MM 32 Poster TU B
(Symposium Tomographic Methods in Materials Research M-32.32-55)

Zeit: Montag 14:30–16:30 Raum: Poster TU B

MM 32.1 Mo 14:30 Poster TU B

Surface morphology changes of 20 - 120 nm thin epitaxial Nb-films during hydrogen uptake — •Kai Nörthemann, Reiner Kirchheim, and Astrid Pundt — Institut für Materialphsysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

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

Because of the different lattice parameter of Niobium and Niobium hydride it is possible to study with the surface sensitive scanning tunneling microscopy (STM) the lateral arrangement of the α-phase and the hydride. STM pictures of thin epitaxial niobium films were taken during hydrogen loading, therefore the time dependency of the hydride formation can be examined. Different types of hydride arrangements were found. Their appearance will be discussed with regard to film thickness and roughness as well as substrate parameters. The stability of the arrangements will also be discussed.

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

MM 32.2 Mo 14:30 Poster TU B

Hydrogen sorption properties of Mg-1wt%Ni-0.2wt%Pd prepared by reactive milling — •O. Gutfleisch[1], S. dal Toe[1], M. Herrich[1], J. Zulkarnain[1], A. Handstein[1], and A. Pratt[2] — [1]IFW Dresden, Institut für Metallische Werkstoffe, Helmholtzstr. 20, D01069 Dresden, Germany — [2]Johnson Matthey Technology Centre, Reading RG4 9NH, UK

Despite the large differences in melting points and the high vapour pressure of Mg, we succeeded in the preparation of induction-melted Mg-1wt.%Ni-0.2wt%Pd alloy. The alloy was then reactively ball milled in 10 bar hydrogen. The structural changes during milling were characterised by XRD and high resolution scanning electron microscopy. The hydrogen sorption properties have been systematically studied by gravimetric analysis in a wide temperature and pressure range for absorption (1-10 bar, 50-300 °C) and desorption (250-350 °C, 50 mbar-1 bar). At 300 °C, the hydrogen absorption in 10 bar proceeds within less than 5 min reaching 6.3 wt% capacity; desorption in 50 mbar is completed within 10 min, whereas 20 min are needed when desorbing into 1 bar. Absorption conditions have been found to be very moderate: e.g. at 200 °C and 4 bar 5.5 wt.% is reached within 5 min, at 150 °C and 2 bar 5.0 wt.% is reached within 60 min and at 100 °C and 10 bar 4.0 wt.% is reached within 60 min. The combined effects of Pd and Ni additions prove particularly useful in providing superior kinetics at moderate charging conditions. Hydrogen capacity and kinetics did not deteriorate over at least 50 cycles. These data are compared with those of nanocrystalline MgH2 powders, obtained by intensive milling in argon atmosphere.

MM 32.3 Mo 14:30 Poster TU B

^{139}La-NMR and the metal-nonmetal transition of lanthanum hydrides — •Sandra Heck, Stephan Leyer, and Elmar Dormann — Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany

^{139}La Knight shift data [1] seemed in conflict with the disappearance of the conduction electron density of states deduced from specific heat measurements [2] for increasing hydrogen content in LaH_x ($2 \leq x \leq 3$) [3,4]. New data for Pauli susceptibility, ^{139} NMR line-width, line-shift and spin-lattice-relaxation are derived. Reliability of the $LaCl_3$ in aqueous solution Knight shift standard is questioned.

A conclusive picture based on NMR is presented.

Acknowledgment: R.G. Barnes and G. Majer for samples, DFG (Do 181/12) for financial support.

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[2] K. Kai et al, Phys. Rev. B **4**0, 6591 (1989)
[3] B. Stalinski, Bull. Acad. Sci. Cl. III **5**, 1001 (1957)
[4] S. Leyer et al, J.Phys. Cond. Matter **1**6, 6147-6158 (2004)

MM 32.4 Mo 14:30 Poster TU B

Herstellung und optische Eigenschaften von Seltenen-Erdhydriden — •H. Schröter und J. Schoenes — Institut für Halbleiterphysik und Optik, Mendelssohnstraße 3, 38106 Braunschweig

Seit längerem ist bekannt, dass Seltene Erdmetalle wie z.B. Yttrium, einen Metall-Isolator-Übergang zeigen, wenn sie einer Wasserstoffatmosphäre ausgesetzt werden. Die damit verbundene, Änderung der optischen Eigenschaften wurde mittels Ellipsometrie, u.a. am VUV-Ellipsometer am BESSY II, untersucht. Um den Mechanismus des Metall-Isolator-Übergangs zu verstehen, wurden Schichten mit unterschiedlicher Konzentration von Wasserstoff im Yttrium hergestellt und an ihnen Messungen durchgeführt. Zur Schichtherstellung wurden dabei verschiedene Methoden eingesetzt. Es wurden zum einem in-situ hydrierte Schichten mittles Molekularstrahlepitaxie (MBE) in einer Wasserstoffatmosphäre hergestellt, des weiteren wurde Schichten hergestellt, die nach dem Wachstum in einer an der MBE-Anlage angebrachten Wasserstoffzelle hydriert wurden. Zudem wurden noch Versuche unternommen, hydrierte Yttriumfilme durch Pulsed Laser Deposition (PLD) herzustellen.

MM 32.5 Mo 14:30 Poster TU B

Optische Untersuchungen an Selten-Erd-Hydriden im Bereich von 5meV bis 5eV — •S. Weber, D. Zur und J. Schoenes — Inst. für Halbleiterphysik und Optik, Mendelssohnstr. 3, 38106 Braunschweig

Viele Seltene-Erd-Metalle durchlaufen bei der Beladung mit Wasserstoff einen Metall-Isolator-Übergang. Neben den damit verbundenen dramatischen Veränderungen der elektrischen Eigenschaften werden die undurchsichtigen Metalle zu einem optisch transparenten Hydrid. Weiterhin geht bei Neodym und Europium eine Veränderung der magnetischen Eigenschaften zu ferromagnetischen Halbleitern einher.

Es wurden dünne epitaktische Filme aus Nd und Eu auf CaF_2(111) und Si(111)-Substraten mittels Molekularstrahlepitaxie hergestellt. Auf CaF_2 wächst Nd im Lage für Lage Wachstum in hcp Struktur, während sich Eu im Stranski-Krastanov Wachstum in bcc Struktur abscheidet. Die Gitterfehlanpassung des Nd beträgt 5,2%. Augerelektronen-Spektroskopie Messungen belegen die chemische Sauberkeit der Filme. Die Transmission und Reflexion der Filme wurde im Energiebereich von 5meV bis 5eV gemessen, und der Metall-Isolator-Übergang anhand Messungen an Proben mit verschiedenen Wasserstoffkonzentrationen untersucht. Der Einfluß von Wasserstoffschwingungen ist im infraroten Spektralbereich anhand von Verschiebungen von Strukturen um den Faktor $\sqrt{2}$ zwischen hydrierten und deuterierten Eu-Filmen zu beobachten. Mit winkelaufgelöster Photoelektronenspektroskopie kann die Veränderung der elektronischen Zustandsdichte untersucht werden. Dazu wurden Messungen an metallischem und *in-situ* hydrierten Proben durchgeführt.

