MM 13: Topical Session: Quasicrystals & Complex Metallic Alloys III

Time: Monday 15:45–18:00 Location: H25

MM 13.1 Mon 15:45 H25

Dealing with the complexity of complex matter — •Peter Häussler — University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Describing the structure of complex systems is difficult enough but, due to the huge unit cell and unknown decoration of the lattice sites, what often happens, calculating their properties is even worse. Understanding their structural evolution from e.g. the gaseous or liquid state and the reasons where structural peaks finally arise is far out of this range. One way, to reduce the tremendous number of parameters and hence to understand their structural development as well as the evolution of physical properties, is to give up a microscopic understanding based on a detailed description of all the individual atoms. We may even ask, is it really necessary to know all these details which we may, probably, never be able to get? Can we tread the complexity with reduced information? If we are able to find global subsystems, consisting of many species which are acting collectively, we would be able to reduce the tremendous number of independent parameters to a few only. If we are further able to describe with these parameters the major effects causing the atomic distances as well as main physical properties, we may have understood a lot. I will talk in this presentation on global effects of different subgroups of electrons. The combined s/p-electrons, the s-electrons alone, as well as the d-electrons, all have their own effects on structural features. Together with the structure they cause the metallic, insulating or semiconducting properties, are defining the atomic density and many more quantities.

MM 13.2 Mon 16:00 H25

Single-crystal growth of various complex metallic alloy phases — •Michael Feuerbacher, Marc Heggen, and Carsten Thomas — Forschungszentrum Juelich, 52349 Juelich, Germany

Complex metallic alloys (CMAs) are intermetallic compounds with large lattice parameters and unit cells containing some tens to some thousands of atoms. Their local order is in most cases dominated by icosahedral atom coordination, which distinguishes CMAs from simple metals and compounds. In order to be able to establish intrinsic structure-property relations characteristic of the particular local order, the availability of high-quality single crystals is of particular importance. In this presentation we report on single-crystal growth approaches on various different, mostly Al-based CMAs. We present the growth techniques applied and the resulting single crystals along with critical primary characterizations. The strategy of phase selection, which is essential to achieve comprehensive structure-property relations by comparative studies, is discussed.

MM 13.3 Mon 16:15 H25

Metadislocation core structure in the complex metallic alloy $\mathbf{Al_{13}Co_4}$ — •Marc Heggen and Michael Feuerbacher — Peter Grünberg Institut, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

We have analysed metadislocations in the complex alloy $Al_{13}Co_4$. The core structure is studied using aberration-corrected high-resolution scanning transmission electron microscopy. Different types of metadislocations with Burgers vectors of b = +/-tau^{-n} b (0 1 0) (n = 3, 4) are found which are associated to four and six planar defects, respectively. They are escorted by phason defects and move, in contrast to metadislocations in most other complex alloys, by pure glide.

MM 13.4 Mon 16:30 H25

Structure of a decagonal Al–Pd–Mn quasicrystal with 16 Å periodicity — •Benjamin Frigan[1], Marek Mihalkovič[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

We present the first detailed structure solution for a decagonal quasicrystal in the Al–Pd–Mn system by means of *ab initio* energy minimization. It is based on structure models of the ε_6- and other approximant phases. All phases consist of columns of pseudo-Mackay icosahedra (PMI), whose projections form tilings of the plane. In between there are glue atoms in the form of large bicapped pentagonal prisms (LBPP). In the past, we have optimized the structure of the ε-phases, where the tilings consist of pentagons, hexagons and nonagons. These can be represented as subsets of a hexagon-boat-star (HBS) tiling. The decagonal phase comprises further HBS-tiles. We have constructed several HBS approximants and decorated them with PMI and LBPP clusters. Whereas the PMI clusters were kept essentially unchanged, each LBPP is adjusted in occupancy depending on its position in the various tiles. In this way we obtain cluster decorations for all tiles of the decagonal quasicrystal. The structures were optimized by molecular dynamics annealing with specially developed EAM-potentials, followed by further relaxation with *ab initio* calculations. The quality of the structures is judged by their position within the convex hull of stable, experimentally known phases of the Al–Pd–Mn phase diagram.

MM 13.5 Mon 16:45 H25

Cu–Sn Cluster Compounds — •Saskia Stegmaier, Thomas F. Fässler, and Karsten Reuter — Technische Universität München, Germany

Nanostructured intermetallic materials attract wide interest because of their structural and physical properties and the related potential for applications, for example in catalysis or electronics.

The intermetallic compounds $A_{12}Cu_{12}Sn_{21}$ (A = Na, K, Rb, Cs) [1] and $Na_{2.8}Cu_5Sn_{5.6}$ [2] feature intriguing new Cu–Sn cluster species. These are onion-skin-like $\{Sn@Cu_{12}@Sn_{20}\}$ clusters with quasi-icosahedral symmetry and related pseudo-five-fold symmetric $^1_\infty\{Sn_{0.6}@Cu_5@Sn_5\}$ rods, respectively. In the solid state structures of the A–Cu–Sn phases the polyanionic Cu–Sn clusters or rods are separated from each other by alkali metal cations. The ternary phases thus represent promising precursors for the synthesis of new nanostructured binary Cu–Sn materials.

In view of this perspective we perform density functional theory calculations to computationally search for such potential Cu–Sn compounds—including discrete clusters and wires, as well as 3D periodic structures.

