

X-ray absorption fine structure calculations for copper

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Extensions of the Finite Difference Method for Near Edge Structure (FDMNES) are employed to calculate X-ray Absorption Fine Structure (XAFS) for solid state copper. These include the incorporation of a Monte Carlo frozen phonon technique to simulate the effect of thermal vibrations under a correlated Debye-Waller model, as well as a consideration of the XAFS broadening induced by the finite photoelectron inelastic mean free path. Spectra are obtained over an energy range in excess of 300eV above the K absorption edge, which is more than twice the greatest energy range previously reported for a solid state calculation using this method.

The dominant theoretical techniques currently used in the literature to model these systems in the XAFS region are the muffin-tin approach, the discrete variational method and the full linear augmented plane-wave approach. The near-edge region is considered in order to examine the applicability of FDMNES. We find that FDMNES can be extended successfully from the near edge region to the dominant XAFS regime.

These calculations are compared to high precision measurements of the x-ray mass attenuation coefficient for copper. This paper relates to experimental data measured on an absolute scale to high accuracy, and reveals considerable agreement but also particular areas of discrepancy. Results agree with current experimental data to within ~3%, a significant improvement over previous non-muffin tin calculations.