MM 32.6 Mo 14:30 Poster TU B

Mg-Ni-Y alloys as new negative electrode materials for Ni-MH rechargeable batteries — •Bogdan Khorkounov, Angelika Teresiak, Margitta Uhlemann, Annett Gebert, and Ludwig Schultz — IFW Dresden, Postfach 270116, 01171 Dresden

Mg_2Ni has a large theoretical discharge capacity, but slow hydrogen sorption kinetics and poor corrosion resistance. Microstructural refinement and further alloying are needed. Mg-Ni-Y alloys with amorphous/nanocrystalline structure are investigated regarding their hydrogenation behaviour and cyclic electrode performance. $Mg_{63-x}Ni_{30}Y_x$-alloys absorb electrochemically up to 2,2 wt. % [H]. The thermal behaviour of Mg-Y-Ni ribbons in the as quenched and hydrogen-charged state was studied by in situ XRD. Crystallisation starts at 423 K with formation of Mg_2(Ni,Y), metastabile Mg_6Ni, Mg. Samples with [H] < 0.6 wt. % show the same phase formation during heat treatment. The formation of Mg_6Ni is inhibited by increasing [H]. Mg_6Ni decomposes at $>$ 523 K into Mg, Mg_2Ni. [H] = 1.42 wt. % leads to the formation of the fcc complex compound Mg_2NiH_4 at 523 K under a hydrogen atmosphere of 0.5 MPa besides $Mg_2NiH_{0.2-0.3}$, YH_2, YH_3, MgH_2. Y improves the corrosion and cycle life stability of Mg_2Ni-based electrodes, but decreases the discharge capacity. The effects of alloy composition, microstructure and electrode preparation on the discharge characteristics are discussed.

MM 32.7 Mo 14:30 Poster TU B

Structure and Chemical Bonding in High Pressure Phases of the Heavy Pnictides, Sb and Bi — •Alim Ormeci and Helge Rosner — MPI CPfS Dresden, Germany

In recent years the high-pressure structures of Sb and Bi have been determined by very accurate experimental techniques. The sequence of the

observed structural phase transitions are, in general, reproduced correctly by first-principles electronic structure methods. In this work we combine first-principles total-energy calculations with the topological analysis of the electron localization function (ELF) in order to study how crystal structure and bonding properties change as pressure is applied. Total-energy calculations are carried out by using the (i) full-potential linear muffin-tin-orbital method (FP-LMTO), and (ii) full-potential local orbital (FPLO) method. The ELF is calculated by using the FPLO method.

A particular issue is the importance of the relativistic effects to the electronic structure and to the crystal structure in Bi. This issue is investigated systematically by performing calculations based on the following approaches: (i) scalar relativistic Hamiltonian, (ii) spin-orbit coupling treated variationally, (iii) full Dirac Hamiltonian in a four-component implementation.

MM 32.8 Mo 14:30 Poster TU B

Electronic structure of Ga_{84} cluster compounds — •Johannes Frenzel, Sibylle Gemming, and Gotthard Seifert — Institut für Physikalische Chemie, TU Dresden, D-01062 Dresden

Semi-conducting and metal clusters as building blocks for organised structures are potential candidates for devices in nano electronics. In this field various aluminium and gallium clusters where synthesized with $[Al_{77}(N(SiMe_3)_2)_{20}]^{2-}$ and $[Ga_{84}(N(SiMe_3)_2)_{20}]^{4-}$ as the largest ones of this kind. Density functional calculations were carried out to study large bare and ligated gallium clusters and their packing in a three-dimensional crystal structure. In the single clusters, the electronic states are delocalised over the whole cluster and the gallium atoms exhibit no noticeable charge. Band structure calculations of the crystal do not yield any significant dispersion of the electronic bands. Thus it is concluded that the observed macroscopic electric conductivity is mediated by a hopping mechanism between the clusters rather than by the presence of states, which are delocalised over the whole crystal.

MM 32.9 Mo 14:30 Poster TU B

Diffusion und Viskosität in unterkühlten Metallschmelzen — •Alexander Bartsch[1], Klaus Rätzke[1], Volker Zöllmer[1], Andreas Meyer[2] und Franz Faupel[1] — [1]Technische Fakultät, Univ. Kiel, Kaiserstr. 2, 24143 Kiel — [2]TU München, Physik Department E13, James-Franck-Str., 85747 Garching

Seit der Entwicklung von Legierungen, die in der tief unterkühlten Schmelze stabil sind, werden Viskosität, Diffusion und Diffusionsmechanismus intensiv erforscht [1]. In der Gleichgewichtsschmelze gilt die Stokes Einstein Relation, nicht aber im Glaszustand. Daher bleibt offen, wo die Abweichung beginnt und welche Legierungskomponente die Viskosität bestimmt. An $Pd_{43}Cu_{27}Ni_{10}P_{20}$ wurden zwischen der kalorischen Glastemperatur $T_g = 582$ K und der kritischen Temperatur $T_c = 715$ K der Modenkopplungstheorie die Phosphor- und Cobalt-Diffusion gemessen. Der Vergleich von Co-Diffusion [2] und Viskosität [3] zeigt eine gute Übereinstimmung in der Gleichgewichtsschmelze. Mit fallender Temperatur beginnt ab T_c eine Divergenz von bis zu vier Größenordnungen bei T_g. Da die P-32-Diffusion in diesem Temperaturbereich fast so schnell wie Co-Diffusion ist, bestimmt erstere nicht die Viskosität; weitere Versuche mit Pd werden auf der Tagung präsentiert.

[1] F. Faupel et al. Rev. Mod. Phys. 75 (2003) 237 [2] V. Zöllmer et al. Phys. Rev. Lett., 92, 195502-1 (2003) [3] I.-R. Lu et al. J. Non-Cryst. Solids 312-314, 547 (2002)

MM 32.10 Mo 14:30 Poster TU B

Mechanical spectroscopy of Zr65Al7.5Cu27.5 thin films and first evidence for an excess-wing in metallic glasses — •Peter Rösner and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The double-paddle oscillator is used for the study of mechanical properties of thin amorphous Zr65Al7.5Cu27.5-films in the tempe-rature range from 300 to 650 K under ultra high vacuum conditions. The oscillator is driven in its secondary torsional eigenmode at about 5.4 kHz and the temperature dependence of the complex shear modulus of the film is measured. At temperatures above the glass transition, the loss modulus can be mathematically described by a Havriliak-Negami function. In the vicinity of the glass transition, our data clearly differ from this mathematical model. The temperature dependence of the mechanical loss modulus is very similar to the dielectric loss modulus of many other glass forming materials, where the deviation from the viscous alpha-process is described with an excess wing. Our experimental results give rise to the assumption that there exists a wing also in amorphous metals and could therefore be a universal property of glasses. One interpretation for the wing is to postulate density fluctuations and dynamic heterogeneities. Cooperative movement of groups of atoms that are called clusters and formed in the vicinity of the glass transition lead to a deviation of the alpha-process that is due to single-atom movement. The authors would like to thank P. Lunken-heimer and A. Loidl for many stimulating discussions. This work was supported by the Deutsche Forschungsgemeinschaft SFB 602, B8 and the Graduiertenkolleg 782.

MM 32.11 Mo 14:30 Poster TU B

DFT investigation of free and supported Mo_mS_n clusters — •Sibylle Gemming, Igor Popov, Jelena Tamuliene, and Gotthard Seifert — Institut für Physikalische Chemie, TU Dresden, D-01062 Dresden

The electronic and structural properties of clusters (Mo_nS_m) of the layered semiconductor MoS_2 were studied using density-functional based methods. For small Mo_nS_m clusters the evolution of structural elements, resembling the corresponding structure motifs of the layered bulk compound MoS_2 was found. Among the small clusters a highly symmetric Mo_4S_6 cluster features an outstandingly high stability and a large HOMO-LUMO gap. Thus, this cluster can be characterized as a "magic cluster". Mo_4S_6 forms stable, regular arrays on the Au(111) surface with a preferential adsorption of three sulphur atoms at Au-Au bridging positions. With increasing cluster size the stabilization of platelet structures is indicated. In the platelet structures the edges determine the deviation from the bulk properties. The binding energies increase smoothly with increasing cluster size towards the bulk limit. Small clusters and platelet structures have a HOMO-LUMO gap comparable with the gap of the semiconductor bulk material, whereas larger platelet structures show a metallic-like behaviour.

