MM 12: Postersitzung I

Time: Monday 17:30–19:00 Location: P5

MM 12.1 Mon 17:30 P5

Molecular dynamics studies on amorphous CuTi nanoparticles — •Susanne Fichtner and S.G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

It is generally well established that physical properties of materials in reduced dimensions deviate from their macroscopic behavior – particularly due to surfaces and dimensionality. For metallic glasses influences on structure, mechanical properties and the glass transition have to be expected.

We employ classical molecular dynamics simulations using embedded atom method (EAM) potentials for the model glass, CuTi, to address the influence of dimensionality and open surfaces on structure. Starting from an amorphous CuTi cell, which is prepared by quenching from liquid, amorphous particles are prepared by cutting out clusters of various sizes, ranging from 1.4nm to 4nm. After relaxation at different temperatures, changes in the pair and angular distributions are followed. Influences of surfaces and dimensionality, as well as the underlying physical origins on the atomic scale are discussed.

This project is financially supported by the DFG - PAK 63.

MM 12.2 Mon 17:30 P5

Nonlinear effects of damping behavior and activation volume of metallic glasses below to above the glass transition temperature — •Moritz Schwabe, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The idea of a potential energy landscape (PEL) from Stillinger and Weber describes relaxation processes in two ways of stimulation: α-relaxations as a changeover to a new metabasin and β-relaxation as changes within the fine structure of the metabasin. External stress can vary these barriers as discussed by W.L. Johnson and K. Samwer. [1,2] With this background we analyzed creep- recovery measurements at constant temperature to investigate the damping behavior of amorphous PdCuSi below Tg. Furthermore we compare the relation of the glass transition temperature and the apparent activation volume for plastic deformation to external stress and temperature of the fragile glass former PdCuSi and the strong ZrAlCu. Then an exponential, multiplicative relationship of stress and temperature dependence can be suggested. [3] [1] P.G. Debenedetti and F.H. Stillinger, Nature, 2001, 410, 259 [2] W.L. Johnson and K. Samwer, Physical Review Letters, 2005, 95, 195501 [3] M. Schwabe, S. Küchemann, H. Wagner, D. Bedorf and K. Samwer, Journal of Non-Crystalline Solids, doi:10.1016/j.physletb.2003.10.071

MM 12.3 Mon 17:30 P5

Combined in-situ SAXS/WAXS and HRTEM Study on Crystallization of $(\mathrm{Cu}_{60}\mathrm{Co}_{40})_{1-x}\mathrm{Zr}_x$ Metallic Glasses — •B. Schwarz[1], U. Vainio[2], N. Mattern[1], S.W. Sohn[3], D. H. Kim[3], and J. Eckert[1] — [1]Leibniz-Institute IFW Dresden, Institute for Complex Materials — [2]HASYLAB at DESY, Hamburg — [3]Department of Metallurgical Engineering, Center for Noncrystalline Materials, Yonsei University, Seoul, South Korea

The binary Cu-Co system exhibits a metastable liquid-liquid miscibility gap and therefore the ternary Cu-Co-Zr system is a promising candidate to form phase separated glass-glass composites. In this work $(\mathrm{Cu}_{60}\mathrm{Co}_{40})_{1-x}\mathrm{Zr}_x$ metallic glasses with $x = 37$ and $x = 32$ were investigated by in-situ small-angle and wide-angle x-ray scattering (SAXS/WAXS) and differential scanning calorimetry (DSC). Certain heat treated samples were additionally investigated by high-resolution transmission electron microscopy (HRTEM). Even for $x = 32$ there are no indications for any kind of phase separation in the as-quenched state within experimental resolution, i.e. the critical temperature T_c for liquid-liquid phase separation has already decreased from 1556 K for binary $\mathrm{Cu}_{60}\mathrm{Co}_{40}$ to a temperature below the glass transition temperature $T_g = 762(5)K$ found for $(\mathrm{Cu}_{60}\mathrm{Co}_{40})_{68}\mathrm{Zr}_{32}$. Combined in-situ SAXS/WAXS and HRTEM investigations reveal that thermal annealing induces the formation of a composite consisting of nano crystallites embedded in an amorphous matrix.

nano

MM 12.4 Mon 17:30 P5

Combined in-situ SAXS/WAXS and HRTEM Study on Crystallization of $(\mathrm{Cu}_{60}\mathrm{Co}_{40})_{1-x}\mathrm{Zr}_x$ Metallic Glasses — •B. Schwarz[1], U. Vainio[2], N. Mattern[1], S.W. Sohn[3], D. H. Kim[3], and J. Eckert[1] — [1]Leibniz-Institute IFW Dresden, Institute for Complex Materials — [2]HASYLAB at DESY, Hamburg — [3]Department of Metallurgical Engineering, Center for Noncrystalline Materials, Yonsei University, Seoul, South Korea

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MM 12.5 Mon 17:30 P5

Combined in-situ SAXS/WAXS and HRTEM Study on Crystallization of $(\mathrm{Cu}_{60}\mathrm{Co}_{40})_{1-x}\mathrm{Zr}_x$ Metallic Glasses — •B. Schwarz[1], U. Vainio[2], N. Mattern[1], S.W. Sohn[3], D.H. Kim[3], and J. Eckert[1] — [1]Leibniz-Institute IFW Dresden, Institute for Complex Materials — [2]HASYLAB at DESY, Hamburg — [3]Department of Metallurgical Engineering, Center for Noncrystalline Materials, Yonsei University, Seoul, South Korea

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MM 12.6 Mon 17:30 P5

Investigation of the viscosity for Bi-Sn(Zn) liquid alloys — •Andriy Yakymovych, Oleg Volkov, and Petro Yakibchuk — Department of Metal Physics, Ivan Franko National University of Lviv, Lviv, Ukraine

In the present study we have determined the viscosity with use of expressions for a polydisperse hard-sphere fluid (theory) and the high-temperature viscometer (experiment). According to the used theory, we present atoms in binary metallic alloy as a mixture of two subsystems of polydisperse hard spheres which interacts each other via contact potential only. Such assumptions lead us to the fact that we can express viscosity of this system using analytical equations and integrals they contains can be presented by simple mathematic functions for well-defined size distributions of polydisperse particles or by simple numeric scheme in general. Studding different cases of size-distribution in one-component systems we found that viscosity limit (value of average hard sphere volume fraction when viscosity turns to infinity) slightly moves down to zero.

In this work we provide calculations for binary alloys and try to analyze our results by comparison them with real alloys. The experimental measurements were carried out by a torsional oscillation viscometer. The viscosity of Bi-Sn liquid alloys has been studied in the vicinity of eutectic concentration and in vicinity of the demixing curve for Bi-Zn system, respectively.

MM 12.7 Mon 17:30 P5

Vitreous tantalum oxide films on glassy tantalum thin film — •Michael Scheele, Kevin Stella, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Thin amorphous tantalum films are prepared on Si(111) substrates in a metallic glassy state. The amorphous monoatomic state of the film is characterized by X-ray diffraction studies. The glassy state leads to a negative **t**emperature **c**oefficient of the **r**esistivity (TCR) for low sample temperatures < 200 K which is attributed to incipient localization. Above 200 K a positive TCR is observed as expected for a normal Boltzmann transport regime. The glassy metal tantalum can be oxidized by an electrochemical method, forming a vitreous highly temperature stable tantalum oxide. These oxides can be used as an internal barrier in thin film electronic devices.

MM 12.8 Mon 17:30 P5

Interfacial tension and wetting at the liquid-liquid interface in Al-Bi, Al-In and Al-Pb monotectic alloys — •Ivan Kaban[1], Markus Köhler[2], Lorenz Ratke[2], Walter Hoyer[3], Norbert Mattern[1], and Jürgen Eckert[1] — [1]IFW Dresden, Institute for Complex Materials, P.O.B. 270116, D-01171 Dresden, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), D-51170 Köln, Germany — [3]Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany

Aluminium alloys with Bi, In or Pb are characterized by a large miscibility gap in the liquid state. They solidify at normal conditions into layered structures, which is the main shortcoming in a view of practical applications. A crucial role in the demixing process is played by the wetting, liquid-liquid interfacial energy and density difference of the coexistent liquid phases. In this contribution we present the results of the experimental investigations of the density, interfacial tension, and wetting of Al2O3, ZrO2 and TiB2 ceramics at the liquid-liquid interface in Al-Bi, Al-In and Al-Pb alloys. The wetting experiments suggest that Al2O3, ZrO2 and TiB2 particles could be used for the nucleation of a minority phase in the Al-In and Al-Pb immiscible alloys.

