculated the porosity and two-point correlation functions of the structures. In order to compare them to numerically and experimentally measured elasticity tensors, we also determined the complete set of Minkowski tensors which are motion covariant and allow for a characterization of anisotropic pore spaces.

MM 41.3 Fri 13:00 IFW D

CORRAX - A TI-FREE STAINLESS MARAGING STEEL INVESTIGATED BY 3 DIMENSIONAL ATOM PROBE — •Stefan Höring[1], Nelia Wanderka[1], Wolfgang Neumann[2], John Banhart[1], Harald Leitner[3], and Helmut Clemens[3] — [1]Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [3]Institut für Metallkunde und Werkstoffprüfung, Montanuniversität Leoben, Franz-Josef-Strasse 18, A - 8700 Leoben

Maraging steels are widely used for aerospace parts as well for tools and dies because of their good mechanical properties. Stainless maraging steels can be used as dies in the glass industry because of its good surface properties. The high strength of these steels is achieved by a precipitation hardening process. Typically these precipitates are in nanometer scale. An alloy with the technical name Corrax with the chemical composition 73.46 Fe-12.76 Cr-8.52 Ni-3.39 Al-0.79 Mo-0.58 Si-0.39 Mn-0.11 C (in at. %) was solution heat treated at 850 °C for 1/2 h and subsequently aged at 525 °C for 3 h, 10 h and 100 h. The microstructural evolution after annealing was studied by high resolution methods such as three dimensional atom probe (3DAP) and high resolution transmission electron microscopy (HRTEM). After 3 h annealing time small precipitates of nearly spherical morphology and of about 3-4 nm in diameter were formed. They are enriched in Ni and Al with an atomic ratio close to 1. While further heat treatment these precipitates grow to plates along one fixed direction.

MM 42 Diffusion II

Time: Friday 11:00–12:00 Room: IFW B

MM 42.1 Fri 11:00 IFW B

Diffusion-induced recrystallization in Au/Cu thin films — •Britta Kruse, Dietmar Baither, and Guido Schmitz — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str.10, 48149 Münster

Diffusion-induced recrystallization (DIR) was investigated in the Au-Cu system. Double layers of Cu and various AuCu alloys were deposited in (111) thin film texture on glass substrates. The as-prepared composition of the alloys varied from pure Au to 87at.% Cu in six steps, in order to control the lattice mismatch between the two diffusing materials. Heat treatments were performed at 435°C, which is well above the highest ordering temperature, so that the formation of intermetallic compounds is excluded. Nevertheless, XRD demonstrates intermediate intensity maxima after the heat treatments. Comparison with simulated XRD spectra and TEM demonstrate that these are related to newly formed grains of distinct compositions inside the diffusion zone. The sequence of the intermediate grain compositions depends characteristically on the initial mismatch. This behaviour may be understood by taking into account elastic stress and its relaxation.

MM 42.2 Fri 11:15 IFW B

Towards the influence of bulk solubility on grain boundary segregation: a case study of Fe and Ni diffusion in Cu — •Jens Ribbe, Sergiy Divinski, Guido Schmitz, and Christian Herzig — Institut für Materialphysik, Universität Münster

^{59}Fe and ^{63}Ni grain boundary (GB) diffusion in high-purity Cu was measured by the radiotracer method combined with mechanical sectioning in an extended temperature interval. At higher temperatures the conditions of Harrison's B kinetics were satisfied and the triple product $P = s \cdot \delta \cdot D_{gb}$ of the segregation factor s, GB width δ, and the GB diffusivity D_{gb} was determined at selected temperatures. Performing GB diffusion measurements at lower temperatures under C regime condition, the GB diffusion coefficient D_{gb} was directly measured. Using the estimate of the GB width deduced from GB self-diffusion measurements on FCC metals, $\delta \approx 5 \cdot 10^{-10} m$, the segregation factor s of Fe and Ni was determined as $s = P/\delta D_{gb}$. Fe reveals strong segregation and very slow diffusivity D_{gb} in Cu high-angle GBs. The measured triple product P^{Fe} for Fe GB diffusion is by orders of magnitude larger than the GB diffusivity P^{Ni} of Ni and many other elements. Small bulk solubility and strong segregation resulted in unusual penetration profiles of GB diffusion of Fe in the B kinetics. The nature of this phenomenon is discussed.