MM 32.12 Mo 14:30 Poster TU B

Phase-field model for binary alloys solidifying under stress — •Bo Liu and Klaus Kassner — Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg Postfach 4120, D-39016, Germany

A phase-field approach is developed to investigate the effect of compositionally-genarated elastic stresses on the morphological instability during directional solidification of a binary alloy. We present a detailed thermodynamic derivation of the model with antitrapping solute current in the mass convervation relation[A. Karma, Phys. Rev. Lett **87**, 115701 (2001)]. This antitrapping current counterbalances the physical, albeit artificially large, solute trapping effect generated when a mesoscopic interface thickness is used to simulate the interface evolution on experimental length and time scales. Furthermore, all spurious effects that scale with this thinkness can be suppressed after we introduce the different diffusivity of concentation evolution and elastic field evolution. The asymptotic analysis of the model recovers previous Gibbs-Thomson condition with compositionally-genarated elastic stresses [B.J. Spencer et.al, Acta metall. mater. **40**, 1599 (1992)]. The performance of the model is demonstrated by calculating accurately for the first time within a phase-field approach the oscillatory instability of a planar interface.

MM 32.13 Mo 14:30 Poster TU B

Strahlungsinduziertes Glätten innerer und äußerer Grenzflächen und Kornwachstum in Ni-Ag-Bilayern — •J. Petersen[1], K. Zhang[2] und S. G. Mayr[1] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, D-37073 Göttingen — [2]II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, D-37073 Göttingen

Es wurden Ni(45nm)-Ag(45nm)-Bilayer mit 300keV Xe^+-Ionen unterschiedlicher Fluenzen bestrahlt. Ionenbestrahlung bietet die Möglichkeit, innere und äußere Grenzflächen zu modifizieren und optimieren. Die wesentlichen morphologischen Änderungen in metallischen Systemen umfassen Glättung bzw. Aufrauung von Grenzflächen, sowie strahlungsinduziertes Kornwachstum. Neben Weitwinkel- und Kleinwinkelröntgenbeugungsmessungen wurde versucht, mittels Rastersondenmikroskopie und chemischen Ätzens direkt die Grenzfläche zu untersuchen. Das Ziel ist, die der Grenzflächenmodifikation zugrunde liegenden atomaren Mechanismen zu identifizieren. Eine wesentliche Rolle kommt hierbei dem thermal spike zu, der einerseits eine Strukturglättung durch viskoses Fließen hervorrufen kann, andererseits auch Rauigkeit und Ionenmischen induziert. Dieses Projekt wird im Rahmen des SFB 602 von der DFG gefördert.

MM 32.14 Mo 14:30 Poster TU B

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

The multilayered system $SrTiO_3(001)|LaAlO_3(001)$ was investigated by density-functional band-structure calculations. For layers of equal and low thickness the optimised lattice constant equals the average of the ones of the two constituents. The system contains two different interface terminations with differing physical properties. For $SrO(001)|AlO_2$ (I) the interface spacing amounts to 1.90 Å, for $TiO_2(001)|LaO$ (II) the spacing is reduced to 1.86 Å. 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.

MM 32.15 Mo 14:30 Poster TU B

Curvature Driven Grain Boundary Motion in Aluminum. — •V.A. Ivanov[1], D.A. Molodov[1], L.S. Shvindlerman[1,2], and G. Gottstein[1] — [1]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow Distr., 142432 Russia

The motion of individual grain boundaries under a constant driving force was studied in Al-bicrystals. In this technique the curved grain boundary moves along the lateral surface of the specimen forming a triple junction "free surface - boundary - free surface" during its motion.

Migration of different grain boundaries was measured *in-situ* utilizing orientation contrast in the SEM. The character of grain boundaries studied was described in terms of the crystallographic planes of the adjacent grains. In the current study, both effects the "surface" triple junction and the boundary character on steady state motion are considered. The effect of the junction is discussed with the criterion Λ which defines the influence of a triple junction on the motion of the attached grain boundaries. To describe the effect of boundary character, the shape of moving grain boundary was analyzed.

MM 32.16 Mo 14:30 Poster TU B

Dry sliding of copper tested by microtribometers in air and in vacuum — •Y. Liu, M. Gubisch, M. Himmerlich, S. Krischok, M. Scherge, and J.A. Schaefer — Institut für Physik und ZMN, TU Ilmenau, 98684 Ilmenau

At low speed and low load, mild wear was found in sliding tests of copper and its alloys. The mild wear is usually related to the formation of oxide films and influenced by the hardness of the substrates. If the oxide film remains after slider passes, and the substrate is hard enough to support the oxide film, the sliding occurs between the oxides, and thus a low wear and low coefficient of friction are expected. We examined this scenario by dry sliding tests of pure copper using microtribometers in air and in vacuum. The oxide films in the wear tracks were studied with scanning electron microscopy and photoelectron emission microscopy combined with locally resolved photoelectron spectroscopy. The deformation band underneath the wear tracks was revealed by conventional metallographic method and was observed by orientation imaging microscopy. The effect of the surface finishing and the atmospheric pressure on the coefficient of friction was examined, and discussed with reference to the formation of oxide films and the development of deformation band.

MM 32.17 Mo 14:30 Poster TU B

Defekte in extrem verformten CuZn-Legierungen - Experimente und Simulationen — •Kai Klement, Rolf Anders und Ferdinand Haider — Universität Augsburg

Durch das ECAP-Verfahren wird in den Proben eine hohe Zahl von Nichtgleichgewichtsdefekten wie Leerstellen und Versetzungen erzeugt. Das Ausheilen dieser Defekte wurde durch dilatometrische und thermoanalytische Methoden untersucht. Die Leerstellen haben einen größeren Anteil am Exzessvolumen, die Versetzungen liefern einen größeren Enthalpiebetrag. Bei diesen Messungen wurde je nach Zusammensetzung der CuZn-Proben (Cu mit bis zu 10 Gew.% Zn) eine Ausheilstufe zwischen 200°C und 300°C beobachtet. TEM-Aufnahmen sollen Aufschluss über die mikroskopischen Vorgänge geben.

Um den Beitrag der Versetzungen zur Volumenvergrößerung zu bestimmen, wurden außerdem Computersimulationen durchgeführt. Hierfür wurde ein fcc-Gitter mit zwei Stufenversetzungen erzeugt. Durch eine Relaxation mittels Molekulardynamik mit periodischen Randbedingungen und variabler Zellengröße wurde das mittlere Exzessvolumen der Versetzung bestimmt und mit einer entsprechenden Simulation ohne Versetzung verglichen. Darüberhinaus liefert die Konstruktion von Voronoi-Polyedern um die einzelnen Atome genauere Informationen über die Volumenvergrößerung in Abhängigkeit vom Abstand vom Versetzungskern.

MM 32.18 Mo 14:30 Poster TU B

Monte Carlo Simulation of Phase Separation Including Elastic Relaxations — •Rolf Anders[1], Gururajan Mogadalai Pandurangan[1,2], and Ferdinand Haider[1] — [1]Univ. Augsburg, Institut f. Physik — [2]Indian Institute of Science, Dept. f. Metallurgy

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 of the vicinity of the jumping atom are relaxed in order to minimise the total energy. This method was applied to a Lennard-Jones alloy to study the microstructure evolution of two systems with respect to misfit parameter and temperature. In the first one the shape of the emerging precipitate phase was analysed, using a randomly mixed initial configuration. In the second one the changing shape of an initially spherical precipitate was investigated.

MM 32.19 Mo 14:30 Poster TU B

Novel conductor materials for high field pulsed magnets — •Alexander Gaganov, Jens Freudenberger, Ekaterina Botcharova, Elias Mohn, and Ludwig Schultz — Leibniz-Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01099 Dresden Germany

There is a need for high-strength and highly-conducting materials for applications such as pulsed high magnetic field coils. Three different approaches were studied in order to strengthen copper-based conductor materials. First, microcomposite Cu-Ag alloys yield high strength as a consequence of their nanoscale microstructure and, on the other hand, a Cu-based macrocomposite can be strengthened by the use of a steel jacket. Last, but not least Cu-Nb mechanically alloyed microcomposited bear large potential to be the futures material for this type of application. In all three cases the increase of strength coincides with a decrease of conductivity. Thus, the ideal material balances between these two competing properties. The actual results will be presented.