MM 12.9 Mon 17:30 P5

Investigation of Real Space Orbital Free Density Functional Theory for the Study of Large Systems — •Jade Mackay, Rainer Backofen, and Axel Voigt — Institute for Scientific Computing, Dresden, Deutschland

A frequently encountered issue in computational materials science is the balance of calculation size and accuracy. The accuracy of the popular Kohn-Sham DFT methods is very impressive. However, interest in systems consisting of tens of thousands, or millions of atoms is growing. Alongside the drive for larger systems, attention is being paid to the consideration of real space formulations. Such formulations have value not only in terms of performance for the study of non-periodic systems (surfaces, clusters, defects), but also when integration with macroscopic modelling is being considered. The Orbital Free DFT (OFDFT) approach of Thomas and Fermi has significant potential for the study of large systems, and readily facilitates a real space implementation. In this we work present results obtained from our implementation of a real space OFDFT formulation using the AMDiS parallel finite elements toolkit.

MM 12.10 Mon 17:30 P5

Generation of polarizable force fields for molecular dynamics simulations of metal oxide systems with long-range interactions — •Philipp Beck, Peter Brommer, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

The simulation of oxide systems is computationally much more demanding than that of metals or covalent materials due to long-range electrostatic interactions. We use the Wolf [1] direct, pairwise r^{-1} summation method with spherical truncation for Coulomb interactions and in addition extend it to dipolar interactions. The polarizable oxygen atoms are described with the Tangney-Scandalo [2] (TS) interaction force field where the dipole moments are determined by iteration to a self-consistent solution. After first simulation results [3] for microstructural and thermodynamic properties of silica with the original TS force field, we now present a method to develop polarizable force fields which reparametrize the potentials of the TS approach. The method can be applied to arbitrary metal oxides. Our results agree with experiment and former simulation issues, but reduce the simulation time dramatically due to the linear scaling properties of the Wolf summation.

[1] D. Wolf *et al.*, J. Chem. Phys. **110**, 8254 (1999).
[2] P. Tangney and S. Scandalo, J. Chem. Phys. **117**, 8898 (2002).
[3] P. Brommer, P. Beck, A. Chatzopoulos, F. Gähler, J. Roth and H.-R. Trebin, J. Chem. Phys. **132**, 194109 (2010).

MM 12.11 Mon 17:30 P5

Frozen phonon calculations confirm electron-phonon coupling in $\mathbf{Fe_{1-x}Co_xSi}$ — •Wilfried Wunderlich[1] and Dirk Menzel[2] — [1]Tokai University, Fac. Eng., Material Science Department, Kitakaname 4-1-1, 259-1292 Hiratsuka, Japan — [2]TU Braunschweig, Inst. f. Physik d. Kondensierten Materie, Mendelssohnstr. 3, 38106 Braunschweig, Germany

Thermoelectric measurements of the Seebeck voltage were performed on $Fe_{1-x}Co_xSi$ single crystals under large temperature gradient [1]. They show an increase of a positive Seebeck coefficient as a function of Co-concentration for $x < 0.05$ up to 0.2 mV/K and a decrease for $0.05 < x < 0.2$, and again an increase until $x < 0.5$ and a decrease for $x > 0.7$. The first increase is related to the semiconductor-metal transition, while the second increase around $x = 0.6$ corresponds to a paramagnetic ordering state and is discussed as caused by magnon-phonon-coupling. For each phonon mode several **q**-vector variants were generated, and using these frozen phonons DFT-GGA calculations using VASP were performed. The difference in bond-length spectrum in the presence of phonons changed the electronic bandstructure remarkably. Instead of the 200 meV wide band-gap in the case without phonons, flattening of the electronic bands and broadening of the DOS is observed. From these investigations the electron-phonon coupling constant can be derived.

[1] W. Wunderlich et al., Mater. Res. Soc. Symp. Proc. (2009) Vol. 1128-U01-10 pp. 1-6.

MM 12.12 Mon 17:30 P5

***Ab initio* calculation of variable saddle point energies for atom jumps in $\mathbf{L1_2}$ ordered $\mathbf{Ni_3Al}$** — •Martin Leitner[1,2], Doris Vogtenhuber[3], Raimund Podloucky[1], Wolfgang Pfeiler[2], and Wolfgang Püschl[2] — [1]University of Vienna, Faculty of Chemistry, Department of Physical Chemistry — [2]University of Vienna, Faculty of Physics, Department Dynamics of Condensed Systems — [3]University of Vienna, Faculty of Physics, Department of Computational Materials Science

Kinetic Monte-Carlo simulation (KMC) in alloys is as good as the jump frequencies provided. According to transition state theory they are determined by a Boltzmann factor with the energy barrier to be surmounted, which is the difference between a saddle point and the initial state. This energy barrier explicitly depends on the atomic neighborhood of both states, especially on the configuration of the saddle point state. As an example for our arguments we take $L1_2$-ordered Ni_3Al. It represents a class of technologically interesting intermetallic compounds where the highly ordered state leads to favorable properties (high-temperature strength, corrosion resistance,...). As in all fcc-type structures, atoms which jump into a nearest neighbor vacancy have to pass a four-atom window of common nearest neighbors. We discuss the substantial influence of the occupancy of this window on jump probabilities. For a classification of jump types, energy profiles were calculated from *ab initio* by using the VASP code. These results were entered into example KMC-simulations, demonstrating the large impact of variable saddle point energies on overall and detailed kinetics.

MM 12.13 Mon 17:30 P5

$\mathbf{FeN_4}$ defects in carbon nanostructures: a comparative study with Fe-porphyrin and Fe-phthalocyanine molecules. — •Ingrid Ibagon[1] and Hélio Chacham[2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Deutschland — [2]Universidade Federal de Minas Gerais, Belo Horozinte, Brazil

In this work we conducted a comparitive study between the Fe-porphyrin and Fe-phthalocyanine molecules and carbon nanostructures with FeN_4 defects using first principles calculations based on the Density Functional Theory. For all systems, we performed calculations varying the total charge. In the case of Fe-porphyrin and Fe-phthalocyanines we studied the neutral systems and those resulting from the addition or remotion of one electron and, in the case of the carbon nanostructures we added a quantity of charge per carbon atom equivalent to each case studied for the molecules. We observed a tendency of the iron atom to maintain its charge constant when the total charge of the system changes, while the spin magnetic moment of the system changes with the total charge. The systems have spin magnetic moment equal to $2\mu_B$ when they are neutral, but it increases (decreases) when electrons are removed (added) from (to) the system.

MM 12.14 Mon 17:30 P5

Preliminary theoretical results on the solubility of ZnO — •Svea Sauer, Susan Köppen, Lucio Colombi Ciacchi, Christof Köhler, and Thomas Frauenheim — Bremen Center for Computational Materials Science, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany

The toxicity of zinc oxide nanoparticles towards macrophage and epithelial cells is directly linked to their solubility in the surrounding solute. In this context a higher solubility was found for nanoparticles dissolved in cell culture media compared to nanoparticles in pure water [1]. Therefore it is crucial to understand the interactions at the solid-water interface that lead to the particle dissolution. Our work puts a focus on the adsorption of different ions on the (10-10) zinc oxide surface in an aqueous environment. The employed ions range from simple anions to more complex molecules like dihydrogen phosphate. Ab-initio Molecular Dynamics simulations using a (4x2) slab model with a pre-adsorbed water layer are carried out in order to investigate the adsorption geometries. To simulate the dissolution of single Zn-atoms from the surface in the presence of different adsorbates a Metadynamics approach as implemented in CPMD is chosen. As the starting point we chose the dissolution of a single Zn-atom from the surface in the absence of adsorbed ions. Preliminary results are shown.

