

Pressure effects in DebyeWaller factors and in EXAFS

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Abstract: Anharmonic correlated Einstein model (ACEM) and statistical moment method (SMM) have been developed to derive analytical expressions for pressure dependence of the lattice bond length, effective spring constant, correlated Einstein frequency and temperature, DebyeWaller factors (DWF) or second cumulant, first and third cumulants in Extended X-ray Absorption Fine Structure (EXAFS) at a given temperature. Numerical results for pressure-dependent DWF of Kr and Cu agree well with experiment and other theoretical values. Simulated EXAFS of Cu and its Fourier transform magnitude using our calculated pressure-induced change in the 1st shell are found to be in a reasonable agreement with those using X-ray diffraction (XRD) experimental results. ?? 2010 Elsevier B.V. All rights reserved.

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