MM 32.20 Mo 14:30 Poster TU B

Molecular dynamics simulation of aluminium diffusion in decagonal quasicrystals — •Stephen Hocker and Franz Gähler — Universität Stuttgart, Institut für theoretische und angewandte Physik, 70550 Stuttgart

Aluminium diffusion in decagonal Al-Ni-Co and Al-Cu-Co quasicrystals is investigated by molecular dynamics simulations, using newly generated EAM potentials. As in our previous work with classical effective pair potentials, above two thirds of the melting temperature strong aluminium diffusion is observed. Compared to pair potentials, the diffusivities in the decagonal plane are enhanced, which is attributed to additional diffusion processes. Furthermore, with EAM potentials the transition metal atoms are more mobile, so that their diffusion is also measurable. The activation enthalpies and the activation volumes are determined by measuring the diffusivities as a function of temperature and pressure. The qualitative behavior of the dynamics is confirmed by ab-initio simulations.

MM 32.21 Mo 14:30 Poster TU B

Effective potentials from ab-initio data for decagonal Al-Ni-Co — •Peter Brommer and Franz Gähler — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Binary and ternary quasicrystalline alloys show remarkable mechanical and transport properties which one would like to reproduce and analyse in more detail in numerical experiments. Unfortunately, the required systems are several orders of magnitude too large for quantum mechanical methods. Classical molecular dynamics with effective potentials allow the simulation of much larger configurations, but for complex systems phys-

ically justifiable effective potentials are scarce. In the Force Matching method, data like forces, cohesive energies and stresses in small systems are calculated with ab-initio methods, and the parameters of an effective potential are adjusted to optimally reproduce these quantum mechanically determined data. In this work an effective potential for decagonal Al-Ni-Co obtained by Force Matching is presented and the application to other quasicrystalline systems is discussed.

MM 32.22 Mo 14:30 Poster TU B

Homogenous nucleation in supersaturated iron vapour, a molecular dynamics study — •Norbert Lümmen and Thomas Kraska — Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Str. 116, D-50939 Köln

The nucleation rate is an important input parameter for the modelling of particle processes by continuum models such as population balances. With increasing nucleation rate more nuclei are formed in a given time range. The remaining atoms in the vapour phase are distributed over these particles over the course of the surface growth process. As result one obtains primary particles which are smaller than in case of a lower nucleation rate.

The experimental investigation of the nucleation at extreme conditions such as high temperature or high pressure is often difficult. In this work we show how molecular dynamics simulations can be employed for the investigation of the homogeneous nucleation and the calculation of nucleation rates for such systems. It is also shown how the obtained nucleation rate can be compared with available experimental data.

MM 32.23 Mo 14:30 Poster TU B

New Expression for the Diffusivity of Carbon in Fe-C Austenite — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt

In engineering technology of particularly case or through hardenable low-alloyed steels, precise mathematical prediction and analysis of carbon solid-state diffusion profiles is of special importance to proper heat treatment process control (carburization) and failure inspection (decarburization). Thus, reliable input data is required for correct simulations. Evaluating three discrete literature sources, for the concentration dependence of the carbon diffusivity in austenite linearized representations suitable for computing-time saving iterative calculations are derived between 0 and 1.4 m.% C and fitted with respect to temperature in the practically most relevant range form 1073 to 1373 K by means of two equivalent defining equations based on a simple polynomial expression and a physically founded Arrhenius approach, respectively. An extensive comparison to available literature references, which are partly inconsistent with each other, is drawn. The mathematical analysis of an industrial two-step gas carburizing experiment demonstrates the potential of the new expression.

MM 32.24 Mo 14:30 Poster TU B

New Computer Model for Decarburization of Steels with Simultaneous Carbide Dissolution — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt

Decarburization, i.e. outward diffusion of carbon caused by oxidation reactions, seriously impairs the mechanical edge zone properties of the affected material. This process represents the most important undesirable side effect to common heat treatment (e.g. austenitizing, soft annealing) and hot-working operations (e.g. forging, upsetting) of particularly low-alloyed steels. Reliable simulation tools are thus required for substantiated failure analyses. If the initial carbon content of the steel exceeds its solubility in austenite, decarburization is accompanied by carbide dissolution and thus becomes a complex diffusion process with simultaneous chemical reaction. A realistic computer model for the involvement of this background process, based on an iterative solution of Fick's law, is developed. Applying the novel calculation tool, the effect of the rate constant of carbide dissolution on the carbon profiles is discussed in detail considering decarburization of standard rolling bearing steel 100Cr6 (SAE 52100) in contaminated protective atmosphere under usual austenitizing conditions at 1123 K as example.

MM 32.25 Mo 14:30 Poster TU B

Thermo-physical properties of thin film and FIB modified NiTi shape memory alloys — •Jürgen Gibkes[1], Ch. Zamponie[2], R. Wernhardt[3], B.K. Bein[1], and J. Pelzl[1] — [1]Solid State Spectroscopy, Experimantal Physics 3, Ruhr-University, D-44780 Bochum — [2]Cesar Research Center, D-53175 Bonn — [3]Experimental Physics 6, Ruhr-University, D-44780 Bochum

Thermal transport parameters are key parameters for the functionality of shape memory (SM) material. The need of miniaturisation of the SM devices requires alternative preparation techniques of the base material affecting the thermal transport parameter. We have investigated films of a few microns thickness and bulk samples laterally surface modified by FIB (focus ion beam). The NiTi films were prepared by sputtering. After removing the amorphous films from the substrate they are thermal treated in order to induce a crystalline structure. The thermal transport properties were investigated by frequency dependent photothermal infrared radiometry. The annealed films exhibit different thermal parameters as the bulk materials of the same composition. The FIP prepared samples were investigated with a scanning thermal microscope (SThM). Local changes of the thermal transport properties with different doses were measured with a resolution of about 50 nm.

This work was performed in the frame of the Sonderforschungsbereich 459.

MM 32.26 Mo 14:30 Poster TU B

Microstructure, phase sequence, and superelasticity in highly oriented MBE-grown NiTiCu shape memory thin films — •R. Hassdorf[1], J. Feydt[1], S. Thienhaus[1], M. Boese[2], L. Buforn[3], N. Conté[3], and M. Moske[1] — [1]Forschungszentrum caesar, 53175 Bonn, Germany — [2]Universität Bonn, Institut für Anorganische Chemie, 53117 Bonn, Germany — [3]CSM Instruments SA, 2034 Peseux, Switzerland

Using MBE deposition highly oriented NiTiCu shape memory thin films were accomplished. The austenite-martensite transition in these films, single or two-stage transformation depending on the quantity of the Cu additions, occurs with comparable transition temperatures as known for sputter-deposited films. Mechanical stress measurements reveal a deformation recovery in the order of 400 MPa. Superelasticity spans to about 3% strain as referred to spherical indentation data. The microstructure is remarkable in that the crystallites are oriented within $\pm 5^\circ$ along the film plane normal as observed by X-ray diffraction. The occurrence of this preferential order is deduced to the formation of a Ti-rich (Ti_2Ni) phase at the film-substrate interface providing a highly oriented initial crystallization template. The results described in this study outline the perspectives for tailoring the microstructure and transformation performance of shape memory thin films, especially in regard to technological applications.

Supported by BMBF under contract no. 03N4031A.

MM 32.27 Mo 14:30 Poster TU B

Fluid Flow Effects on Phase Formation and Microstructural Evolution in Nd-Fe-B Melts — •Sven Reutzel[1,2], Takeshi Okutani[3], Thomas Volkmann[2], Jianrong Gao[4], Jörn Strohmenger[2], Heinrich Bach[1], and Dieter M. Herlach[2] — [1]Ruhr-University, Bochum — [2]German Aerospace Center, Cologne — [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan — [4]Northeastern University, Shenyang, China

Experiments on peritectic and hyper-peritectic $Nd_xFe_{100-1.5x}B_{0.5x}$ alloy melts (x = 11.8, 14, 16 and 18) were performed under microgravity during parabolic flight campaigns using the TEMPUS facility (Tiegelfreies elektromagnetische Positionieren unter Schwerelosigkeit) to elucidate the effect of melt convection on critical undercooling levels for the occurrence of metastable phases and the different solidification pathways which were observed in ground-based electromagnetic levitation experiments. Furthermore, the experiments were carried out to improve the knowledge on the relationship between undercooling, fluid flow, magnetic field, metastable phase formation and the structural properties, such as the homogeneity and crystallite orientation. Our main focus was (I) to analyse the influence of fluid flow in the undercooled melt on phase selection and on volume fraction of competing phases in the solidified samples and (II) to evaluate the influence of convection and static magnetic fields with respect to the crystallographic alignment of grains and homogeneity of microstructure.