[1]T. Xia et al. ACS Nano 2(10), 2121 (2008)

MM 12.15 Mon 17:30 P5

Structures of metal electrodes at the solid-liquid interface studied by density functional theory — •Xiaohang Lin — Institut für Theoretische Chemie of Universität Ulm, Ulm

Recently, the operation of an electrochemical atomic-scale quantum conductance switch has been demonstrated, which is controlled by an external electrochemical voltage applied to an independent third gate electrode [1]. However, the microscopic processes underlying this atomic switch are still unclear. Using density functional theory (DFT) calculations, we have addressed the structure of Ag and Pb metal surfaces which are both used as electrode materials for the switch. We have considered the presence of water layers and the self-diffusion on flat and stepped metal surfaces in order to contribute to the understanding of electrodeposition. We find that the substantial difference in the lattice constants between Ag and Pb leads to significant changes, as far as the stable water structure at the metal-water interface is concerned. With respect to the metal diffusion, the DFT results indicate that exchange processes can have considerably lower barriers than hopping processes.

MM 12.16 Mon 17:30 P5

A variable charge transfer model for the molecular dynamics code IMD — •Andreas Chatzopoulos and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

For the efficient simulation of solids which contain electric charges and dipole moments and where, hence, the atoms interact by long-range forces, suitable algorithms must be developed. Examples are oxides or metal-oxide interfaces. For this purpose, our molecular dynamics code IMD[1] was enlarged by a dynamic charge transfer model according to Streitz and Mintmire (SM)[2].

In the model of SM the electrostatic energy contains the charges in second order. The charges are determined by minimization of this energy, taking the constraint of charge neutrality into account. In contrast to SM we solve the minimization by the conjugate gradient method. The long-range interactions are handled by the Wolf summation method[3].

[1] J. Stadler et al. *Int. J. Mod. Phys. C* 8, 1131, 1995.

[2] F. H. Streitz and J. W. Mintmire *Phys. Rev. B*, 50(16): 11996-12003, 1994.

[3] D. Wolf et al. *J. Chem. Phys.*, 110(17): 8254-8282, 1999.

MM 12.17 Mon 17:30 P5

Modellierung digitaler Kornmikrostrukturen — •Stefan Schäfer und Dana Zöllner — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Eine Methode zur Generierung digitaler Kornmikrostrukturen polykristalliner Materialen wird vorgestellt. Basierend auf dem Problem der Kreispackungen in zwei Dimensionen wurde ein Algorithmus entwickelt, der eine dichte Kreislagerung generiert, die einer vorgegebenen Größenverteilung folgt. Die daraus entwickelten Mikrostrukturen auf Kornebene wurden bezüglich der Homogenität metrischer und geometrischer Parameter untersucht. Der Generierungsalgorithmus ist dabei so gestaltet worden, dass einer Erweiterung auf drei Dimensionen problemlos möglich ist.

Anschließend wurden ausgewählte Korngefüge, die jeweils einer anderen Verteilungsfunktion folgen, Kornwachstum mithilfe der Monte Carlo Potts Modell Simulation unterworfen. Besonderes Augenmerk lag dabei auf dem frühen Zeitraum des Wachstums, der dem quasistationären Zustand normalen Kornwachstums vorangeht. Es wurde festgestellt, dass durch geeignete Parameterwahl Mikrostrukturen so erzeugt werden können, dass sie dem späten selbstähnlichen Wachstumsregime der Simulation entsprechen.

MM 12.18 Mon 17:30 P5

Cluster Expansion study of $\mathbf{Fe}_x\mathbf{Ni}_y\mathbf{Al}_{1-x-y}$ alloys — •Georg Kastlunger, David Reith, Markus Stöhr, and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

Cluster expansion (CE) is the state of the art tool to derive concentration dependent properties of alloys with the precision of density functional theory calculations. In this work we apply CE for a ternary system to study thermodynamical phase stabilities for $\mathrm{Fe}_x\mathrm{Ni}_y\mathrm{Al}_{1-x-y}$ alloys crystallizing in bcc-based structures. For studying Ni-Al precipitations in Fe (steel) the concentration range was defined correspondingly. On the basis of DFT total energy calculations for about 350 compounds we derived the effective cluster interaction energies (ECI) by a genetic algorithm employing the UNCLE (UNiversal CLuster Expansion) code[1]. After an extensive ground state search the stable phases and their convex free energy hull were identified. For constructing the phase diagram at finite temperatures the converged ECIs were used in both, canonical and grand-canonical Monte-Carlo simulations.

[1] D. Lerch, O. Wieckhorst, G.L.W. Hart, R.W. Forcade, and S. Müller, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009).

MM 12.19 Mon 17:30 P5

Molecular dynamics simulations of tensile tests in $\mathbf{Al_2O_3}$ with new polarizable force field — •Stephen Hocker[1], Philipp Beck[2], Siegfried Schmauder[1], and Hans-Rainer Trebin[2] — [1]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre, Universität Stuttgart, Germany — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

We apply the force matching method to generate a potential for molecular dynamics simulations of $\mathrm{Al_2O_3}$. The Wolf summation method is used for Coulomb interactions. In contrary to previous potentials the polarizability of oxygen atoms is taken into account by iteration to a self-consistent solution of the dipole moments. The potential is optimized to reproduce the forces in relaxed and strained $\mathrm{Al_2O_3}$ configurations. We apply the developed potential to simulate tensile tests of $\mathrm{Al_2O_3}$ with (0001), $(10\bar{1}0)$ and $(11\bar{2}0)$ tension axes. Stress strain curves are compared with ab initio results and previous molecular dynamics simulation results of $\mathrm{Al_2O_3}$.

MM 12.20 Mon 17:30 P5

Phonon Contribution to the Thermodynamics of Pure and Mixed Clusters in bcc-Fe — •Mina Talati[1], Matthias Posselt[1], Giovanni Bonny[2], Ahmed Tamer Al-Motasem[1], and Frank Bergner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O.Box 510119, D-01314 Dresden, Germany — [2]Nuclear Materials Science Institute, SCK-CEN, Boeretang 200, B-2400 Mol, Belgium

The irradiation-enhanced nanostructural evolution in reactor pressure vessel steels is a multiscale phenomenon. It can be effectively studied by rate theory for which necessary parameters must be obtained through atomistic simulations. The present work focuses on the phonon contribution to the thermodynamics of nanoclusters consisting of vacancy and/or Cu. In all calculations the most recent Fe-Cu interatomic potential developed by Pasianot and Malerba is employed. The vibrational density of states determined by the dynamical matrix method is used to calculate the phonon contribution to free energy of formation and free binding energy of the clusters. Pure bcc-Fe and pure fcc-Cu are used as references in the calculation of the free energy of formation. The vibrational contribution to the total free energy of these metals determined in this work is compared with available CALPHAD data and with literature data obtained by first-principle methods or interatomic potentials. In the case of pure vacancy clusters and for many mixed vacancy-Cu clusters the absolute value of the total free binding energy decreases with increasing temperature. Pure Cu clusters show the opposite behavior.

MM 12.21 Mon 17:30 P5

Electronic Structure of the Doped fcc- C60 Compound of Solid fcc-C60: Ab Initio Calculations — •Samaneh Javanbakht[1] and Saied Jalali Asadabadi[2] — [1]Department of Physics, Faculty of Science, University of Isfahan (UI), Isfahan 81744, Iran — [2]Department of Physics, Faculty of Science, University of Isfahan (UI), Isfahan 81744, Iran

Electronic and structural properties were calculated for the fcc-C60 compound. The calculations were performed within the density functional theory (DFT) employing the augmented plane waves plus local orbital (APW+lo) method as implemented in the WIEN2k code. The C60 clusters were then positioned on the lattice sites of the fcc taking into account the highest symmetry. The carbon atoms were fully relaxed to minimize the interatomic forces. Single and double bond lengths were then calculated using the relaxed atomic positions. Total density of states (DOS) was calculated. We also doped an additional carbon atom as an impurity into the C60 clusters. Recalculating the bonds of this doped structure, we observed that the distinction between double and single bonds becomes less important as charge transfer proceeds in the fcc crystal. Moreover; we have calculated the bang gap of fcc-C@C60,and we realized that it is reduced incredibly.

