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Anharmonic phonons at elevated temperatures in Al: experiment and ab initio predictions

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The importance of anharmonicity for describing fundamental materials properties, starting from finite heat conductivity due to phonon-phonon scattering, can hardly be overemphasized. For crystalline matter, the pertinent information is captured to a large part by considering q-dependent phonon lifetimes, leading to a broadening in energy of the phonon dispersions. The prevalent way of computing these broadenings theoretically is by employing perturbation theory, being of comparable effort as the computation of the dispersions in the harmonic approximation. Conversely, the experimental determination of phonon linewidths is much more involved, and only a small number of data sets covering large parts of reciprocal space at elevated temperatures, where anharmonic effects will be most pronounced, have been reported. Thus, theoretical computations today go largely unvalidated.

Here I will consider the case of elemental Al at temperatures up to the melting point. I will present experimental data obtained by inelastic neutron scattering with consideration to the necessary steps in data analysis for being able to extract the inherent linewidths. Further, I will present calculations of q-dependent line broadenings on the basis of density-functional theory, both in the standard approach of perturbation theory as well as via ab initio molecular dynamics, and discuss their discrepancies. Finally, I will analyse the short-range atomic interactions and show how numerically efficient phenomenological potentials can be constructed that allow to compute anharmonic properties beyond the limitations of perturbation theory at very small computational effort.

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