MM 42.3 Fri 11:30 IFW B

Study of Electrochemical Dissolution of Ternary Ag-Au-Dy Alloy — •VISWANATH RAGHAVAN NADAR[1], HARALD RÖSNER[1], DOMINIK KRAMER[1], and JÖRG WEISSMÜLLER[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany

We report results for the microstructure evolution during the dealloying of Ag-Au-Dy ternary alloys. The nature of the transport path during the formation of the nanoporous structure in dealloyed Ag-Au is the sub-

ject of current research, and in particular the role of bulk diffusion is debated. By exploring the dealloying of a supersaturated solid solution we aim at verifying the suggestion of an enhanced bulk diffusion coefficient due to excess vacancy injection at the dissolution front: the conceivable formation of solvent-rich precipitates in the alloy ahead of the dissolution front would support an enhanced diffusivity. In fact, the results for Ag-Au-Dy supersaturated in the rare earth Dy are not incompatible with this expectation. The suction-cast specimens were selectively dealloyed in 1M $HClO_4$ solution at different durations and investigated at each stages ex-situ using TEM, XRD and AC magnetometer. The material is two phase in its initial state, with a Ag-rich ternary solid solution as the majority phase and a Au- and Dy-rich ternary intermetallic as the minority phase. During dealloying a repartitioning of Dy between the solid solution and the ternary compound is found, a process which may suggest accelerated bulk transport, since Dy would oxidize immediately when brought in contact with the electrolyte.

MM 42.4 Fri 11:45 IFW B

Element Specific Defect Investigation on Mg-Alloys with Coincident Doppler Broadening Spectroscopy — •Martin Stadlbauer[1], Christoph Hugenschmidt[2], Klaus Schreckenbach[2], and Peter Böni[1] — [1]Physikdepartment E21, James-Franck-Straße, 85748 Garching — [2]ZWE FRM-II, Lichtenbergstraße 1, 85748 Garching

A new coincident Doppler broadening spectrometer (CDBS) at the high intense positron source NEPOMUC [1] in Garching was set into operation. The Doppler broadening of the 511 keV annihilation line reveals not only information about the defect concentration of the sample but also the chemical surrounding at the annihilation site. Since positrons are efficiently trapped at open volume defects, it becomes feasible to identify the elements in the vicinity of these defects. For this purpose, two collinear Germanium detectors are used in coincidence in order to reduce the background efficiently. Annealed samples of Magnesium, Aluminum, Zinc and AZ31 were investigated with CDBS in order to compare the shape of the annihilation line in the high momentum region and to get reference spectra. Furthermore, ion irradiated samples of AZ31 were measured to reproduce the defect profile by quantifying the S-parameter versus sample potential between 1 and 30 keV and position. Additionally coincidence spectra were recorded in order to detect any changes in the chemical surrounding of the defects.

[1] Hugenschmidt, C., G. Kögel, R. Repper, K. Schreckenbach, P. Sperr, B. Strasser und W. Triftshäuser: NEPOMUC - The New Positron Facility at FRM II, Mat. Sci. Forum, in press, 2004

MM 43 Diffusion III

Time: Friday 12:30–13:30 Room: IFW B

MM 43.1 Fri 12:30 IFW B

Imaging of defect structure in fatigued carbon steel C45E — •Patrick Eich, Matz Haaks, and Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16,D-53115 Bonn, Germany