MM 12.22 Mon 17:30 P5

Extending the Cluster Expansion by vibrational free energies — •David Reith, Markus Stöhr, and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

The Cluster Expansion technique allows to carry over the precision of density functional theory (DFT) calculations to systems consisting of 10^6 - 10^9 atoms [1]. It is based on DFT total energies of properly chosen input structures with a common basic lattice. The effective cluster interaction energies (ECI) are derived from CE fitting criteria and then enter into Monte Carlo (MC) simulations for e.g. deriving phase boundaries. By adding vibrational free energies to DFT total energies the ECIs become temperature dependent which strongly influences the CE+MC treatment. The temperature dependent extension of CE is demonstrated on the binary $\mathrm{Fe}_{1-x}\mathrm{C}_x$ alloy system, for which it turns out that including the vibrational free entropy strongly increases the solubility of Cu in Fe-rich (steel) alloys. We discuss the complications and strategies which have to be followed for deriving the ECIs and for combining CE with temperature dependent ECIs and MC. For the CE+MC calculations we used the UNCLE code [1] and a direct force constant approach for deriving the phonon spectra [2] for each of the DFT input structures.

[1] D. Lerch, O. Wieckhorst, G.L.W. Hart, R.W. Forcade, and S. Müller, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009).

[2] D. Reith, program package fPHON based on PHON by D. Alfè, 1998.

MM 12.23 Mon 17:30 P5

Molecular dynamics simulations of femtosecond laser ablation in copper — •Carolina Trichet Paredes, Steffen Sonntag, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

Femtosecond laser ablation of copper is investigated by using a hybrid simulation scheme. Two equations are solved simultaneously: One for the electronic system, which accounts for laser energy absorption and heat conduction, the other for the dynamics of the lattice where the ablation process takes place. For the electron-temperature a generalized heat-conduction equation is solved by applying a finite difference scheme. For the lattice properties, e.g. pressure, density or temperature, we use common molecular dynamics. Energy transfer between the subsystems is allowed by introducing an electron-phonon coupling term.

Spallation instead of ablation as a ruling phenomenon for thin copper films of various thicknesses was observed. However, it will be shown that the heat conduction plays a crucial role: By changing its value a transition from spallation to ablation occurs. Besides, the ablation rates and cluster size distribution of the ablated material will be compared to recent experiments.

MM 12.24 Mon 17:30 P5

Heat capacity of aluminum nitride phases from *ab initio* calculations — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The ability to calculate thermodynamical material properties on *ab initio* level is an important preliminary for the accurate prediction of phase diagrams.

We present results on the heat capacity of the wurtzite and rocksalt phases of aluminum nitride. The isochoric heat capacity C_V is obtained from harmonic phonon calculations using density functional perturbation theory. In the quasi-harmonic approximation, the isobaric heat capacity C_p is then obtained from C_V via the thermal expansion coefficient. The latter is calculated (i) directly from the mode Grüneisen parameters using phonon calculations at several volumes and (ii) estimated from molecular dynamics.

We would like to thank the DFG for financial support within the DFG Priority Program 1236: *Strukturen und Eigenschaften von Kristallen bei extrem hohen Drücken und Temperaturen*

MM 12.25 Mon 17:30 P5

Density functional theory study of LO-TO splitting of vibrational modes of insulating compounds — •Marcel Hieckel, David Reith, and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

We present results of density functional theory (DFT) calculations for vibrational properties of insulating compounds derived by the force constant method [1]. For the exchange-correlation functional the generalized gradient approximation as well as a hybrid functional were used. The LO-TO splitting in ionic solids is due to the long range Coulomb interactions which is caused by the coupling of atomic displacements to the thus generated electrostatic field [2]. The modelling is based on an additional nonanalytic term to the dynamical matrix which depends on the Born effective charges and the dielectric constant whose tensors are derived from DFT calculations of the macroscopic electronic polarization [3]. The results for nonmagnetic ionic compounds are as well as for the transition metal oxides MnO and NiO are presented and compared to experiment. [1] D. Reith, program package fPHON based on PHON by D. Alfè, 1998. [2] M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford University Press, 1954. [3] R.W. Nunes and X. Gonze, Xavier, Phys. Rev. B **63**, 155107 (2001).

MM 12.26 Mon 17:30 P5

Comparative analysis of hydrogen-vacancy interactions in Mg and Al based on density functional theory — •Lars Ismer[1], Min Sik Park[2], Anderson Janotti[1], and Chris G Van de Walle[1] — [1]University of California at Santa Barbara, CA 93106 — [2]Missouri University of Science and Technology, Rolla, MO 65409

For hydrogen storage in metals the presence of vacancies in the bulk of the metal and their interactions with atomic hydrogen (H) plays an important role. Using density functional theory we have studied the H-vacancy interactions in hcp-Mg and fcc-Al, two prototypic systems for H storage. We show that a single vacancy can host up to 9 H atoms in Mg and 10 in Al. In going beyond previous theoretical studies we evaluate the concentration of the H-vacancy complexes for different H loading conditions, ranging from low pressures to high pressures of H2 gas. We find strong differences between Mg and Al. In the case of Al, up to 15 % of H atoms are trapped in single vacancies even for very low H pressures, which slows down the diffusion of H atoms. In the case of Mg, these trapping effects are negligible for low H pressures. However, vacancies containing multiple H atoms and H-induced superabundant vacancy formation are predicted to occur in Mg at much lower H loading pressures (about 1 GPa) than in Al (about 10 GPa).

MM 12.27 Mon 17:30 P5

$\mathrm{LAMMPS}_{\mathrm{CUDA}}$ - A general purpose MD code — •Christian Trott and Lars Winterfeld — Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany.

Molecular dynamics (MD) simulations are one of the most common computational methods to explore the structure and dynamics of condensed matter systems. They form the basis for investigating many types of materials, ranging from simple atomic liquids, over metal systems to bio-molecules. The advent of easily programmable graphic card processors (GPUs) allows for the development of new codes, which increased the potential workstation performance by more than an order of magnitude. Most of the codes though, are of limited capabilities compared to the well established MD packages like LAMMPS and NAMD. We present our own code, $\text{LAMMPS}_{\text{CUDA}}$ (`www.tu-ilmenau.de/lammpscuda`), which aims at providing GPU support for the full LAMMPS functionality. Besides useability and scope of features the main focus of $\text{LAMMPS}_{\text{CUDA}}$ is to provide good scaling behavior on GPU based supercomputers such as the Japanese 7168 GPU Supercomputer Tsubame 2.0 (rank 4 in the 2011 TOP500 list of supercomputers). As a result of our development efforts, $\text{LAMMPS}_{\text{CUDA}}$ allows for the effective parallel usage of hundreds of GPUs for a single simulation. We present details of the implementation, benchmarks for various material classes such as inorganic glasses, metals and bio-molecules and an investigation of the scaling behavior of $\text{LAMMPS}_{\text{CUDA}}$ with varying system size and number of GPUs.

MM 12.28 Mon 17:30 P5

Construction of High-Dimensional Neural Network Potentials Based on Atomic Pairs — •Jovan Jose Kochumannil Varghese and Jörg Behler — Ruhr-Universität Bochum, D-44780 Bochum

An accurate description of the interatomic potential is the crucial step in theoretical simulations. Consequently, a large number of potentials of varying form and complexity has been reported in the literature. Still, for some systems the accuracy that can be achieved is not satisfying. Artificial Neural Networks (NN) have become a promising new tool for the construction of efficient and accurate potentials due to their flexible functional form. We present a new high-dimensional NN approach based on an expansion of the total energy in terms of environment-dependent atom pairs. The advantages and drawbacks of this approach are discussed and compared to the alternative approach employing a summation of atomic energy contributions.

