

A new anharmonic factor and EXAFS including anharmonic contributions

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Abstract: A new anharmonic factor and the extended X-ray absorption fine structure (EXAFS) including anharmonic contributions have been developed based on the cumulant expansion and the single-shell model. Analytical expressions for the anharmonic contributions to the amplitude and to the phase of the EXAFS have been derived. The EXAFS and its parameters contain anharmonic effects at high temperature and approach those of the harmonic model at low temperature. Numerical results for Cu agree well with experiment. Peaks in the Fourier transform of the calculated anharmonic EXAFS for the first shell at 297 K and 703 K agree well with the experimental ones and are shifted significantly compared to those of the harmonic model. ?? 2003 The Physical Society of Japan.

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