This work is funded by the Space-flight Management of the German Aerospace Center, Bonn under contract No.50WM9930.

MM 32.28 Mo 14:30 Poster TU B

Hochtemperaturkorrosion von Überhitzerrohren in Kraftwerken — •Barbara Waldmann[1], Bernhard Stöcker[1], Christoph Mocker[1], Ferdinand Haider[1], Siegfried Horn[1] und Ragnar Warnecke[2] — [1]Institut f. Physik, Univ. Augsburg — [2]GKS Gemeinschaftskraftwerk, Schweinfurt

Die Korrosion von Stählen in Wärmetauschern von Kraftwerken ist nach wie vor nicht in allen Einzelheiten verstanden. Insbesondere in Müllverbrennungsanlagen ist die Korrosion ein erhebliches technisches und auch wirtschaftliches Problem. Am Beispiel eines häufig eingesetzten niedrig legierten Kohlenstoffstahls (15Mo3) wurde in einem Modellexperiment der Korrosionsangriff in einer chloridhaltigen Atmosphäre bei ca. 400°C (der typischen Arbeitstemperatur) mittels Rasterelektronenmikroskopie und EDX untersucht. Daneben werden Korrosionsstrom und -spannung mit elektrochemischen Methoden registriert. Es zeigt sich, dass sich auf dem Stahl zunächst eine Eisenchloridphase bildet, oberhalb derer als stabiles Korrosionsprodukt Eisenoxide wachsen. Diese Ergebnisse stimmen qualitativ mit den Befunden an aus einer MVA entnommennen Stahlproben überein.

MM 32.29 Mo 14:30 Poster TU B

Molekulardynamik-Simulationen zum Skalenverhalten der Schmelztemperatur von metallischen Nanopartikeln — •Magnus Kreth und Peter Entel — Universität Duisburg-Essen, Institut für Physik, 47048 Duisburg

Das Schmelzen von metallischen Nanopartikeln wurde mit Hilfe von Molekulardynamik-Simulationen untersucht. Wir studieren das Skalenverhalten der Schmelztemperatur für eine Reihe von metallischen Systemen. Die interatomaren Wechselwirkungen in den Simulationen werden durch empirische tight-binding second moment Potentiale beschrieben.

MM 32.30 Mo 14:30 Poster TU B

Microstructure of Fe2Re (Re=Tb, Nd) spherical alloy produced by containerless solidification in drop tube — •Shumpei Ozawa[1,2], Kazuhiko Kuribayashi[1], and Dieter Herlach[2] — [1]Institute of Space and Astronautical Science, 3-1-1 Yoshinodai, Sagamihara, 229-8510, JAPAN — [2]Institute of Space Simulation, German Aerospace Center, 51170 Cologne, GERMANY

Fe2TbxNd1-x alloy were containerlessly solidified in a drop tube. Droplets of various diameters were formed and collected at the bottom of the drop tube. The microstructures of the Fe2Tb samples consist of two regions. One is properitectic Fe3Re phase in the Fe2Tb matrix and the other is primary Fe2Tb dendritic grains. The region that consists of Fe2Tb dendrite expands due to the enhancement of the undercooling and cooling rate with decreasing the sample diameter. In the Fe2Tb0.5Nd0.5 samples, the Fe3Re phase crystallized from the melt directly. The Fe2Re phase is peritectically formed from Fe3Tb and liquid phases. The further improvement in the solidification conditions such as the ejection gas pressure and temperature of the molten metals together with the composition modifications should be favorable to increase the undercooling level for the direct crystallization of the Fe2Re phase. This will be a challenge to produce the Fe2Nd Laves phase directly from the undercooled melt, which has been theoretically predicted to exhibit the highest magnetostrictive strain.

MM 32.31 Mo 14:30 Poster TU B

Martensitic transformation behavior of compression aged Ni-rich NiTi shape memory alloys — •J. Michutta[1], Ch. Somsen[1], A. Dlouhy[2], K. Neuking[1], and G. Eggeler[1] — [1]Institute of Materials Science, Ruhr-University Bochum, 44780 Germany — [2]Institute of Physics of Materials, Zizkova 22, 61662 Brno, Czech Republic

In the present study we investigate the martensitic transformation behavior in Ni-Ti single crystals with a nomin al Ni content of 50.8at.% aged under compression of 50MPa in [111]-direction for aging times from 2ks up to 360ks at 550°C. The martensitic transformation behavior of the compression aged single crystals is mainly characterize d by differential scanning calorimetry (DSC) and in-situ transmission electron microscopy (TEM) on cooling the sa mples. Compression aging at 550°C in [111]-direction leads for all investigated aging times to the growth of only one family of Ni_4Ti_3 precipitates. In order to reduce internal stresses the Ni_4Ti_3 precipitates grow in an autoc atalytic process resulting in B2-type channels in between the precipitates. On cooling three peaks are present in the DSC charts, more distinct for the longer aging times from 16ks up to 360ks. In-situ TEM shows that the first peak on cooling is attributed to a martensitic transformation of the high temperature B2-phase to the martensiti c R-phase starting at the particle matrix interface all over the sample. In contrast the second peak is associate d with the formation of B19′ in favorite regions of the single crystal appearing in a burst like event on cooling in some channels. On further cooling from this transformed channels the martensitic B19′-phase growth, which exp lains the third peak in the DSC-measurements.

MM 32.32 Mo 14:30 Poster TU B

NON-DESTRUCTIVE TESTING WITH NEUTRON PHASE CONTRAST IMAGING — •Klaus Lorenz[1], Erich Steichele[1], and Eberhard Lehmann[2] — [1]FRM-II, 85748 Garching, Germany — [2]Paul-Scherrer-Institut, 5232 Villigen, Switzerland

At the NEUTRA facility (SINQ), a great variety of objects was investigated with phase contrast radiography, for instance metal foams and casted objects. The phase contrast effect is now well understood and great efforts are made to improve the existing setup and to exploit all the possibilities offered by this technique. The tomography facility ANTARES at the FRM-II in Garching was designed to perform phase contrast measurements with neutrons as a matter of routine.

A big goal is to do quantitative phase contrast radiography and the step towards phase contrast tomography. By performing phase retrieval for every slice of a tomographic data set it becomes possible to assign every voxel the imaginary (attenuation coefficient) and the real part of the refractive index. This allows the separation of materials, which could not be separated hitherto in conventional tomographies.

MM 32.33 Mo 14:30 Poster TU B

Conceptual design and construction of the cold neutron tomography facility at HMI — •André Hilger[1,2], Nikolay Kardjilov[1], Lounis Mokrani[1], Rudolf Ringel[1], Wolfgang Treimer[1,2], and John Banhart[1] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin — [2]Technische Fachhochschule Berlin, Luxemburger Str. 10, 13353 Berlin

Neutron tomography is a powerful non-destructive method for the investigation of a large variety of different objects. It allows to visualize the inner volume of a sample without destroying or dismantling it. The different interaction mechanisms of neutrons and X-rays with matter make neutron tomography a complementary technique to classical X-ray tomography. Tomographic imaging with cold neutrons is on one hand highly sensitive to light elements and organic materials. On the other hand, cold neutrons pass easily through metals and other materials composed of heavy elements. A new tomography facility with cold neutrons is under construction at the reactor BER II of the Hahn-Meitner-Institut, Berlin. The new instrument is placed at the end of a curved neutron guide which faces the cold neutron source of the reactor. Two measuring positions are planned. The first one is directly at the end of the neutron guide where an extremely high cold neutron flux of approximately $10^9 n/cm^2 s$ is available. The second measuring position is intended for high-resolution tomography and is located 5 m away from the neutron guide where the flux is only $10^7 n/cm^2 s$ but the beam collimation is much better. The first test experiments at these measuring position have been performed and will be presented.