MM 12.29 Mon 17:30 P5

The solubility of carbon in bcc iron under volumetric strain: comparison of DFT and empirical methods — Elisaveta Hristova, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, Germany

With the aim of investigating the interaction of C with dislocations in Fe by large scale molecular dynamics, we evaluate the transferability of different semi-empirical potentials. As a test case the carbon solubility in bcc Fe as a function of lattice strain is studied by ab-initio calculations based on density-functional theory (DFT) and by four different empirical potentials of the embedded-atom method as (EAM) well as the modified EAM (MEAM). Both DFT and (all but one) empirical potential calculations predict that the carbon solubility increases with increasing volumetric strain, up to the maximum applied strain of five percent. However, the enthalpy of formation for this interstitital defect remains positive throughout the whole range of strains. Interestingly, the enthalpy of formation obtained by DFT is much more strain-sensitive than the one obtained by the empirical potentials. The different description of the carbon solubility in the presence of strain fields by the four empirical potentials is due to different parametrization, construction and fitting of the EAM potentials, and in the case of the MEAM to the different formalism including angular dependent bonding.

MM 12.30 Mon 17:30 P5

Efficient ab-initio characterisation of the parameter space of grain boundaries — Naveed Ahmed, Xueyong Pang, Christian Kellermann, •Rebecca Janisch, Holger Dette, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, Germany

A grain boundary is characterised by at least five macroscopic and three microscopic degrees of freedom, the orientation of the grain boundary plane, the misorientation axis and the misorientation angle, as well as the interface translation state. At the same time, continuum modeling of polycrystals requires knowledge of the elastic and plastic properties of all kind of interfaces in their microstructure. To capture the physics of grain boundary sliding, migration and decohesion, these processes should be investigated by atomistic calculations. Especially if the influence of segregated impurities, which can alter the bond character, shall also be described, a quantum mechanical treatment is necessary. However, sampling the above mentioned parameter space ab initio remains a formidable task, even with today's computers. In this paper we will introduce our investigation of the mechanical properties of grain boundaries in aluminum, which aims at replacing such a comprehensive sampling by as few representative calculations as possible. For this we are evaluating a "design of experiment scheme" combined with insight on the role of crystallography that we gain from our ab-initio calculations: On the one hand we are investigating discriminating features in the elastic and plastic response of tilt and twist grain boundaries. On the other hand we are looking for common behaviour that enables a unified treatment and a separation of variables.

MM 12.31 Mon 17:30 P5

Molecular Dynamics Simulations on Carbon Nanoclusters — •Andrew Aird and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

Bulk- as well as nanodiamonds containing impurities are promising candidates for a broad range of applications (quantum computing, magnetometry). A positioning accuracy on the nanometer scale and very small, nanometer sized diamonds containing stable defects are prerequisites. Nowadays, molecular dynamics (MD-) simulations allow the atomistic description of devices with system sizes in the range of 10-100 nm. Using MD simulations together with potentials to describe covalent materials, carbon clusters with and without defects are investigated. The effect of external mechanical as well as kinetic stress on the structure and stability of the nanodiamonds are of special interest. In addition, low energy implantation processes of nitrogen into bulk- as well as nanodiamonds are explored. The main goal is to optimize these processes with respect to requested target structures.

MM 12.32 Mon 17:30 P5

Quantitative study of the effect of local ordering on the growth kinetics of metallic alloys — M. Guerdane[1], B. Nestler[1], and •H. Teichler[2] — [1]Institute of Reliability of Components and Systems, Karlsruhe Institute of Technology (KIT) — [2]Institute for Materials Physics, University of Göttingen

We illustrate how local ordering in a metallic melt (NiZr) can transform into a massive in-plane ordering at the surface of a crystal (bcc Zr) when commensurablity is given between the solute-centered clusters of the melt and the periodic potential of the crystal surface for a given orientation. Combined molecular dynamics and phase-field simulations allow to estimate quantitatively the influence of the surface effect on the growth kinetics. This study provides a more complete understanding of the relation between the undercooling ability (e.g. in the case of glass forming alloys) and the pronounced local ordering in the melt.

MM 12.33 Mon 17:30 P5

A study of ice crystal growth based on diffuse interface modeling using extended anisotropy formulations — •Marcel Huber, Frank Wendler, and Britta Nestler — Institute of Materials and Processes, Karlsruhe University of Applied Science, Moltkestr. 30, 76133 Karlsruhe, Germany

Though a phenomenon of daily experience, the precise description of ice crystal growth is still lacking. Progress in technical application like ice slurry for cooling, cryodesiccation and freeze casting process in the synthesis of porous ceramics motivate further research. In this work we study equilibrium and off-equilibrium growth of ice crystals in pure water. The solid interfaces evolve due to an interplay of a driving force (pressure change or undercooling) and interface anisotropies with a normal velocity depending on chemical potential, kinetic coefficient and surface stiffness. To define the location of each ice-crystal (of different orientation) and the phase in the computational domain, we introduce non-conserved order parameters, so that the equation for the velocity can implicitly be solved by using a phase-field model of Allen-Cahn type. We pay special attention to the definition of an adequate anisotropy formulation for interface energies and kinetics. We present numerical studies of various formulations including expansions with respect to cubic harmonics and compare the resulting growth shapes under equilibrium conditions to experimental observation. Using these findings, simulations of strongly undercooled dendritic growth of ice are carried out, where the thermal field is also solved in the domain to account for the transport of latent heat.

MM 12.34 Mon 17:30 P5

Phocphate Crystallisation — •Paul Schneider, Andreas Erbe, and Frank Renner — Max-Planck-Institut für Eisenforschung, Düsseldorf, Deutschland

Chemical reactions forming surface coatings are an important way to protect metals against environmental attack. Besides the relevance for applications, there is a considerable fundamental interest in the nucleation of crystals on surfaces in complex environments. As modern steels contain silicon and aluminium as elements forming passive layers, phosphate crystal growth under acidic conditions on surfaces of aluminium, silicon, and steels containing silicon and aluminium has been investigated. Different fluoride treatments were employed. On Silicon(100) with native oxide layer, a strong etching of pits was observed, with only few phosphate crystals formed on the surface. Results on a steel with aluminium/silicon coating also show a strong etching, and deposition of fluorides on the surface. Differences between pure aluminium and silicon on the one and surfaces in which aluminium and silicon coexists are attributed to the coexistence of metallic and semiconducting crystalline structures in the initial surface. Such coexistence leads to a substantial modification of the pickling attack.

MM 12.35 Mon 17:30 P5

Impact of Ni on degradation of 8.5 mol% Y_2O_3-doped ZrO_2 (8YDZ) — •Benjamin Butz[1], Andreas Lefarth[2], Heike Störmer[2], Annika Utz[3], and Dagmar Gerthsen[2] — [1]CENEM, Universität Erlangen-Nürnberg — [2]Laboratorium für Elektronenmikroskopie, Karlsruhe Institut für Technology (KIT) — [3]Institut für Werkstoffe der Elektrotechnik, KIT

The efficiency of solid oxide fuel cells is influenced by the electrochemical performance of the anode (8YDZ/Ni composite). One criterion is the ionic conductivity of the 8YDZ. Pure 8YDZ degrades by 40 % (950°C) within thousands of hours due to the decomposition on the nanoscale. Moreover, the degradation of 8YDZ in the presence of Ni proceeds 50 times faster. To clarify this, NiO thin films were deposited onto 8YDZ substrates by electron-beam evaporation. Sintering (1400 °C, 5 h, air) facilitated the incorporation of Ni into the 8YDZ. The influence of annealing under reducing conditions (950 °C) was studied by transmission electron microscopy. The decreased solubility of Ni in 8YDZ under reducing atmosphere led to the nucleation and growth of Ni crystallites within the 8YDZ. Typical chemical variations on the nanoscale after degradation were revealed by analytical TEM techniques (FEI Titan 80-300 microscope). The enhancement of the cation mobility and thus the accelerated decomposition of 8YDZ are explained by the electron capture of dissolved Ni under reducing atmosphere. The strain field due to the increase in size ($r_{\mathrm{Ni}^{2+}}$=69 pm, r_{Ni^0}=125 pm) leads to larger displacements of the surrounding ions, which effects the diffusivity of ions in the vicinity of the exsolving Ni.

