INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

Prof. Hans-Rainer Trebin

Institute for Theoretical and Applied Physics
University of Stuttgart, Germany

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Phason paradigms tested on a virtual quasicrystal

Phasons are a special kind of elementary excitations in quasicrystals. They show up as correlated flips of atoms between neighboring split positions. Phason fluctuations have been observed by quasielastic neutron scattering, in x-ray speckle patterns and in electron microscopy. Phason walls follow dislocations. Since the early stages of quasicrystal research speculations exist that there is a phason induced diffusion of atoms [1] and that phasons contribute to an entropic stabilization of quasicrystals [2]. We have found a simple double well interaction potential that makes a monatomic two-dimensional melt grow into a decagonal quasicrystal upon cooling by molecular dynamics simulations [3]. This virtual quasicrystal allowed us to perform numerical experiments of phason dynamics and to determine the free energy. Indeed, it could be verified that phason induced diffusion exists. The temperature dependence of the phason elastic constants could be measured. It could be confirmed that at low temperatures an energetically stabilized periodic structure exists, that turns into a quasicrystal due to the configurational entropy of the phasons.

[1] Kalugin P.A., Katz A. 1993 Europhys. Lett. 21, 921
[2] Elser V. 1989 in: Extended Icosahedral Structures, Eds. Jaric M.V. and Gratias D., pp. 105-136, Academic Press
[3] Engel M., Trebin H.-R. 2007 Phys.Rev.Lett. 98, 225505