MM 32.34 Mo 14:30 Poster TU B

Tomography with Monochromatic Neutrons — •Markus Strobl[1,2], Wolfgang Treimer[1,2], André Hilger[1,2], and Nikolay Kardjilov[1] — [1]Hahn-Meitner-Institut Berlin, Glienickerstr. 100 14109 Berlin — [2]Technische Fachhochschule Berlin, Luxemburger Str. 10, 13353 Berlin

A perfect Si monochromator placed in the cold neutron beam of the BER II reactor at the Hahn-Meitner-Institute provides a highly monochromatic beam. The ratio $\Delta\lambda/\lambda$ is in the range of a few percent for a wavelength $\lambda = 0.45nm$ that is fulfilling the Bragg condition for the asymmetric reflection. Although the resulting flux density is low i.e. approximately $5 \times 10^3 cm^{-2} s^{-1}$ this beam has advantages for special radiography and tomography applications. On one hand the effect of beam hardening can be avoided and hence a better sensitivity concerning slight density differences can be achieved. On the other hand the irradiation of samples can be reduced compared to high flux instruments in spite of the fact that the exposure time is necessarily increased. The spatial resolution of the instrument can be given with $125\mu m$ in horizontal respectively $200\mu m$ in vertical direction. Some examples of successful applications will be given.

MM 32.35 Mo 14:30 Poster TU B

Combination of neutron tomography and X-ray tomography at FRM-II — •Michael Schulz and Burkhard Schillinger — Technische Universität München, 85747 Garching, Germany

The combination of neutron tomography and x-ray tomography can greatly enhance the field of application of computed tomography in non-destructive testing. Having different absorption coefficients for x-rays and neutrons, respectively more materials can be distinguished than with only one of the two methods. One of the major problems of combining different imaging methods is the alignment of the 3D datasets to each other (image registration). This difficulty can almost completely be avoided by using the same measuring geometry and detector setup for both measurements. For neutron tomography the radiographies are made in parallel beam geometry. As a detector we use a neutron sensitive scintillation screen and a CCD camera to record the scintillation image. Increasing the distance between our 320kV x-ray source and the sample position to approx. 12m, a nearly parallel beam geometry can be achieved for x-ray tomography, either. Thus it is possible to use the same reconstruction algorithm for the two datasets. This minimizes the differences in shape and orientation of the two 3D datasets. The detector is the same CCD camera as for neutron tomography in combination with a scintillation screen which is sensitive to both x-ray and neutrons. In this talk we will present the new x-ray tomography facility at the experimental reactor FRM-II in Garching. First experimental results will be shown and our experience with the new facility will be discussed.

MM 32.36 Mo 14:30 Poster TU B

Einfluss auf die Relaxationraten T_1 und T_2 durch Kombination von NMR und NAR — •David Tyler Hartman, André Engelbertz und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms- Universität zu Bonn

NMR ist heutzutage ein vielfältig eingesetztes Werkzeug in der naturwissenschaftlichen Forschung bis hin zum Klinikalltag. Durch die physikalisch begründeten Relaxationszeiten ist diese Methode für Betrachtungen von dynamischen Prozessen in der Bildgebung bisher ungeeignet. An Festkörpern kann auf die Relaxationszeiten mit Hilfe von eingestrahltem und resonantem Ultraschall Einfluss genommen werden. Desweiteren werden Messungen an weicher Materie und Flüssigkeiten vorgestellt. Dafür wurde der Ultraschall mit der Lamorfrequenz unter dem optimalen Winkel von 54,7° eingestrahlt. Die Ultraschallpulse erzeugen über periodische Druckschwankungen Wechselfelder, vergleichbar zum B_1-Feld, welche mit dem Kernspinensemble wechselwirken. Die Resultate an den verschiedenen Proben werden hier vorgestellt.

MM 32.37 Mo 14:30 Poster TU B

Nonlinear registration of series of atomic force microscopy images of nanostructured materials — •Sabine Scherdel[1], Stefan Wirtz[2], Nicolaus Rehse[1] und Robert Magerle[1] — [1]Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth — [2]Mathematisches Institut, Universität zu Lübeck, 23560 Lübeck

Nanotomography is a new method to map the complex spatial structure of modern materials. Here a series of two-dimensional atomic force microscopy images is obtained. To reassemble these to a volume image image distortions must be corrected. We have modified a more general registration method [1] for our applications, which was mainly applied to medical science so far. Our atomic force microscopy images are cutouts of an object and show not a single object that is clearly separated from the background. Furthermore the selected section is slightly shifted in each image. Inevitable contaminations of the specimen are another problem. They appear in just one layer and contribute with high grey values to the calculation of the distortion field, even though they comprise no three-dimensional image info rmation at all. By the use of this nonlinear registration we are able to picture nanostructured materials over large ranges (1 mum) with a resolution of 10 nm per pixel. Examples are a 20 nm wide rack in a nickel based super alloy as well as several crystalline lamellae in a semi-crystalline polymer film.
[1] B. Fischer, J. Modersitzki, J. of Math. Imag. Vision 2003, 18, 81.

MM 32.38 Mo 14:30 Poster TU B

Tomographic atom probe (TAP) study of the chemical ordering in amorphous alloys — •Ahmed Shariq, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich hund platz 1,D 37077, Göttingen, Germany

Amorphous alloys are characterized by the absence of atomic long range order and reveal only topological and sometimes chemical short range order. The attractive properties offered by these alloys triggered intensive microstructural investigations in the last few years. The wider supercooled liquid region in new amorphous alloys allows to explore the kinetics and thermodynamics in this region. 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. The data from TAP has been used to elucidate the atomic distance between neighbouring atoms. The chemical ordering in the Fe, Pd and Zr based amorphous alloys are discussed in this contribution.

MM 32.39 Mo 14:30 Poster TU B

Analysis of Ordering and Site Occupancies in TiAlNb — •Torben Boll[1], Talaat Al-Kassab[1] und 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, Nanjing 210093, China

Titanium-aluminium-alloys with small amounts of Niobium were prepared under high vacuum conditions by means of levitation melting. Heat treatment in the temperature range of 1250 K for several hours were performed.

The samples were investigated with field ion microscopy (FIM) and tomographic atom probe (TAP). Special attention was paid to the distribution of Nb in the γ-phase, where it, as FIM-analysis indicates, preferentially occupies Ti-sites. A new algorithmic approach based on TAP-data was developed to evaluate the site occupancies in ordered structures. Preliminary results, obtained with this method, will be presented and discussed for the site occupancy of Nb along a <001>-direction in these alloys.

MM 32.40 Mo 14:30 Poster TU B

New aspects of the decomposition in CuCo observed with different field ionisation-based tomographic techniques — •Alexander Heinrich, Talaat Al-Kassab und Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

CuCo has been of great interest as an ideal model system for decomposition in binary alloys. Specimen of Cu2at.%Co have been examined using the Tomographic Atom Probe (TAP), Field Ion Microscopy (FIM) and a recently developed method for Field Ion Image Tomography (FIIT). In this method sequences of field evaporation images are digitally registered. A three dimensional reconstruction of the imaged volume is followed via an advanced algorithm. This enables the examination of large analysis volumes with respect to the volume analysed in the TAP. New aspects of the decomposition behaviour at lower annealing temperatures (703K and 763K) could be observed with this technique. Nucleation is observed initially along the elastic soft direction in Cu, forming needle-shaped precipitates which are subsequently subject to coarsening reactions. In contrast to this phase separation at higher annealing temperatures (853K) was observed to take a different path of decomposition. Small agglomerates of atoms form which then coarsen to larger precipitates. The results will be discussed in terms of phase decomposition theory.

