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Chains of coupled clusters arranged in a quasiperiodic sequence are analyzed with respect to the dynamics of wave packets. The recurrence probability is shown to show characteristic plateaus described by an interplay of localization and dominant motion. A three-mode model is developed which allows to understand the features of the recurrence probability as well as of the time-dependent width of the wave packets. The relation to waiting probabilities and anomalous diffusion is worked out. The consequences for the transmission coefficient realizable in experiments by sequences of quasiperiodic chains are discussed and the generalizations towards two-dimensional tilings are presented.

MM 21.5 Tue 12:45 H 0111

Phase behavior of colloidal particles on a 2D quasicrystalline substrate — ●MICHAEL SCHMIEDEBERG and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623

Berlin, Germany

By using Monte-Carlo simulations, we study charged-stabilized colloidal particles in a two-dimensional decagonal potential and calculate their phase diagram as a function of the particle density and the strength of the substrate potential, which in experiments is realized by interfering laser beams.

As one expects, we find a triangular to liquid phase transition for small laser intensities and a ten-fold symmetric quasicrystalline phase for high potential strengths. For intermediate intensities, however, where the colloidal ordering is influenced by both the colloidal interaction and the substrate potential, we identify a series of interesting phases: For systems with low densities, where the number of colloidal particles is less than the number of potential minima, there is a quasicrystalline phase which exhibits bond orientations in 20 different directions. When the number of colloids exceeds the occurrence of minima, we usually find a solid phase without any bond-orientational order. However, for certain densities the system locks into a highly ordered phase that is close to an Archimedean tiling.

MM 22: HV Paxton

Time: Tuesday 14:00–14:30

Location: H 1058

Invited Talk MM 22.1 Tue 14:00 H 1058

Grain boundary embrittlement and cohesion enhancement in copper — ●ANTHONY PAXTON¹, ALEXANDER LOZOVOI¹, RAINER SCHWEINFEST², and MICHAEL FINNIS³ — ¹Atomistic Simulation Centre, Queen's University Belfast, BT7 1NN, UK — ²Science+Computing ag, Hagellocher Weg 71-5, 720270 Tübingen, Germany — ³Imperial College London, Exhibition Road, London SW7 2AZ, UK

There has been a long standing debate surrounding the *mechanism* of grain boundary embrittlement and cohesion enhancement in metals. Embrittlement can lead to catastrophic failure such as happened in the

Hinkley Point disaster, or indeed in the case of the Titanic! This kind of embrittlement is caused by segregation of low solubility impurities to grain boundaries. While the accepted wisdom is that this is a phenomenon driven by *electronic* or *chemical* factors, using language such as *charge transfer* and *electronegativity difference*; we believe that in copper, at least, both cohesion enhancement and reduction are caused by a simple *size effect*. We have developed a theory that allows us to separate unambiguously, if not uniquely, chemical and structural factors. We have studied a large number of solutes in copper using first principles atomistic simulation to support this argument, and the results of these calculations will be presented here

MM 23: Poster session

Time: Tuesday 14:45–18:00

Location: Poster B

MM 23.1 Tue 14:45 Poster B

Nanotomography of Biomaterials — ●STEPHANIE RÖPER¹, CHRISTIAN ZEITZ², CHRISTIAN DIETZ¹, NADINE DRECHSEL¹, ANKE BERNSTEIN³, NICOLAUS REHSE¹, and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken — ³Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Biomaterials such as bone and teeth are nanocomposites of proteins and minerals. At the molecular length scale these materials have a stiff inorganic component (hydroxylapatite) that reinforces the soft organic matrix (type I collagen) through a recurring structural motif. To gather information of the nanometer scaled structure of these materials we use nanotomography. For this scanning probe microscopy (SPM) based method the specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode SPM after each etching step. In our experiments we focus on cortical human bone (embedded and native) and human teeth. The stepwise etching is done in-situ in the SPM with an automated setup. We will present our latest volume images of human bone and teeth and discuss new concepts for adjusting the imaging parameters to maintain a good imaging quality.

