MM 24 Quasicrystals

Time: Wednesday 14:00–15:15 Room: IFW D

MM 24.1 Wed 14:00 IFW D

Formation of quasicrystals and complex periodic intermetallics in the Al-Pd-Ru and Al-Pd-Rh alloy systems — •Benjamin Grushko[1], Dmytro Pavlyuchkov[1,2], and Bartosz Przepiórzyński[1,3] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]I.N. Frantsevich Institute for Problems of Materials Science, 03680 Kiev 142, Ukraine — [3]Institute of Materials Science, Silesian University, 12 Bankowa, 40007 Katowice, Poland

This work continues the study of formation of complex intermetallics, including quasicrystals, in ternary Al-Pd-TM systems. The Al-Pd-Ru system is related to extensively studied Al-Pd-Fe [1, and Al-Pd-Rh to Al-Pd-Co [2]. We confirmed the thermal stability of the icosahedral (I) phase. The ternary extension of the Al-Pd Epsilon-phases is comparable to that in Al-Pd-Co. Three ternary cubic phases isostructural to C, C1 and C2 in Al-Pd-Fe were revealed. No stable quasicrystals were revealed in Al-Pd-Rh. The Al-Pd and Al-Rh Epsilon-phases form a continuous range. Also C-Al5Rh2 exhibited significant solubility of Pd. Two ternary phases structurally related to C-Al5Rh2 phase were revealed: cubic C2, isostructural to that in Al-Pd-TM (TM=Fe,Co,Ru) and hexagonal C3. The latter has a wide compositional range along about constant Al. [1] S. Balanetskyy, B. Grushko, T.Ya. Velikanova and K. Urban, J. Alloys Comp. 376, 158 (2004). [2] M. Yurechko, B. Grushko, T. Velikanova and K. Urban, J. Alloys Comp. 337, 172 (2002).

MM 24.2 Wed 14:15 IFW D

Molecular dynamics simulation of diffusion processes in decagonal quasicrystals — •Stephen Hocker, Franz Gähler, and Peter Brommer — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Diffusion in decagonal Al-Ni-Co and Al-Cu-Co quasicrystals is investigated by molecular dynamics simulations using newly developed EAM potentials. The potentials are determined with the force matching method: For a selection of small reference configurations, the cohesion energies, stresses, and forces on individual atoms are calculated by ab-inito methods, and the parametrized potentials are adjusted to optimally reproduce these data. One difficulty with these aluminium-rich ternary alloys is that short distances between transition metals are rare in realistic reference structures, so that there is not enough data to determine the short-range part of the transition metal potential accurately. The diffusion properties, however, depend sensitively also on these parts of the potential. Nevertheless, for a number of important diffusion processes the energy barriers determined by molecular statics simulations agree well with the activation enthalpies determined by ab-initio simulations and experimental data.

MM 24.3 Wed 14:30 IFW D

Planar binary dipolar colloidal quasicrystals — •Johannes Roth and Ulrich Koschella — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

The stability of planar binary decagonal quasicrystals interacting by dipolar potentials has been studied recently [1] with the help of computer simulations. Here we present new results from the search for possible decagonal and dodecagonal ground states. We discovered a path linking the quasicrystal structures with the best crystalline configurations. Although this proves that the quasicrystals cannot be the ground state in general we can argue that the quasicrystal structures have an advantage if the energy of grain boundaries between different phases and structural relaxations are taken into account. The results are confirmed by Monte-Carlo simulations.
[1] F. Scheffler, P. Maass, J. Roth, and H. Stark, European Physical Journal B **42**, 85 (2004)

MM 24.4 Wed 14:45 IFW D

Structure factor of the harmonic Fibonacci chain — •Steffen Sonntag, Michael Engel, Hansjörg Lipp, and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

In quasicrystals peculiar dynamic modes, the phasons, are existing in addition to the usual phonons. However, experimentally little is known about their precise nature. In order to investigate the interplay between phasons and phonons on an elementary level we resort to various one-dimensional model systems and study them with a special molecular dynamics code. Our main observables of the dynamics are the coherent and the incoherent dynamical structure factor. In a first talk we present simulation results for harmonic chains, (i.e. chains without phason flips), especially the harmonic Fibonacci chain. The structure factor consists of one-phonon and multi-phonon branches arranged periodically or quasiperiodically and is resolved in great detail by our algorithm. Comparison is made to analytical calculations which can be performed for certain approximations. The examination of the harmonic Fibonacci chain is prerequisite for separating phonon and phason dynamics in a chain with flippable atoms.

MM 24.5 Wed 15:00 IFW D

Structure factor of the dynamic Fibonacci chain — •Michael Engel, Steffen Sonntag, Hansjörg Lipp, and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

We have constructed an anharmonic chain, denoted "dynamic Fibonacci chain", where neighbouring atoms interact by double-well potentials. Thus they are able to perform both harmonic motions and phason flips where short and long atomic separations are exchanged. Molecular dynamics simulations show that the difference between the coherent and incoherent structure factors of the dynamic and the harmonic Fibonacci chain is in general tiny and has the form of a characteristic broadening of the phonon branches. We ascribe it to the phasons flips. The temperature dependence of the broadening is discussed. Attempts are made to filter out the flip dynamics by suppressing the harmonic motion. If a bias is introduced in the well depth, broadened optic phonon bands split off. In direct space we observe correlated phason flips propagating with phonon excitations.