Anharmonic correlated Einstein-model Debye-Waller factors

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Abstract: An anharmonic correlated Einstein model is derived for local vibrational amplitudes in x-ray-absorption fine structure (XAFS) that takes into account all near neighbors of absorber and backscattering atoms. The model is based on quantum thermodynamic perturbation theory and includes anharmonic effects based on empirical potentials. Calculations are presented for the second and third cumulants in XAFS as well as the net thermal expansion and thermal expansion coefficient. This model avoids full lattice dynamical calculations yet provides reasonable agreement with experiment. The generalization to displacement-displacement correlation functions and multiple-scattering Debye-Waller factors is also discussed.

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