MM 23.2 Tue 14:45 Poster B

Neutron Reflectometry Studies on Self-diffusion in Nano-Crystalline Fe Films: First Results — ●SUJOY CHAKRAVARTY¹, MICHAEL HORISBERGER², THOMAS GUTBERLET², JOCHEN STAHN², and HARALD SCHMIDT¹ — ¹Institut für Metallurgie, AG Materialphysik, TU Clausthal, Germany — ²Laboratorium für Neutronenstreuung, ETH Zürich & PSI, Villigen, Switzerland

Nano-crystalline metals show in comparison to their coarse grained counterparts improved mechanical properties like high hardness and fracture toughness and also interesting magnetic properties. At low

temperatures mechanical deformation (grain boundary creep, grain boundary sliding), grain growth, and also thermal stability are essentially controlled or influenced by self-diffusion. For an understanding of these processes close to room temperature, we carried out self-diffusion measurements on nanocrystalline Fe films using neutron reflectometry. This method enables to determine extremely low diffusivities down to $10^{-25} \text{ m}^2/\text{s}$ and also extremely small diffusion lengths $< 1 \text{ nm}$, not possible with conventional methods. For diffusion studies, isotopic multilayers of the form $\text{Si}(\text{substrate})/[\text{57-Fe}(5 \text{ nm})/\text{nat-Fe}(10 \text{ nm})] \times 10$ were deposited by using magnetron sputtering. The multilayers were annealed in the temperature range between 473 and 673K for different periods of time and neutron reflectivity has been measured in-situ. Further, structural characterization has been done by grazing incidence X-ray diffractometry, Moessbauer spectroscopy, atomic force microscopy, and electron microscopy. First results are presented and are discussed in the framework of grain boundary diffusion in the type C regime.

MM 23.3 Tue 14:45 Poster B

Nitrogen Diffusion in Amorphous Silicon (Carbo)Nitride Probed by Neutron Reflectometry — ●ERWIN HÜGER¹, THOMAS GUTBERLET², JOCHEN STAHN², MICHAEL BRUNS³, and HARALD SCHMIDT¹ — ¹Institut für Metallurgie, AG Materialphysik, TU Clausthal, Germany — ²Laboratorium für Neutronenstreuung, ETH Zuerich & PSI, Villigen, Switzerland — ³Institut für Materialforschung III, Forschungszentrum Karlsruhe GmbH, Germany

Covalently bound amorphous solids are distinguished by extremely low self-diffusivities, which necessitates the detection of extremely short diffusion lengths in order to prevent an overlapping of crystallization and diffusion processes during annealing. We present nitrogen diffusion studies on amorphous SiN_x and SiC_xN_y materials, which were carried out by neutron reflectometry on isotope heterostructures. Here, a se-

quence of 14-N and 15-N enriched layers are deposited by magnetron sputtering on silicon substrates. Due to the different coherent neutron scattering lengths of 14-N (9.37 fm) and 15-N (6.44 fm) a scattering contrast for neutrons occurs between chemically identical layers. Self-diffusivities are determined from the modification of the reflectivity due to interdiffusion of the two nitrogen isotopes after annealing at elevated temperatures. We present a systematic study on samples with 3, 5, 12 and 40 single layers and demonstrate that it is possible to detect minimum diffusion lengths of 0.7 nm and self-diffusivities of $5 \times 10^{-25} \text{ m}^2/\text{s}$. The temperature and annealing time dependence of the diffusivities is analyzed and explained in the framework of structural relaxation processes.

MM 23.4 Tue 14:45 Poster B

Exciton formation in graphene bilayer — ●RAOUL DILLENSCHNEIDER — University of Augsburg, Germany

Graphene, layers of two-dimensional honeycomb-array of carbon atoms, has attracted much interest these last few years due to its recent experimental accessibility and a wide variety of interesting properties. As the engineering application of the graphene layers attracts increasing significance, we need to explore, experimentally and theoretically, ways to enrich graphene's electrical properties and to control them. One way to achieve some control over the electrical properties is to change the number of layers and/or the bias applied across the layers.

