

Study of EXAFS cumulants of crystals by the statistical moment method and anharmonic correlated Einstein model

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Abstract: The moment method in statistical (SMM) dynamics and anharmonic correlated Einstein model (ACEM) are used to study the cumulants of crystals taking into account the anharmonicity effects of the lattice vibrations. Analytical expressions for the mean square displacement (MSD) $\langle u^2 \rangle$, and the cumulants ($\sigma^{(1)}$, $\sigma^{(2)}$) of crystals in the X-ray absorption fine structure (XAFS) have been derived. We have presented the SMM formalism and ACEM by using the Lennard-Jones and Morse interaction potentials. Numerical results for $\sigma^{(1)}$, $\sigma^{(2)}$ of Cu, Pt, and Fe crystals are found to be in good agreement with experiment and other theoretical calculations. © 2010 Elsevier B.V. All rights reserved.

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