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Temperature dependence and linewidths of Al phonon dispersions

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The availability of accurate phonon dispersions for all temperatures up to the melting point is essential for the prediction of thermodynamic stabilities of crystal structures. Standard ab initio approaches are based on a quasiharmonic (QH) approximation of the interaction potential, where temperature dependencies enter only via the volume expansion. We have recently developed an extension of the QH approach [1] that uses the asymmetry of the nearest-neighbor potential. The approach allows us to perform computationally efficient molecular dynamics simulations with full ab initio accuracy. The predictive power of the resulting temperature dependencies and phonon linewidths is determined in this study. We have chosen Al for this purpose, since it is isotopically pure, non-magnetic and its electronic structure is known to be adequately described by density-functional theory.
Here, we report for the first time measurements of the entire phonon dispersion of Al at temperatures of 293 K, 700 K, 800 K and 900 K, as well as of high symmetry points at additional temperatures between 15 K and 700 K. The experiments were performed at the thermal triple axis neutron spectrometer PUMA at FRM II in Garching, Germany. The presented results give access to the temperature dependent longitudinal and transversal phonon branches in the high symmetry directions including the evaluation of phonon broadening. The combination of the comprehensive theoretical and experimental data allows an evaluation of anharmonic contributions beyond Grüneisen theory to the phonon dispersion and of the temperature dependence of phonon linewidths in metals.

[1] A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer, to appear in Phys. Rev. Lett. (2015)

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