[1] S. Stegmaier, T. F. Fässler, *J. Am. Chem. Soc.* **2011**, *133*, 19758.

[2] S. Stegmaier, T. F. Fässler, *Angew. Chem. Int. Ed.* **2012**, *51*, 2647.

MM 13.6 Mon 17:00 H25

Thermal Conductivity in Type-I Clathrate Systems — •Daniel Schopf and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart

Intermetallic clathrates are currently actively investigated due to their special thermoelectric properties. They are composed of periodically arranged cages, formed by host atoms, which enclose single guest atoms. The low thermal conductivity of these structures has been attributed to the scattering of the phonons on the local vibration modes (“rattling”) of these guest atoms.

Molecular dynamics simulations can be used to study the influence of complexity on the thermal conductivity. To model the strongly directional atomic interactions in clathrates, angular dependent potentials are required. Effective potentials have been determined with the force-matching method and will be presented.

The Green-Kubo method has been used to calculate the thermal conductivity of clathrate systems with different levels of complexity. The influence of the size of the unit cell and the arrangement of vacancies as sources of the low conductivity are discussed.

MM 13.7 Mon 17:15 H25

Medium-range structure of $\mathbf{Zr_{50}Cu_{45}Al_5}$ Bulk Metallic Glass from Fluctuation Electron Microscopy — •Paul Voyles[1,2,3], Jinwoo Hwang[1], Zenon Melgarejo[1], Irena Kalay[4], Eren Kalay[4], Matt Kramer[4], and Don Stone[1] — [1]University of Wisconsin, Madison, United States — [2]Forschungszentrum Jülich, Jülich — [3]RWTH Aachen, Aachen — [4]Ames Lab, Iowa, United States

By combining fluctuation electron microscopy data sensitive to medium-range order (MRO) with an empirical interatomic potential sensitive to short-range order (SRO) in a single hybrid reverse Monte Carlo structural refinement, we have found two types of structural order in $Zr_{50}Cu_{45}Al_5$ bulk metallic glass [1]. One structure consists of icosahedral nearest-neighbor SRO clusters, arranged in chains at the

MRO length scale of 1 nm. The other structure is more crystal-like, consisting of SRO clusters with more 4- and 6-sided faces on their Voronoi polyhedra. The crystal-like SRO clusters organize into compact MRO clusters with distinct 4- and 6-fold rotational symmetry. Experimentally, structural relaxation shifts the cluster population from crystal-like to more icosahedral. In molecular dynamics, the structural models are stable under annealing at temperatures well below T_g. The structural evolution of the models through the simulated glass transition will be discussed.

[1] J. Hwang, Z. Melgarejo, Y. Kalay, I. Kalay, M. J. Kramer, D. S. Stone, P. M. Voyles, Phys. Rev. Lett. 108, 195505 (2012)

MM 13.8 Mon 17:30 H25

How atomic structure forms - a general principle — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

The evolution of atomic structure on large scales is still not well understood. In principle one has to deal with approximately 10^{23} individual atoms, but even a few hundreds are still too much to apply microscopic techniques - the number of parameters would still be horrible. Subsequently, one is left with simulations and techniques which implement the final results in advance. On the other hand, we observed that structure formation is to a great extent an ordering process where a few global subsystems, like the outer electrons as one, and the remaining ions as the other one, are behaving collectively. Both are connected by global resonances. Using collectivity allows the reduction of the number of independent parameters to a few only - to understand the most important principle, the formation of gaps or pseudo gaps at the Fermi energy. Redistributing electrons at the Fermi energy causes very effective reductions of the total energy of the system and, hence, stabilizes particular structures. I will talk about this principle for completely different systems as all the liquid elements along the periodic table (molecular and elemental liquids, liquid insulators, metals, or semiconductors), and the rising complexity, whenever alloys have to be understood. Complexities as charge transfer, hybridization effects, phase separation, the formation of quasi- or nano-crystalline inclusions are described as well. We became able to predict mayor structural motif of not yet measured systems and their electronic properties

MM 13.9 Mon 17:45 H25

On the evolution of structure and electronic transport properties in Al-Mn — •Syed Sajid Ali Gillani and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

A systematic study of thin films of Al-Mn, evaporated at $T = 4\,\mathrm{K}$, shows mixtures of amorphous, quasi-crystalline, as well as nano-crystalline phases. Their structures have been investigated by electron diffraction, their transport properties and thermal stability by resistivity measurements, indicating clear evidences of resonance effects between global subsystems as there are the Fermi gas as one, and the forming static structure as the other one. The global resonances are self-organizing via their exchange of characteristic momenta and angular momenta, respectively and dominate all the properties including phase stability and phase separation. The amorphous phase shows in r-space spherical periodic order, predominately based on an exchange of characteristic momenta alone. Al-rich alloys show, in addition, features of quasi-crystalline order and Mn-rich alloys an enhanced content of nano-crystalline periodic order. The characteristic distances between theses phases are related among each other and to half the Fermi wavelength λ_F, indicating resonance effects in all of them. In k-space the corresponding structure factor $S(K)$ shows a resonance peak at scattering vector $K_\mathrm{pe} = 2k_\mathrm{F}$ with an additional prepeak in the range of the quasi-crystalline phase and further peaks in the range of enhanced nano-crystallinity.