Nowadays all used construction parts have a finite lifetime under alternate conditions. Hence, a precise damage prediction would be very useful. The observation of the microscopic process of fatigue in a metal is a condition for a reliable damage prediction. Physically, the reason for fatigue is the accumulation of lattice defects, like dislocations, vacancies and vacancy clusters. The increase of the defect concentration due to alternate load fatigue can be observed by positron annihilation spectroscopy. The deformation state at higher load cycle numbers can be estimated from the defect concentration in the early stages of fatigue. [1] Even if a homogeneous stress field is applied, heterogeneous structures in the defect concentration are formed during fatigue. These structures can be imaged using the fine focus positron beam of the Bonn Positron Microprobe. Samples of the carbon steel C45E were tested with alternate load fatigue. At different stages the defect density was examined with a spatial resolution in the micrometer range. [1] M. Haaks, K. Maier in V. Jentsch et al. *extreme events*, Springer 2005, in press

MM 43.2 Fri 12:45 IFW B

The effect of low stresses on creep and surface profiles of thin copper wires — •Vivek Srivastava[1], Howard Jones[2], and Geoffery Greenwood[2] — [1]Otto-von-Guericke-University Magdeburg, Institute of Materials Engineering & Testing, PO Box 4120, D-39016 Magdeburg, Germany — [2]Department of Engineering Materials, University of Sheffield, Mappin Street, Sheffield S1 3JD, UK

At low stresses and high temperatures, materials creep by stress directed diffusion of vacancies, i.e. diffusional creep. The creep rates and surface profile changes of wires, of diameters from 25*500 microns of high purity (99.995%) copper, have been investigated close to their melting temperature under stresses up to 0.4 MPa. Strain rate always varied linearly with stress. For the thinnest wires the rate was about twice the rate expected from Nabarro*Herring creep and more than one order of magnitude larger than expected from Harper*Dorn creep. For 500 microns wires, the measured rate was initially close to Harper*Dorn prediction but became constant only after longer durations at a level five times lower than this. The wire profiles near the closely perpendicular boundaries showed a smooth diameter increase or decrease depending on whether the stress was sufficient or insufficient to overcome the effect of the surface tension forces tending to shrink the wire. These profile changes indicated the location of vacancy sources and sinks and the measured steady state creep rates could be accounted for by the direction and magnitude of the vacancy fluxes.

MM 43.3 Fri 13:00 IFW B

Radiation damage in fused quartz — •Poornnima Anbalagan[1], Christine Negrini[1], Andre Engelbertz[1], Bernd Habenstein[2], and Karl Maier[1] — [1]Helmholtz - Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn — [2]General Electric, Köln

Radiation damage has always been a topic of great interest in various fields of sciences. We have made an attempt to probe into the effect of subthreshold ultrasonic waves on the radiation damage created by irradiation of protons and alpha particles in the model system fused quartz. Three independent techniques were used to visualize the radiation damage. The polarization microscope shows the so-called Bragg-Peak, which is the region of maximum damage indicating internal stress in the sample. Positron annihilation spectroscopy was used to analyze the suppressed positronium generation due to the reduced positron diffusion as a result of radiation damage. UV-absorption spectroscopy shows a dominant absorption peak at an optical wavelength of 210nm. This corresponds to the E'-Centers and is an observable electronic defect. Surprisingly, the Bragg-Peak (which is identical with the particle range) is observable with the polarization microscope but not in the case of UV-absorption spectroscopy. A comparison between the samples that were irradiated and the samples that were exposed to ultrasonic waves simultaneously with irradiation shows the influence of the standing ultrasonic wave.

MM 43.4 Fri 13:15 IFW B

Surface nano-structural modifications in Mo by nitrogen ion implantation as a function of temperature — •Hadi Savaloni[1,2], Mariam Motmaen Dadgar[2], Mahmood Ghorannevis[2], and Mohamad-Reza Hantehzadeh[2] — [1]Dept. Of Physics, University of Tehran, North-Kargar Street, Tehran, Iran — [2]Plasma Physics Research Center, Science and Research Campus of I. A. University, P. O. Box 14665-678, Tehran, Iran.