MM 32.41 Mo 14:30 Poster TU B

Segregation and Clustering of Phosphorus at Grain Bounderies of Nanocrystalline Cobalt — •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-37075 Göttingen — [2]Chalmers University of Technology, Department of Material Science and Engeneering, SE-412 96 Göteborg, Schweden

Nanocrystalline Co-1.2at%P and Co-2.1at%P layers with a thickness of 70-200 μm and a grain size of around 10 nm were prepared by pulsed current electrodeposition. These specimens were investigated by Field Ion Microscopy (FIM), Tomographic Atom Probe (TAP) and Transmission Electron Microscopy (TEM) both in the as prepared state and after different heat treatments.

The results reveal already a P-segregation at the grain boundaries in the as prepared state. In addition to normal and abnormal grain growth, the Co-1.2at%P alloy exhibited the formation of Co_2P- and CoP-precipitates at grain boundaries after isochronal thermal annealing. In this paper, preliminary results of grain growth and segregation behavior as a function of temperature and time of annealing for the Co-2.1at%P alloy will be presented. The findings will be compared to the ones observed in the Co-1.2at%P alloy.

MM 32.42 Mo 14:30 Poster TU B

Analysis of the ageing of metallic foams by means of quantitative micro-computed tomography (μCT) — •Oliver Brunke[1], Stefan Odenbach[1], and Felix Beckmann[2] — [1]ZARM Universität Bremen, Am Fallturm, 28359 Bremen — [2]GKSS-Forschungszentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht

Metallic foams, and especially those made from Al and its alloys, have become a major topic for both industrial and basic research throughout the last decade. The physical properties of solid metallic foam which are relevant for most applications like e.g. in automotive or aerospace industry are strongly affected by its structure parameters, like for instance pore size, shape and distribution, the location of inhomogeneities or the distribution of solid material between films and Plateau borders. On the other hand, these parameters directly depend on the temporal development, stability and ageing of the liquid foam system. The ageing behaviour of Al foams produced by a powder metallurgical route has been observed by means of Synchrotron- as well as cone beam μCT. We will present methods for the analysis of the development of the structure of metallic foams using 3D image processing techniques. This allows us the three dimensional and non-destructive determination of the temporal behaviour of e.g. the pore size or the cell wall material of the foam system.

MM 32.43 Mo 14:30 Poster TU B

High resolution synchrotron tomography on Nickelbase superalloys — •Thomas Link[1] und Alexander Epishin[2] — [1]Dr. T. Link, TU Berlin BH18, Ernst-Reuter-Platz 1, 10587 Berlin — [2]Dr. A. Epishin, BAM-Berlin, Unter den Eichen 87, 12205 Berlin

Single crystals of Nickel base superalloys contain micro pores, resulting from solidification, heat treatment and creep deformation. The investigated specimens have rod shape. They are grown by directional solidification, resulting in a dendritic structure along the rod axis. SEM images of cross sections through the rods gave an indication, that the pores are arranged preferably in the interdendritic region. Because the pore volume fraction is quite low, about 0.3 percent, this is difficult to be seen in a 2D image. Therefore tomography was applied. The pores under interest are quite small, around 5 microns, and the density of the superalloys high. This restricted the thickness of the specimens to about 0.5mm. They were investigated at the ID19 beamline, ESRF, Grenoble under 50 keV. The main points of interest were: Porosity in undeformed superalloys of the 3 generation (SRR99, CMSX-4, CMSX-10). Development of porosity in CMSX-4 during creep. Influence of the creep stress on the creep porosity. We could show, that porosity is most pronounced in the newest superalloy. Porosity increases during creep. With rising creep stress the creep pores form also in the primary and secondary dendrite arms.

MM 32.44 Mo 14:30 Poster TU B

Development and construction of an X-ray nano-tomography facility for interdisciplinary research at the Ghent University — •Bert Masschaele[1], Manuel Dierick[2], Jelle Vlassenbroeck[2], Luc Van Hoorebeke[2], Patric Jacobs[1], and Veerle Cnudde[1] — [1]Krijgslaan 281, S8, B-9000 Gent — [2]Proeftuinstraat 86 B-9000 Gent Belgium

Development and construction of an X-ray nano-tomography facility for interdisciplinary research at the Ghent University

Bert Masschaele b, Manuel Dierick a, Jelle Vlassenbroeck a , Luc Van Hoorebeke a, Patric Jacobs b, Veerle Cnudde b

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Since very recent is has become possible to manufacture X-ray tubes with high energy and high flux with focal spot sizes below 1 micrometer. These sources make it possible to investigate samples with a resolution below 1 micrometer and a detail detectability of 200nm non-destructively and in three dimensions. In the paper we will discuss the development of a nano-tomograph for multidisciplinary research. We will also discuss the latest evolutions of the detectors and manipulation motors for sub micrometer tomography.

MM 32.45 Mo 14:30 Poster TU B

Server/Client Distributed Cone Beam Reconstruction algorithm — •Jelle Vlassenbroeck, Bert Masschaele, Manuel Dierick, and Luc Van Hoorebeke — Proeftuinstraat 86 B-9000 Gent Belgium

Server/Client Distributed Cone Beam Reconstruction algorithm

Jelle Vlassenbroeck, Bert Masschaele, Manuel Dierick, Luc Van Hoorebeke

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During the last 10 years micro-CT has gained much popularity in industry and research. A lot of efford was put into the development of fast reconstruction algorithms and dedicated hardware to improve the CT reconstruction calculations in terms of speed and quality. In the past year we have developed a dedicated FDK algorithm using LabVIEW for the Octopus package. The paper will explain the new algorithm and the server/client implementation for network reconstruction.

MM 32.46 Mo 14:30 Poster TU B

Chemical processes in commercial batteries studied by synchrotron-tomography and 3D image analysis — •A. Rack[1], A. Haibel[1], I. Manke[2], S. Zabler[2], H. Riesemeier[3], G. Weidemann[3], J. Goebbels[3], and J. Banhart[1,2] — [1]Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung, Glienicker Str. 100, 14109 Berlin — [2]Institut für Metallphysik, Hardenbergstr. 36, 10623 Berlin — [3]Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, Haus 60, 12205 Berlin

Batteries are playing a major role in everybody's daylife: laser pointers, walkmen, mobile telephones - all are working with a power pack. Here we are focusing on manganese-zinc batteries (type AAA/micro) as they are widely used and therefore investigations are interesting for all kind of applications. By working with the high resolution tomographic setup of the BAMline @ BESSY II we obtained 3D images of one battery in different discharging stages. Due to the use of monochromatic radiation we are able to distinguish between the different materials within our tomographic image. All chemical components are separated from the greyscaled data into Boolean images and then evaluated by 3D image analysis methods derived from stochastic geometry [1]. We can quantify the time-dependent decay of the battery's manganese as well as changes of the zinc powder's morphological structure.

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

MM 32.47 Mo 14:30 Poster TU B

Study of semi-solid casting and processing with X-ray phase-sensit ive tomography — •S. Zabler[1], A. Haibel[2], A. Rack[2], A. Rueda[1], H. Riesemeier[3], G. Weidemann[3], J. Goebbels[3], and J. Banhart[1,2] — [1]Institut für Werkstoffe (TU), 10623 Berlin — [2]Hahn-Meitner-Institut Berlin, Abteilung SF3, 14109 Berlin — [3]Bundesanstalt für Materialforschung und -prüfung, 12205 B erlin

Alloys with a *globular microstructure* are the feedstock for industr ial components processed in the *semi-solid state* which requires thi xotropic behaviour of the melt. The fundamental link between alloy micros tructure and *thixotropic breakdown*, occuring when shear stress is a pplied, was first reported for Sn-Pb15 (Spencer 1972). During the past th ree decades thixo-processing has been established for a wide range of all oys but structural analysis remained however limited to metallography (2D images) and rheology (global measurement of viscosity as a function of s hear rate, temperature and shear time). Non-destructive three-dimensional structure analysis was first performed at the ESRF in 2000. It initiated a new rush for the investigation and modelling of the semi-solid casting process. In a first approach we use alloys with higher absorption contra st than common Al-Si in order to characterize the three-dimensional image s of *dendritic* and *globular* structures. Then we show recent e xperiments from the tomography setup of *BAMline* at the synchrotron BESSYII. The setup provides high spatial resolution using X rays with a *partial spatial coherence* thus allowing 3D *phase-sensitive imag ing* of neighbouring elements that are undistinguishable to absorption to mography.

