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Lattice anharmonicity revealed by nuclear resonant inelastic x-ray scattering

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Nuclear Resonant Inelastic X-ray Scattering (NRIXS) is a spectroscopy method to study atomic vibrations and dynamics, currently done with synchrotron radiation at a few high energy third generation facilities. It finds a wide range of applications in condensed matter physics, materials science, chemistry, biophysics, geosciences, and high-pressure researches. Many atomic dynamics and lattice thermodynamics information can be derived from NRIXS measurements. Phonon Density of States (DOS) characterizes lattice dynamics of a material and can be derived under the {\it quasi}-harmonic approximation. Combined with modelling and simulations, results from NRIXS can provide unique and clarifying insights into many fields of research.

The interpretation of NRIXS measurements has been done mostly in the context of {\it quasi}-harmonic approximation. Phonon density of states and dynamic properties like mean kinetic energy and mean force constant can be derived.

Going beyond the harmonic lattice model, we show that the anharmonic terms in the lattice potential can be measured. This opens up the NRIXS method to study anharmonicities in materials.

Given any {\it ab initio} model or specific model of lattice potentials, one can calculate the moments of a would-be measured NRIXS spectrum. Comparing them with NRIXS measurement results will help to restrict and adjust the models and calculations.

We will present a study of lattice anharmonicity in the sigma phase of Fe-Cr alloy, particularly the anomalous effect of magnetic structure on lattice dynamics.

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