The structural characteristics of nitrogen ion implanted MO massive samples (0.5 mm foils) are studied by SEM, XRD, AFM, and SIMS. 20 KeV nitrogen ions with a dose of $1 \times 10^{18} N^{+} cm^{-2}$ were implanted in Mo samples at different temperatures. XRD patterns clearly showed MoN(031) line very close to Mo(200). AFM images showed the formation of grains on Mo samples, which grew in size with temperature. The surface roughness variation with temperature, decreased to a minimum, and further increase in temperature increased the surface roughness. SIMS analysis of the density of implanted N+ ions, and the depth of N+ ion implantation in Mo, showed a minimum for both the N+ density and depth of N+ ions, at a certain temperature consistent with XRD results (i.e., IMo(200) /IMo(211) and IMoN(031) /IMo(200)). These observed

minimums in XRD and SIMS results are again similar to those obtained for N+ ion implanted W (Savaloni et al., 2005) and for XRD results in different thin films(Physica B, 349(2004)44; Vacuum, 77(2005)245).

MM 44 Mechanical Properties II

Time: Friday 11:00–12:00 Room: IFW A

MM 44.1 Fri 11:00 IFW A

Bolometric detection of strain solitons in Sapphire, Si and GaAs — •Anthony Kent and Nicola Stanton — School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK.

We show that superconducting bolometers possess sufficient temporal resolution to detect strain soliton pulses propagating over mm distances in c-axis Sapphire and [001] Si and GaAs crystals. Using imaging techniques we show that the soliton pulses propagate as a narrow collimated beam. Strain pulses of up to 1% amplitude were generated by absorption of 100 fs light pulses from a Ti:Sapphire regenerative amplifier in a Cr-film deposited on the crystal surface. As these travel in the crystal, the combined effects of nonlinearity and dispersion results in the formation of a train of strain solitons. We use superconducting Aluminium bolometers to detect the pulses reaching the back surface of the crystal (opposite the Cr film). When the fluence of the laser pulse exceeds a certain threshold value, a sharp pulse arrives just ahead of the leading edge of the longitudinal phonon heat pulse. The speed of the sharp pulse is slightly faster than the normal speed of sound, as predicted for soliton propagation. The advantage of bolometers is that they can be used for high-resolution phonon imaging. Using this technique we find the solitons propagate as a collimated wavefront over cm distances in Sapphire and Si, but only mm in GaAs due to strong scattering.

MM 44.2 Fri 11:15 IFW A

Advances in Neutron Tomography — •Wolfgang Treimer[1,2], Nikolay Kardjilov[2], Andre Hilger[1,2], Ingo Manke[2,3], and Markus Strobl[1,2] — [1]University of Applied Sciences (TFH) FB II Berlin — [2]Hahn-Meitner-Institut Berlin — [3]Technical University Berlin, Faculty III

The experimental possibilities of neutron tomography at the BER II reactor in Berlin were improved by several options: The *classical* cold neutron radiography and tomography facility *CONRAD* got a parallel option for CT with monochromatic neutrons in the range of 0.23nm<lambda<0.65nm. With this option the same beam line geometry, sample and detector system can be used as for the whole cold spectrum. The extracted energies cover the most interesting range of 15.5meV<E<1.94meV, that contains the Fe, Cu, ß-Tin and Al Bragg edges, which are important for e.g. investigations of textures or more complex materials. Real time radiography and tomography can be performed at two different sample positions, having either a high neutron flux of 3x10ˆ9n/cmˆ2.s but low L/D˜70 or 5x10ˆ7n/cmˆ2.s and a L/D ˜500 as well as phase contrast imaging either with polychromatic or with monochromatic neutrons. With two high resolution double crystal systems refraction tomography and ultra small angle scattering tomography can be performed with a constant wave length of 0.524nm, USANS-CT shows clusters and inhomogeneities of 10nm - 500nm particles in a sample, both work with a spatial resolution of <1mm.

