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.

[1] J.C. Hulteen, and C.R. Martin, J. Mater. Chem., 7(7), 1075 (1997)
[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.

[1] S.I. Ben-Abraham, Ferroelectrics, 305 (2004) 29-32. [2] S.I. Ben-Abraham, Y. Lerer, Y. Snapir, J. Non-Cryst. Solids, 334&335 (2004) 71-76.

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.