MM 12.36 Mon 17:30 P5

Theoretical and experimental structure analysis of the (1 0 -1 -1) ZnO twin boundary — •Viktor Hrkac[1], Viola Duppel[2], Yogendra Kumar Mishra[3], Rainer Adelung[3], and Lorenz Kienle[1] — [1]Synthesis and Real Structure, Institute for Materials Science, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart — [3]Functional Nanomaterials, Institute for Materials Science, CAU Kiel, Kaiserstr. 2, 24143 Kiel

The II-VI semiconductor zinc oxide (ZnO) has been the subject of intensive research due to its wide spectrum of properties which results in a plethora of applications including optoelectronic and piezoelectric technologies. In particular, the morphology and thereby the physical properties of ZnO are significantly affected through defect structures induced by twinning. Thus, a comprehensive understanding of twin interfaces is a pivotal for a future optimization of controlling and device performance. Based on analytical electron microscopic observations, a three dimensional model of the (1 0 -1 -1) twin boundary interface is derived which allows a convincing simulation of experimental micrographs. In addition, dynamic effects at the twin interface can be studied in simulated diffraction patterns via the model. The authors would like to thank the DFG for funding via the SFB 855.

MM 12.37 Mon 17:30 P5

Characterization of Complex Structures by means of Precession Electron Diffraction — Ulrich Schürmann[1], Viola Duppel[2], Saskia Buller[3], Wolfgang Bensch[3], and •Lorenz Kienle[1] — [1]Synthesis and Real Structure, Christian Albrechts University, Kaiserstr. 2, D-24143 Kiel, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [3]Institute of Inorganic Chemistry, Christian Albrechts University, Max-Eyth-Straße. 2, D-24118 Kiel, Germany

Precession electron diffraction (PED) became a versatile tool for the advanced characterization of nanoscaled materials in the last years. The determination of the space group of a material is complicated when applying selected area electron diffraction (SAED) since the zonal and serial reflection conditions are often violated by multiple scattering. This effect can be reduced via PED, so the resulting patterns reflect those which are based on the kinematic approximation. Due to the less dynamic intensity the Laue symmetries and the space groups of the crystals can be determined fast and reliably and enables the ab-initio structure determination of unknown nanoscaled materials. Also the PED gives 3D structural information, e.g. about disorder. An experimental breakthrough related to the PED technique is revealed by the analysis of extremely electron beam sensitive samples like intermetallic phases with melting points around 100 °C. PED is also suitable for the characterization of homologous structures based on variable sequences of building units like in Phase Change Materials (PCM). Financial support by the DFG in the SPP1386 is gratefully acknowledged.

MM 12.38 Mon 17:30 P5

Transmission Electron Microscopy Studies along the Process Chain of Printable Electronics based on Nanoparticulate Systems — •Stefanie Spallek, Benjamin Butz, and Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy (CENEM), Department of Materials Science, University of Erlangen-Nuremberg, Germany

Printable electronics based on nanoparticulate systems is a highly active research field due to its enormous economical potential. The goal is to develop routes for fabrication of electronic and optoelectronic devices on flexible substrates by cheap and scalable printing techniques that use inks (or pastes) containing conducting or semiconducting nanoparticles. The performance of the final device critically depends on each step of the process chain which comprises synthesis of the nanoparticles, their functionalization and dispersion to printing pastes, the fabrication of the devices and possible after-treatments. The structural properties that influence the device performance include the shape and size distribution of the nanoparticles after synthesis, their 3D arrangement and interconnection in the functional layers as well as defects that may be introduced at various steps of the fabrication. In this contribution we show several examples of TEM studies along the process chain of printable electronic devices as well as the challenges of the corresponding sample preparation.

MM 12.39 Mon 17:30 P5

Characterization of ex-situ heated Fe70Pd30 thick films using TEM and STEM techniques — •Andriy Lotnyk[1], Christoph Bechtold[2], Burak Erkartal[1], Lorenz Kienle[1], and Eckhard Quandt[2] — [1]Synthesis and Real Structure, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Inorganic Functional Materials, CAU Kiel, Kaiserstr. 2, 24143 Kiel

The phase transformations in the system Fe-Pd were mostly studied on bulk samples. However, the structural evolutions of Fe-Pd films at the composition of Fe70Pd30 are less examined. Here, Fe70Pd30 films with a thickness of 1-5 micrometer were produced by magnetron sputtering on thermally oxidized Si substrates and on a (001)-oriented MgO substrate. Before deposition, the Si substrates were covered by Au layers for obtaining freestanding films while for the MgO substrate, a Cr/Rh layer was used to enhance epitaxial growth of Fe70Pd30. Polycrystalline bcc Fe70Pd30 films were formed on Si while an epitaxial bct Fe70Pd30 film was grown on MgO. The obtained films were ex-situ heated at 650 °C and at 850 °C for 30 min. After heating of the freestanding bcc Fe70Pd30 film at 650 °C, a film containing the fcc Fe60Pd40 and Fe-rich grains was observed while the transformation from bcc to fcc Fe70Pd30 was found for the films heated at 850 °C. The latter films are decomposing into a Fe-Pd alloy with composition close to 70:30 and Fe-rich precipitates. Heating of the epitaxial bct Fe70Pd30 film at 850 °C also leads to the formation of the fcc structure, however, in this case Fe diffused into MgO and a dissolution of Rh into the Fe70Pd30 phase was observed.

MM 12.40 Mon 17:30 P5

Structural analysis of severly deformed Ni_3Ge — •Andreas Grill, Hans-Peter Karnthaler, and Christian Rentenberger — Physics of nanostructured Materials, University of Vienna, Boltzmanngasse 5, 1090 Wien

Single crystals of the $L1_2$ ordered intermetallic compound Ni_3Ge were severely plastically deformed by high pressure torsion (HPT) and studied by transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron backscattered diffraction and differential scanning calorimetry (DSC). The deformation leads to the formation of nanocrystalline bands (5 to 30 μm wide) that are mainly occurring in regions within 100 μm near the top and bottom surface of the HPT disc. This structural inhomogeneity is shown by SEM images and studied in detail by TEM of focussed ion beam specimens. The analysis shows three different structures occurring next to each other: (i) a highly deformed single crystalline matrix, (ii) a textured nanocrystalline structure inside of the bands and (iii) a nanocrystalline structure with little texture near the surface of the bands in a region of about 3 μm thickness. The grain sizes in the nanocrystalline areas are about 20 nm. The average grade of disordering was investigated by DSC showing an ordering peak at 594 K; with increasing deformation the corresponding values of the enthalpies increase between 10 and 26 J/g. This result agrees with the deformation induced increase of density of bands, that show a much higher degree of disorder than the matrix as resulting from the TEM study.

MM 12.41 Mon 17:30 P5

3D imaging and characterisation of strengthening particles in Inconel 718 using FIB tomography — •Adam Kruk, Adam Gruszczyński, and Aleksandra Czyrska-Filemonowicz — AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Al. A. Mickiewicza 30, 30-059 Kraków, Poland

The Inconel 718 is a commercial nickel-base superalloy, widely used for critical pieces in turbine engines. Its microstructure consists of the γ matrix and strengthening coherent nanoparticles γ' and γ". In the present work FIB tomography technique was used for imaging and characterisation of strengthening particles. FIB tomography is based on a serial sectioning procedure using a FIB/SEM dual beam workstation. Repeated removal of layers as thin as several nm for some hundred times allows to investigate at total a volume of some μm3 with a voxel size as 2.5 nm x 2.5 nm x 2.5 nm. 3D mapping of nanoparticles with high Z-resolution by serial FIB slicing (in a distance of about 2.5 nm) and SEM imaging was performed. Ga ion beam at 30 kV was used to perform a precise in-situ milling. The SEM images at accelerating voltage 1.5 kV were taken with using ESB detector. The real 3D-data of precipitates obtained by FIB tomography, open a new possibility for microstructure analysis of materials for industrial applications.

