MM 57: Complex Materials I

Time: Thursday 15:45–17:00 Location: H 1029

MM 57.1 Thu 15:45 H 1029

Quasikristalle - Clusterkristalle mit Defekten — •Hartwig Schlüter — SCHLÜTER CONSULT, Maschmühlenweg 8-10, 37073 Göttingen

Anders als bisher angenommen, kann eine dichteste Atom-/Kugelgelpackung aus Clustern mit ikosaedricher Symmetrie erzeugt werden. Bausteine sind ein Bergman-Cluster mit 20 Kugeln in der äußeren Schale und ein Mackay-Cluster mit 30 Kugeln auf den 2f-Symmetrieachsen der äußeren Clusterschale. Bei dem Mackaytyp-Cluster 2. Generation(2. Gen.) befinden sich die Bergman-Cluster 1. Gen. auf den Schalen mit geradzahligem Schalenindex und die Mackay-Cluster 1. Gen auf den Schalen mit ungeradem Schalenindex - oder umgekehrt. Nächstenachbar(NN)-Cluster 1. Gen. aus NN-Schalen besitzen 5 Koinzidenzplätze. NN-Bergman-Cluster 1. Gen. besitzen 2 Koinzidenzplätze und NN-Mackay-Cluster 1. Gen. besitzen 4 Koinzidenzplätze. Aus geeigneten Clustern 2. Gen. wird ein Cluster 3. Gen. konstruiert, der aus 20 "Cluster-Einkristallen"besteht. Dieses Strukturmodell erlaubt es, Quasikristalle mit ikosaedrischer Symmetrie als Kristalle mit Defekten zu beschreiben.[1]

[1] Models of the Atomc Structure of Approximants and related Quasicrystals, Hartwig Schlüter, SCHLÜTER CONSULT, Göttingen, 2011 (www.schlueter-consult.de)

MM 57.2 Thu 16:00 H 1029

Studying plastic deformation in brittle complex metal alloys: deformation of Al13Co4 at room temperature — •Sandra Korte[1,2], Volker Schnabel[2], and William J Clegg[2] — [1]Friedrich Alexander Universität Erlangen-Nürnberg, Erlangen, Deutschland — [2]University of Cambridge, Cambridge, UK

In this paper the low temperature deformation behaviour of single crystals of orthorhombic Al13Co4 has been studied using micropillar compression. This technique allows the study of plasticity by suppressing cracking in brittle materials as the sample size is reduced to a few microns. Therefore, a polycrystal of sufficient grain size allows the milling of micropillars as single crystalline samples and the selection of different crystal orientations by correlation with electron backscattered diffraction. The plastic deformation of such small single crystals has been studied in terms of the stresses involved and structures observed by scanning and transmission electron microscopy after deformation. It was found that features correlating to crystallographic slip on the glide planes expected based on experiments at higher temperatures mainly occurred where these were oriented favourably, with a high resolved shear stress. In other orientations deformation bands were observed to form on planes of maximum shear stress. This is discussed in the light of the deformation morphology, strain-rate dependence and similar deformation signatures found in bulk metallic glasses.

MM 57.3 Thu 16:15 H 1029

Quantum Diffusion in Metallic-Mean Labyrinth Tilings — •Stefanie Thiem and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

We present results for the quantum diffusion in quasiperiodic tight-binding models in one, two, and three dimensions. The models are based on a class of one-dimensional quasiperiodic chains, in which the atoms are coupled by weak and strong bonds aligned according to the metallic-mean sequences. The associated labyrinth tilings in d dimensions are then constructed from the direct product of d such chains, which allows us to consider rather large systems numerically. The electronic transport properties are studied by computing the scaling behavior of the return probability and the mean square displacement of wave packets with respect to time. Our results reveal that the systems exhibit anomalous diffusion, where this behavior can be related to the underlying quasiperiodic structure by applying a renormalization group approach and perturbation theory.

MM 57.4 Thu 16:30 H 1029

Role of phason fluctuations for the stability of a quasicrystal model system — •Alexander Kiselev[1], Michael Engel[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Department of Chemical Engineering, University of Michigan, USA

The source of stability of quasicrystals is generally not well understood. A common model assumes that structural fluctuations, which are not present in periodic approximant crystal structures, play an important role by contributing a configurational term to the free energy. Here, we study the influence of phason fluctuations on the stability of a decagonal quasicrystalline model system, where the atoms interact by the Lennard-Jones-Gauss potential [1], and apply molecular dynamics and Monte Carlo simulations. Absolute values of the Free energy were calculated by the Frenkel-Ladd method [2] for the phononic part and by the phason flips decoupling approach for the configurational part. A phase transition from an energetically stabilized periodic Xi-approximant to an entropically stabilized random tiling quasicrystal is observed. We simultaneously have observed the phason elastic constants. One phason elastic constant changes its sign from positive to negative when the temperature at the Xi-quasicrystal transition is lowered, indicating a soft-phason transition.

[1] M. Engel and H.-R. Trebin, Phys. Rev. Lett. **98** 225505 (2007)
[2] D. Frenkel and A.J.C. Ladd, J. Chem. Phys. **81** 3188-3193 (1984)

MM 57.5 Thu 16:45 H 1029

Defects in the monoclinic Al-Pd-Fe complex metallic alloy — •Michael Feuerbacher and Marc Heggen — Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The complex metallic alloy phase m-Al-Pd-Fe, a ternary extension of the Al13Fe4 phase, has a monoclinic structure (space group C1 2/m, lattice constants a = 1.55 nm, b = 0.88 nm, c = 1.25 nm). The unit cell contains 102 atoms, which are coordinated in the form of icosahedral clusters.

We present a characterization of defects in as grown and plastically deformed m-Al-Pd-Fe by means of aberration-corrected high-resolution scanning transmission electron microscopy using a high-angle annular dark-field detector. In the deformed samples we find dislocations trailing stacking faults at a high density, which mediate plastic deformation in the structure. We identify the displacement vectors of the stacking faults and the dislocation Burgers vectors. We demonstrate that the dislocations are metadislocations and discuss their relation to metadislocations in orthorhombic Taylor phases.