MM 32.48 Mo 14:30 Poster TU B

High resolution synchrotron-tomography on human tooth tissue — •H. G. Gräber[1], A. Rack[2], A. Haibel[2], I. Manke[3], H. Riesemeier[4], G. Weidemann[4], J. Goebbels[4], and J. Banhart[2,3] — [1]Medical Faculty, RWTH Aachen — [2]Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung — [3]Institut für Metallphysik, TU Berlin — [4]Bundesanstalt für Materialforschung und -prüfung

Caries and periodontitis are the most frequent infectious diseases at all. Both diseases lead to an irreversible loss of mineralized tissues (bone and tooth). The aim of current and future research projects is to develop regenerative strategies by means of tissue engineering. We examine samples for different stages of the disease with synchrotron-tomography using a high spatial resolution of 1.5 μm pixelsize. The demineralized tissue can be detected in the 3d images due to it's lower density. By quantitative analysis of the data one obtains information about the dis-

ease growing's time-dependence. A comparison of non-treated infected teeth with treated ones (e.g. fluoridation) delivers information about the quality of different regeneration approaches.

MM 32.49 Mo 14:30 Poster TU B

Flaw Types in Metallic samples Analyzed with Computed Tomography — •Juergen Goebbels, Gerd Weidemann, Heinrich Riesemeier, Bernhard Illerhaus, and Yener Onel — BAM, Unter den Eichen 87, 12205 Berlin

Volume characterization of metallic samples with computed tomography requires a broad spectrum of X-ray energies depending on the maximum material thickness to be penetrated. BAM has developed several tomographs from high resolution computed tomography with synchrotron radiation at the BAMline at BESSY in the energy range from 8 to 80 keV, over laboratory equipment using different kind of microfocus X-ray tubes (a 100 kV transmission type X-ray tube, a conventional 225 kV and a world wide unique 320 kV bi-polar microfocus X-ray tube) up to high energy sources like Co-60 and an 12 MeV electron linear accelerator. The limits of spatial and contrast resolution are discussed together with the types of detectors used. The flaw types ranges from different kind of pores and cracks in welding seams to stress corrosion cracking, inclusions and inhomogenities.

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3D reconstruction of an abnormally growing Goss grain in Fe3%Si by FIB serial sectioning and EBSD — •Dorothée Dorner and Stefan Zaefferer — Max-Planck-Institut für Eisenforschung, Abteilung Mikrostrukturphysik und Umformtechnik, 40237 Düsseldorf, Germany

Grain-oriented silicon steel is used in electrical transformers as the core material. It is characterised by a strong crystallographic preferred orientation that develops due to abnormal (discontinuous) growth of {110}<001>-oriented grains (Goss grains). Though various models exist to explain this abnormal growth behaviour, no theory is yet generally accepted. The Σ9 grain boundary theory emphasis the significance of special grain boundaries. The solid state wetting model is based on grain boundary energy considerations and proposes a special grain boundary shape, i.e. wedge-shaped bulges.

In this study, we performed serial sectioning experiments with the focussed ion beam (FIB) technique in combination with crystal orientation measurements using electron backscatter diffraction (EBSD). We investigated the shape of growing Goss grains in 3D as well as the spatial position and crystallography of their grain boundaries. This possibly helps to answer how the anisotropic growth of Goss grains depends on the grain boundary properties.

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3D-analysis of the crystal orientation relationship and growth process of lenticular martensite in Fe-30mass%Ni alloy — •Hisashi Sato and Stefan Zaefferer — Department of Microstructure Physics and Metal Forming, Max-Planck-Institute for Iron Research, Max-Planck-Strasse, 1, Dusseldorf, Germany

The 3-dimensional structure of lenticular martensite in Fe-Ni alloys has been studied by EBSD orientation microscopy on serial sections produced in a focused ion beam - scanning electron microscope (FIB-SEM). With a spatial resolution of 50 x 50 x 50 nm and an orientation resolution of 0.5° very fine details of the microstructure can be observed and a formation mechanism is proposed.

In previous studies [1-2], it has been reported that the crystal orientation relationship (OR) between martensite and austenite in Fe-Ni alloy is Nishiyama-Wassermann. However, this OR is an average one which can only partly be confirmed by our local measurements. The 3-dimensional measurements show that martensite nucleates with a Kurdjumov-Sachs relationship which then rotates towards NW with further growth.

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Investigation of rheological behaviour of binary alloys with synchrotron radiation — •Rueda A.[1], Zabler S.[1], Rack A.[2], Haibel A.[2], and Banhart J.[1,2] — [1]Technische Universität Berlin, Institut für Werkstoffwissenschaften und -technologien, Fakultät III - Fachgebiet Struktur und Eigenschaften von Materialien — [2]Hahn-Meitner-Institut Berlin, SF3, Abteilung Werkstoffe

Thixotropic alloys are characterized by a non-dendritic, i. e. globular, solid phase embedded in a melting liquid matrix. Due to the good casting property of the thixotropic alloys they play an important role for engineering applications. One production route of such alloys is the new rheocasting process. At this, the liquid alloy will be casted in a special container and the accruing shear forces cause the building of the globular solid structure. By using this proceeding and with chemical grain refining (AlTiB) we were able to manufacture thixotropic material (AlGe15%) with around 100μm diameter grains. In order to investigate the static and dynamic, i.e. rheological, properties we used synchrotron radiation at BESSY II. By means of high resolution synchrotron radiography we studied the microstructure of our alloy, which is rich in absorption contrast of X-rays. Tomographic images of the thixotropic alloy are used to quantify their globular shape. In radiographic images of micrometer-thin layers we obtained at real time the rheological behaviour, i.e. the grain formation and movement in the mushy state of the alloy.

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Synchrotron Tomography Investigations on Ceramic Foams — •A. Berthold[1], A. Haibel[2], and H. Schubert[1] — [1]TU Berlin, Institut für Werkstoffwissenschaften und -technologien, Fakultät III - Fachgebiet Keramik — [2]Hahn-Meitner-Institut Berlin, SF3 Abteilung Werkstoffe

Interfacial active properties of special biopolymers, i.e. proteins, allow the generation of ceramic foams with microwaves. This differs obviously from conventional production methods of such foams. By means of synchrotron tomography we investigated the mechanism of accruement of the initial pore distribution in these foams as well as the shape of fully foamed ceramic material. Thanks to the knowledge of the accruement mechanism we are able to influence and control pore accruement and growth.

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Ausbau der Mikrotomographieapparatur für Serienuntersuchungen von Magnesiumimplantaten — •J. Fischer[1,2], F. Witte[1], T. Donath[2] und F. Beckmann[2] — [1]Orthopädische Klinik der Medizinischen Hochschule Hannover, Anna-von-Borries-Str. 1-7, 30625 Hannover — [2]GKSS Forschungszentrum, Max-Planck-Str. 1, 21502 Geesthacht

Die Mikrotomographie mit Synchrotronstrahlung ist in der Materialwissenschaft zu einer festen Größe geworden. Am Deutschen Elektronen-Synchrotron DESY werden unter Verwendung der Tomographieapparatur der GKSS unter anderem Untersuchungen von Magnesiumimplantaten der Medizinischen Hochschule Hannover durchgeführt. Um Serienuntersuchungen zu beschleunigen, wurden ein automatisches Probenwechselsystem, sowie der Umbau auf eine kontinuierlich drehende Rotationsachse realisiert. Es wird das Konzept und die Durchführung der Umbauten dargestellt.