MM 12.42 Mon 17:30 P5

Analytical transmission electron microscopy investigations of Sn-Pd nanoparticals with core-shell structures — •Dietrich Haeussler[1], Bernhard Schaffer[2,3,4], Fu Liu[1,5], Ferdinand Hofer[4], X. B. Zhang[5], and Wolfgang Jaeger[1] — [1]Microanalysis of Materials, Christian-Albrechts-University Kiel, 24143 Kiel, Germany — [2]SuperSTEM Facility, Daresbury Laboratory, Warrington, WA4 4AD, UK — [3]SUPA, School of Physics and Astronomy, University of Glasgow, UK — [4]Institute for Electron Microscopy, Graz University of Technology, 8010 Graz, Austria — [5]Department of Materials Science and Engineering, Zhejiang University, Hangzhou, 310037, China

Metallic core-shell nanoparticles for applications in catalysis and as data storage materials offer the possibility to tailor macroscopic properties generally not obtained by the single-component particles. We show for Pd-Sn nanoparticles that a combination of the analytical techniques of the spectrum-imaging mode with high-angle annular dark-field imaging in Cs-corrected high-resolution scanning transmission electron microscopy enable to precisely analyse and map structure, morphology, and chemical composition of the particles. Beneficial additional information about the particle structure is obtained from electron nanodiffraction patterns. Our analyses of a number of Sn-Pd particles with diameters as small as 20 nm reveal particles with Pd-rich cores and oxidized shells enriched in Sn as well as polycrystalline alloy particles. The study confirms that these methods are useful for monitoring reactions or degradation for composite nanoparticle materials.

MM 12.43 Mon 17:30 P5

Interface studies on carbon nanotubes grown from $Fe_{20}Ni_{80}$ catalysts particles — •Anja Kiessling, Darius Pohl, Christine Täschner, Mark Herrmann Rümmeli, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, D-01069 Dresden, Germany.

Hard-magnetically terminated carbon nanotubes (CNT) are of particular interest for applications in the field of nanotechnology. Recent results obtained on CNT which are grown from and terminated with FePt nanoparticles [1] imply that there is (i) an enrichment of Pt at the particle surface and (ii) an energetically favored facet from which the carbon is released in order to grow the CNT.

In order to further improve the understanding of the physical principles that govern the catalytic growth of the nanotubes, CNT were grown via plasma-enhanced chemical vapor deposition from Ni-rich $Fe_{20}Ni_{80}$ catalyst particles. Likewise prepared CNT are characterized by means of aberration-corrected high resolution transmission electron microscopy (HRTEM). Particular attention is paid to the question as to whether or not there is an indication for a segregation of one of the alloy constituents to the particle surface, as was previously observed in free FeNi particles of close to equi-atomic composition [2]. It is investigated, if there is a preference for the type of facet from which the CNT grow. For the case of CNT growth from Ni particles, MEAM studies indicate that the (111) facet is energetically favored here [3].

[1] F. Schäffel et al., Appl. Phys. Lett. 94 (2009) 193107/1-3. [2] B. Bieniek et al., J. Nanoparticle Res. (submitted). [3] W. Xiao et al., Surf. Sci. 603 (2009) 1985-1998.

MM 12.44 Mon 17:30 P5

Characterization of Al-Si alloy - TiB2 particles composite structure by STEM — •Justyna Grzonka[1], Tomasz Plocinski[1], Pedro Egizabal[2], and Krzysztof Kurzydlowski[1] — [1]Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland — [2]TECNALAI Foundation, San Sebastian, Spain

The paper describes results of structural characterization of an Al-Si alloy matrix composite reinforced with TiB2 particles produced by in situ reaction. The properties of such composites, developed for weight reducing and wear resistant applications, critically depend on the inter-phase boundaries between Al-Si alloy matrix and TiB2 particles.

In order to study Al-Si alloy - TiB2 inter-phase boundaries High Resolution Scanning Transmission Electron Microscopy (HRSTEM) was used. Samples representative of the material before and after thermal treatment were prepared using Focused Ion Beam technique (FIB). The Energy Dispersive X-ray Spectroscopy (EDS) was used to map the spatial distribution of the key chemical elements. Phase analyses were performed using X-ray and electron diffraction patterns.

The results of the investigations show that the Si and TiB2 particles do not change with the applied heat treatment. However, other particles appearing in the composite matrix do. In particular, the heat treatment results in formation of Al2O3 and magnesium oxide particles at the inter-phase boundaries between Al alloy and TiB2.

MM 12.45 Mon 17:30 P5

Characterization of Al-Si alloy - TiB2 particles composite structure by STEM — •Tomasz Plocinski[1], Justyna Grzonka[1], Pedro Egizabal[2], and Krzysztof Kurzydlowski[1] — [1]Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland — [2]INASMET Foundation, San Sebastian, Spain

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MM 12.46 Mon 17:30 P5

TEM diffraction used for 3D profile analysis of nanomaterials — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

Nanocrystalline FeAl was made by high pressure torsion deformation of the B2 ordered intermetallic compound Fe-45at.%Al. In this study it is shown that quantitative results for the 3D analysis of bulk nanocrystalline materials can be obtained using profile analysis of selected area diffraction patterns (PASAD). This method allows a quantitative local scale analysis of a wide range of nanomaterials. TEM diffraction patterns showing rings were recorded with a large range of tilting angles

(±52° along the shear direction). By applying different tilting angles of the incident beam, the morphology of the nanocrystallites was analysed by using the software PASAD-tools (www.univie.ac.at/pasad). It should be pointed out that because of the strong scattering factor in electron diffraction, the diffraction rings can be recorded in seconds thus allowing to cover a large range of tilting angles in a short time. To compare the results gained from diffraction patterns with those from direct images, TEM samples were cut out of the bulk samples to link them directly to the shear direction and to the shear plane. Both, planar and cross sections of nanocrystalline FeAl were investigated to study the shape and morphology of the nanocrystallites. The 3D reconstruction gained from the images of the different cuts agrees very well with the 3D results gained from the diffraction patterns.

MM 12.47 Mon 17:30 P5

Growth of nanosized ordered domains in nanocrystalline intermetallic FeAl studied by TEM methods — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

Severe plastic deformation of intermetallic compounds leads to the formation of a nanocrystalline structure that is frequently accompanied by a loss of the long range order. Up till now this has been monitored by X-ray methods; here it is shown that Transmission Electron Microscopy (TEM) is able to give additional insight. In this study TEM methods are used to reveal that high pressure torsion deformation of FeAl does not lead to a complete destruction of the chemical order B2. It leads to the formation of a structure of a medium range chemical order, composed by nanosized ordered domains of B2 structure (about 2 nm in size). Upon heating the long-range order is recurring by coarsening of the ordered nanodomains until they reach the grain size. The growth of the nanosized ordered domains is studied by using both TEM dark field images and TEM diffraction patterns. The quantitative evaluation of the diffraction ring patterns is carried out with the PASAD method (www.univie.ac.at/pasad). The results deduced from the images and those achieved by PASAD complement each other very well. Furthermore the present example shows that due to the strong scattering factor electron diffraction patterns can be used to evaluate very weak superlattice reflections.

MM 12.48 Mon 17:30 P5

A Method to Locally Determine Layer Dimensions and Interface Roughness for Multilayer Coatings with Ultimate Accuracy — •Dietrich Häussler[1], Ulrich Ross[1], Uwe Heidorn[2], Frank Hertlein[2], Jörg Wiesmann[2], and Wolfgang Jäger[1] — [1]Microanalysis of Materials, Christian-Albrechts-University of Kiel, 24143 Kiel, Germany — [2]Incoatec GmbH, 21502 Geesthacht, Germany

Multilayer coatings consisting of ultrathin bilayers on the nanometer scale are essential components of X-ray optics for advanced X-ray analytical equipment and for synchrotron beamlines. Their functionality is based on X-ray scattering from alternating amorphous layers of materials with differing atomic number Z. The development of those layer systems requires precise monitoring of layer thickness, layer periodicity and uniformity, and of interface quality on different length scales. We describe a method for locally determining layer dimensions and interface roughness of multilayer coatings with ultimate accuracy from intensity profiles obtained from high-angle annular dark-field (HAADF) scanning TEM investigations of multilayer cross-sections. Our procedure allows to obtain separate values for lateral interface roughness and interface broadening. For examples of specially designed W-C multilayer systems it is shown that the layer dimensions can be determined with sub-nanometer precision. Comparisons with spatially averaged data obtained from X-ray reflectivity measurements are in satisfactory agreement with our determination of roughness and layer dimensions. The method fails for heavily disturbed multilayer regions involving growth-induced thickness fluctuations.