The bias can also potentially control the formation of excitons. Since the applied bias leads to the charge imbalance in the two layers, it is natural to suspect that the Coulomb attraction of the excess electrons and holes on opposite layers would lead to an exciton instability

We consider the possibility of an excitonic instability for biased graphene bilayer in the framework of Hartree-Fock theory.

MM 23.5 Tue 14:45 Poster B

Soft absorption edges studied with hard x rays — ●HENNING STERNEMANN¹, CHRISTIAN STERNEMANN¹, JOHN S. TSE², JUHA A. SOININEN³, YONG Q. CAI⁴, SERGE DESGRENIERS⁵, TIMOTHY T. FISTER⁶, NOZOMU HIRAOKA⁴, ACHIM HOHL⁷, ANDREAS SCHACHT¹, GERALD T. SEIDLER⁶, GYÖRGY VANKÓ^{8,9}, SIMO HUOTARI⁸, KEIJO HÄMÄLÄINEN³, and METIN TOLAN¹ — ¹Fakultät Physik / DELTA, TU Dortmund, Germany — ²Dept. Phys. & Engn. Phys., U Saskatchewan, Canada — ³Div. X-ray Phys., Dept. Phys. Sci., U Helsinki, Finland — ⁴NSRRC, Hsinchu, Taiwan — ⁵Dept. Phys., U Ottawa, Canada — ⁶Phys. Dept, U Washington, USA — ⁷Inst. Mat. Sci., TU Darmstadt, Germany — ⁸ESRF, Grenoble, France — ⁹KFKI, Budapest, Hungary

Non-resonant inelastic x-ray scattering is a powerful tool to access shallow absorption edges using hard x-rays. This allows the study of low energy transitions under conditions which do not permit electrons and soft x rays as a probe. We present a variety of non-resonant inelastic x-ray scattering measurements of Si based compounds. Applications range from L-edge studies of elemental Si [1] and bulk amorphous Si monoxide [2] to the study of giant dipole resonances of Ba and I endohedrally intercalated in complex silicon networks. The experimental results are compared to calculations employing a real-space multiple-scattering approach [3]. Implications on the study of high-pressure induced phase transitions will be emphasized.

[1] H. Sternemann *et al.*, Phys. Rev. B **75**, 075118 (2007). [2] C. Sternemann *et al.*, J. Phys. Chem. Solids **66**, 2277 (2005). [3] J.A. Soininen *et al.*, Phys. Rev. B **72**, 045136 (2005).

MM 23.6 Tue 14:45 Poster B

Stability, electronic and magnetic properties of iron oxyhydroxides under high pressure: Insights from first principles — ●KATRIN OTTE¹, ROSSITZA PENTCHEVA¹, and JIM RUSTAD² — ¹Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — ²Department of Geology, UC Davis

Iron oxyhydroxides (FeOOH) play an important role in nature and technology, e.g. in binding heavy metals. The high pressure behavior of water containing minerals is important for understanding the processes in the Earth's crust and lower mantle. Using density functional theory (DFT), we investigate the structural, electronic and magnetic properties of the iron oxyhydroxide-polymorphs (α -, β -, γ - and *hp*-FeOOH) under high pressures. We find that under ambient conditions goethite (α) is the lowest energy phase, while at high pressures the *hp*-phase becomes more favorable. The relative stability of the different phases follows the trend obtained from recent calorimetric measurements [1]. Bond lengths are in a good agreement with available experimental data. While in the ground state Fe³⁺-ions are coupled

antiferromagnetically, at high pressures a transition to a ferromagnetic alignment takes place in *hp*-FeOOH. At ambient conditions all AFM phases are insulating within the generalized gradient approximation (GGA). However, a substantial improvement of the size of the band gap is achieved by including electronic correlations within the LDA+U method.