MM 44.3 Fri 11:30 IFW A

X-rays and Positrons Compared: Plasticity Studies on Deformed Carbon Steel — •Matz Haaks[1], Stephan Roth[2], and Karl Maier[1] — [1]Helmholtz-Institut für Strahlen und Kernphysik, Nußallee 14-16, 53115 Bonn — [2]Hasylab/Desy, Notkestraße 85, 22607 Hamburg

Plastic deformation is based on the movement and multiplication of dislocations, leading to jumps out of the glide plane. The movement of these jogged dislocations is always accompanied by the production of vacancies. In X-ray diffraction pattern the presence of dislocations causes a broadening of the diffraction reflexes. Using a high energy X-ray source with sufficient luminosity, powder-like Debye-Scherrer conditions can be achieved in a polycrystalline carbon steel with optimized geometry by diffracting in a volume containing 20000 grains. Positron Annihilation Spectroscopy (PAS) is used as a complementary method. It is non-destructive and highly sensitive for the detection of the vacancies associated with the dislocations.

We analyzed samples deformed in a three-point bending test with scanning X-ray diffraction in transmission at the high-energy beam line at Petra II/Hasylab as well as with scanning positron microscopy at the Bonn Positron Microprobe. The results from both methods are presented and compared.

As a practical application of transmission X-ray diffraction, the fabrication method of a historical cannon was investigated. We were able to decide between casting and forging.

MM 44.4 Fri 11:45 IFW A

Correlation between acoustic and electromagnetic emissions in plastically deformed LiF — •Konstantin Chishko[1], Tatiana Antsygina[1], Claire Mavromatou[2], and Vassilios Hadjicontis[2] — [1]B.Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., Kharkov 61103, Ukraine — [2]University of Athens, Panepistimiopolis, Zografos, TK 157 84, Athens, Greece

The experiments on plastic deformation (PD) of compressing LiF ionic monocrystals are performed with simultaneously registration of the acoustic emission (AE) and electromagnetic field (EF) near the sample surface measured with piezoelectric transducer and monopole coaxiale antenna, respectively. It has been found that jump-like deformation observed on promoted (rather late) stages of work hardening is accompanied by exclusive powerful AE bursts which can be associated with the break-through and emergence on the crystal free surface of large dislocation pile-ups formed due to evolution and intersection of different slip systems. Most of the acoustical events of such kind are accompanied by the measurable electromagnetic pulse whose appearance is strongly correlated with the front of the corresponding AE burst. The obtained phenomenon is obviously connected with the ionic lattice charge re-distribution controlled by interaction between dynamic dislocations and charged vacancies of the ionic crystal. The theory is proposed to interpret the electromagnetic emission during PD of an ionic crystal and the shape of EF pulse generated by a dynamical dislocation pile-up releasing from vacancy atmosphere is calculated. The theory predictions are in good agreement with the experimental observations.

MM 45 Mechanical Properties III

Time: Friday 12:30–13:30 Room: IFW A

MM 45.1 Fri 12:30 IFW A

Intrinsic plastic deformation behaviour of the complex metallic alloy phase ß-Al-Mg — •Stefan Roitsch, Marc Heggen, Carsten Thomas, Marita Schmidt, and Michael Feuerbacher — Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We have performed macroscopic plastic deformation experiments on the complex metallic alloy ß-Al-Mg. This material is a technologically interesting lightweight alloy (density 2.2 g/cm3) with a face centred structure containing about 1168 atoms per unit cell. For the first time, the intrinsic plastic deformation behaviour of high-quality single crystalline material was characterized. Uniaxial deformation experiments at a constant strain rate of 10-4 s-1 were performed at temperatures between 225 and 375°C. It was found that the single crystalline ß-Al-Mg exhibits

ductile behaviour down to temperatures of 225°C. At this temperature we find upper yield stresses of about 780 MPa. This is a very high value compared to other alloys in the Al-Mg system, for which yield stresses of the order of 300 MPa and below are found. The yield-point is followed by an almost constant flow-stress level up to strains of about 6%. Stress-relaxation tests and temperature changes were carried out in order to determine the thermodynamic activation parameters of the deformation process.