MM 12.49 Mon 17:30 P5

Electron holography of Fe nanoparticles embedded in MgO crystals — •Dorin Geiger[1], Hannes Lichte[1], Artem Shalimov[2], and Kay Potzger[2] — [1]Technische Universitaet Dresden, ISP, Triebenberglabor, Zum Triebenberg 50, 01328 Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany

In Mg-oxide embedded iron nanoparticles [1] show relevant magnetic fields being epitaxially related to the surrounding matrix. Their properties as nano-dimensional objects can strongly differ from those of the macroscopic ones, due to large surface to volume ratios. They were synthesized by Fe$^+$ ion implantation at an energy of 100keV (incidence angle 7°) with varying fluences up to 3×10^{17} cm^2. Both alfa-Fe (body centered cubic) and gamma-Fe nanoparticles (face centered cubic) are formed in a surface layer of about 50nm thickness. The content of the alfa-Fe phase, which seems to be responsible for the magnetic behaviour, increases at higher fluences and after annealing [1].

To investigate the magnetic fields at nano-scale, off-axis electron holography was applied using a Cs-corrected transmission electron microscope (Tecnai F20 Cs-corr) [2] working in a pseudo Lorentz mode. This allows the reconstruction of the object wave phase, which can be interpreted quantitatively in terms of electromagnetic fields.
[1] Shalimov, A. et al., Journal of Applied Physics 105, 064906 (2009)
[2] Geiger, D. et al., Microsc. Microanal. (2008) 14, 68-81.
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MM 12.50 Mon 17:30 P5

In-situ TEM investigation under extreme heat: Gold and hydrocarbon adsorbates on graphene — •Benedikt Westenfelder[1], Jannik C. Meyer[2], Xiaohang Lin[3], Ferdinand Scholz[1], Carl E. Krill III[4], Axel Gross[3], and Ute Kaiser[2] — [1]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany — [2]Central Facility of Electron Microscopy, Ulm University, 89081 Ulm, Germany, — [3]Institute of Theoretical Chemistry, Ulm University, 89081 Ulm, Germany — [4]Institute of Micro- and Nanomaterials, Ulm University, 89081 Ulm, Germany

Atomically resolved studies of the heat-induced evolution of adsorbates on graphene have been enabled due to the development of specifically designed TEM sample carriers. Our concept provides to apply in situ an electrical current to a freestanding graphene membrane. In this way we reach local temperatures exceeding 2000 K enabling to observe the transformation of adsorbated hydrocarbons into atomic layers of amorphous carbon and eventually into polycrystalline graphene. Moreover, we observed the migration of gold nanoparticles and their self-organized alignment along parallel straight lines along the negative temperature gradient. Furthermore, we investigated the periodical arrangement of individual gold atoms into rectangularly shaped atomic monolayers and bilayers as well as entire cuboids of many atomic layers. We found, that their lattice parameter is significantly larger than the value for pure gold articles, which might be caused by the incorporation of excess carbon into the gaps of the gold fcc lattice. DFT calculations suggest that an interstitial gold-carbon compound has been developed.

MM 12.51 Mon 17:30 P5

High Resolution Transmission Electron Microscopy of Organic Molecules on Graphene — •Gerardo Algara-Siller[1,2], Goutam Pramanik[3], Tanja Weil[3], and Ute Kaiser[1] — [1]Group of Electron Microscopy of Materials Science, Ulm University, Ulm, Germany — [2]Technical University Ilmenau, Ilmenau, Germany — [3]Department of Organic Chemistry III/Macromolecular Chemistry, Ulm University, Ulm, Germany

Graphene, a one atom thick material, has been proven to be a perfect substrate for TEM investigations. In this work, a graphene substrate was fabricated via micromechanical cleavage and transfered to a Quantifoil grid. In order to reduce contamination on the substrate, graphene was annealed and treated with H2:O2 ion plasma. Solutions of protein based copolymers, cBSA-PEO-TA coated Au nanoparticles (NPs) with different Au-protein ratios were deposited by drop coating on graphene and investigated using an aberration-corrected FEI TITAN 80-300 operated at 80kV acceleration voltage. HRTEM micrographs of the deposited protein based copolymers corroborated that the particle size distribution of the Au NPs is dependant on the Au-protein ratio. Furthermore, due to the low noise graphene substrate, the surrounding protein and single gold atoms forming the NPs can be easily resolved and counted. Thus, we report an approach of lower voltage aberration-corrected HRTEM imaging on graphene towards unraveling the chemistry of inorganic/organic interfaces.

MM 12.52 Mon 17:30 P5

Influence of chemical bonding on HRTEM images of light elements — •Simon Kurasch[1], Jannik C. Meyer[1,3], Hye Jin Park[2], Viera Skakalova[2], Siegmar Roth[2], and Ute Kaiser[1] — [1]Central Facility for Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm — [2]MPI FKF, 70569 Stuttgart — [3]University of Vienna, Department of Physiks, 1090 Vienna, Austria

We improved the HRTEM image simulation by calculating the electrostatic specimen potential via density functional theory (DFT) [1]. This approach takes into account the electron charge redistribution within the specimen due to chemical bonding. Usually this is neglected by calculating the scattering potential as a superposition of isolated atom potentials.

Here we show that chemical bonding is clearly detected in experimental images of nitrogen doped graphene. We found that single atom nitrogen substitutions can be detected in experimental HRTEM images (dZ=1). According to the isolated atom model this should not be possible. However the observation is in excellent agreement with the DFT based simulation. Therefore the observed contrast from the N atom originates from a polarization effect on the neighbouring carbon atoms.

These experiments reveal that bonding has to be included in the TEM image simulation, and that a TEM can be utilized to obtain information about the electronic configuration of the specimen. This opens a way to discern electronic arrangements in point defects or other non-periodic objects that can not be analyzed by diffraction.

MM 12.53 Mon 17:30 P5

The Unitarily Covariant Formulation of Hedin's Equations

— •Ronald Starke and Georg Kresse — University of Vienna, Faculty of Physics, Comp Mat Phys

The Feynman graph formulary as used e.g. by Hedin's equations depends on the usage of the spacetime domain. E.g., the well-known GW-approximation is usually formulated as $\Sigma(1,2) = \mathrm{i}G(1,2)W(2,1)$ where $G(1,2)W(2,1)$ denotes a point-wise product in the space time domain, i.e. $1 = x_1 = (\boldsymbol{x}_1, t_1)$. For practical calculations, however, it might be useful to work with quantities given as time (frequency) dependent matrices w.r.t. an orbital basis. The resulting expressions for Σ etc. do not carry over directly from the space-time domain. E.g., ${\Sigma^i}_j \neq \mathrm{i}{G^i}_j{W^j}_i$ already because W is given in an arbitrary orbital basis by a 4-point quantity ${W^{ij}}_{kl}$. It is, therefore, desirable to reformulate Hedin's equations such that they hold in an any orbital basis. In analogy to General Relativity, we call this formulation *unitarily covariant.* For the implementation of such an unitarily covariant formulation, it is necessary to clarify the resulting transformation properties induced by a change of basis in the one-particle Hilbert space $\mathcal{H}$. In particular, it turns out that one has to distinguish between 'upper' and 'lower' indices according to the transformation behavior of the respective quantities. The upshot of the fully covariant formulation will be – apart from a certain theoretical insight – the facilitation of explicit calculation especially when it comes to the derivation of useful approximations: the covariant formalism allows for the direct switch to a basis where certain quantities take particularly simple (e.g. diagonal) forms.