[1] C. Laberty and A. Navrotsky, *Geochimica et Cosmochimica Acta* **62**, 2905-2913 (1998)

MM 23.7 Tue 14:45 Poster B

Investigation of Electronic Transport Mechanisms in Phase Change Materials — ●JENNIFER LUCKAS, MARTIN SALINGA, CARL SCHLOCKERMANN, ANDREAS KALDENBACH, URSULA NELLEN, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The non-linearity of the electrical conductivity in the amorphous phase not only states to be the oldest of all puzzles in the field of phase change materials starting with Ovshinsky's discoveries in the 1960s, but also remains likely to be the most controversial one to this date. The most prominent effect in this context is the so-called threshold switching in the amorphous phase describing a sudden break down of resistivity in the presence of a critical electric field. Besides its scientific importance this effect is crucial for the currently most promising application of phase change alloys, i.e. electric memory (PCRAM).

Several theories about electronic transport of this class of materials have been proposed in the last decades, but there is still a lack of quantitative experimental data to validate or disprove them. To fill this gap in this work the mobility of the charge carriers is studied for some representative phase change materials. The dependence of the mobility both on temperature and on the electric field is investigated and compared with existing theories. From this comparison insight into the mechanism of charge carrier transport is obtained.

MM 23.8 Tue 14:45 Poster B

High Kinetic Energy Photoelectron Spectroscopy Study of the Ni 1s Core Level and Satellite Structure — ●MIHAELA GORGOI¹, SVANTE SVENSSON², OLOF KARIS², JAN RUSZ², PETER OPPENEER², FRANZ SCHÄPFERS¹, WALTER BRAUN¹, NILS MARTESSON², and WOLFGANG EBERHARDT¹ — ¹BESSY GmbH, Berlin, Germany — ²Uppsala University, Uppsala, Sweden

The Ni 2p level and its satellite structure have been studied since many years and the mechanisms behind this structure have been addressed in a large number of reports [1, 2 and references within]. In contrast, there is not a modern photoelectron spectrum of Ni 1s and the corresponding satellite structure. Using the HIKE facility at beam-line KMC1 at BESSY we have studied this core level using excitation energies from 9 keV to 12 keV. Our findings show that the satellite *main line energy distance decreases for the Ni 1s level in comparison to the Ni 2p case. Our finding has important implications for the existing theoretical explanations of the classical Ni satellite problem and requires a revision of current models.

[1] A.P. Grosvenor, M.C. Biesinger, R.St.C. Smart, N.S. McIntyre, *Surface Science* **600** (2006) 1771.

[2] A. Bosch, H. Feil, G.A. Sawatzky, N. Märtensson, *Solid State Communications* **41** (1982) 355.

MM 23.9 Tue 14:45 Poster B

The importance of cluster-distortions in the tetrahedral cluster compounds: Ab initio investigations — MARTIN SIEBERER, STEFAN TURNOVSKY, PETER MOHN, and ●JOSEF REDINGER — Center for Computational Materials Science, Vienna University of Technology, Vienna, Austria

We study the electronic and structural properties of selected representatives of the so-called Molybdenum cluster compounds such as GaM₄X₈ with M=Mo as a group VIB element and V, Nb, Ta as a group VB element. X denotes either S or Se. These compounds are known to exhibit semiconducting behavior in the electrical resistivity, caused by hopping of electrons between well-separated metal clusters. The large separation of the tetrahedral metal (M₄) clusters is believed to be the origin of strong correlations. We show that recent calculations neglected an important type of structural distortions, namely those happening only within the M₄ unit upon a fixed angle $\phi = 60^\circ$ of the trigonal (fcc-like) cell. These internal distortions gain a significant amount of energy compared to the cubic cell and they are - to our knowledge - almost undetectable within powder x-ray diffraction. However, they strongly influence the band-structure by opening up a gap at the Fermi-energy, which puts into question whether all