MM 45.2 Fri 12:45 IFW A

Strain rate effects of nano- and microcrystalline nickel measured form the macro- to the nanoscale — •Horst Vehoff, Delphine Lemaire, Bo Yang, and Michael Marx — Saarland University, Department of Materials Science, Building D23, D-66041 Saarbrücken, Germany

Understanding the macroscopic deformation behaviour of metals based on the microscopic mechanisms like grain rotation, grain boundary- and volume diffusion, emission and motion of dislocations and the interaction of dislocations with microstructure elements is one of the main objectives of modern materials science. Due to the different length scales of the deformation mechanisms the active mechanisms change with the grain size. Therefore the grain size dependent deformation behaviour was investigated locally by nanoindentation and macroscopically by incremental strain rate tests with nanocrystalline and microcrystalline nickel. The nanoindentation measurements probe the interaction of dislocations and grain boundaries locally during plastic deformation. It will be shown that with decreasing grain size the pile up of dislocations at grain boundaries as the dominant mechanism of the deformation process which leads to hardening is changed to grain boundary sliding and grain rotation as active mechanisms which leads to softening. The measurements were completed by macroscopic measurement of the strain rate sensitivity as function of the grain size. It will be shown that nanocrystalline materials have a higher strain rate sensitivity and smaller activation volumes than microcrystalline materials which indicates a continuous change of deformation mechanisms with the grain size.

MM 45.3 Fri 13:00 IFW A

High compression strain in bulk metallic glass composites containing low fraction of nanocrystals — •Alban Dubach, Florian Dalla Torre, Marco Siegrist, Kaifeng Jin, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland

A significant difference in compression strain but a similar yield strength has been measured for Zr-based bulk metallic glasses, if cast using two different techniques (casting via arc melting or induction melting). The processing route via arc melting produces samples showing plastic compression strains of 10-20%, whereas the other generates samples with only 0-2% plasticity. Microstructural analysis shows that despite the good glass-forming ability of the alloys chosen, samples with high compressive strain contain nanosized crystals in a glassy matrix. These samples are x-ray amorphous, while transmission electron microscopy clearly reveals the presence of a low fraction of nanocrystals. In contrast, the samples processed via induction melting are fully amorphous, but less ductile. We suggest that the second-phase nanoparticles, despite their low volume fraction not detectable by x-ray diffraction, lead to nucleation and multiplication of shear bands, in turn producing high plastic strain. Such high plasticity allows 'in-situ' probing of deformation kinetics by cycling the strain rate during compression testing. Results show a negative strain-rate sensitivity, which tends to be more pronounced for samples containing a higher fraction of second-phase particles or tested at higher strain rates.

MM 45.4 Fri 13:15 IFW A

Room-temperature embrittlement of Mg-based amorphous alloys — •A. Castellero, D.I. Uhlenhaut, and J.F. Löffler — Laboratory of Metal Physics and Technology, ETH Zürich, Wolfgang Pauli Str. 10, 8093 Zürich, Switzerland

Mg-Cu-Y alloys can be amorphised in a wide range of compositions. When these alloys are produced in bulk form they exhibit high mechanical strength but no ductility. Rapidly quenched ribbons and thin foils show plastic deformation upon bending. However, a dramatic deterioration in mechanical properties is observed after aging at room temperature. A sharp transition from ductile to brittle behaviour can be observed in Mg65Cu25Y10 a few hours after the alloy has been produced. The process becomes slower when Cu is substituted by Mg. Corresponding to this time-dependent embrittlement, differential scanning calorimetry (DSC) curves show a reduction in the relaxation enthalpy that is associated with a structural relaxation (i.e. annihilation of free volume) of the metallic glass. Oxidation as a cause of this embrittlement has been ruled out, since the same behaviour is observed when the samples are stored in a protective atmosphere. The bent as-quenched samples exhibit shear bands on the surface, indicating that the material is able to deform plastically. The aged metallic glass exhibits only elastic deformation, followed by catastrophic failure at a certain critical bending strain which progressively decreases with time. The mechanical properties and the deformation mode were characterized in detail as a function of time.