



Contribution ID: 79

Type: Talk

【161】 Oscillatory dynamics in simple systems at elevated temperatures – beyond a perturbational treatment of anharmonicity

Friday, 3 September 2021 11:15 (15 minutes)

The anharmonicity of atomic couplings, responsible e.g. for finite heat conductivity in crystals due to phonon-phonon scattering, is most fundamentally accessible as broadenings of phonon dispersions or finite lifetimes.

Here we will compare inelastic neutron scattering on fcc-Al up to the melting point to ab initio calculations of q -dependent line broadenings [1]. Further, an analysis of the atomic interaction constants will show how to construct numerically efficient phenomenological potentials that accurately reproduce anharmonic properties as computed by DFT at very small computational effort, and finally the limitations of perturbation-derived linewidths will be elucidated.

[1] A. Glensk et al., Phys. Rev. Lett. 123, 235501 (2019)

Primary author: LEITNER, Michael (Technische Universität München)

Co-author: Dr GLENSK, Albert (Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland and Max-Planck- Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany)

Presenter: LEITNER, Michael (Technische Universität München)

Session Classification: Condensed Matter Physics

Track Classification: Condensed Matter Physics (KOND)