Treatment of disorder in XANES by RMC simulations

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X-ray absorption spectroscopy (XAS) is a powerful tool to probe the local, atomic and electronic structure of a material. Extended X-ray absorption fine structure (EXAFS) contains information on local structure around absorbing atom (interatomic distances, bond angles, means-square relative displacements (MSRD factors)). X-ray absorption near-edge structure (XANES) gives insights in to the chemical bonding and local environment (valence, coordination, structural disorder) in a material. The interpretation of EXAFS and XANES spectra is not straightforward and often requires the use of advanced simulation tools. Treatment of thermal fluctuations and static disorder in XAS is a complex task, which can be successfully addressed by reverse Monte Carlo (RMC) method [1, 2].

In this study, we first apply RMC simulations based on evolutionary algorithm (EA) to analyse the temperature-dependent (23-700°C) Cu and Mo K-edge EXAFS spectra of $CuMoO_4$. This method allows one to obtain structural model of such complex material as copper molybdate accounting for multiple-scattering effects as well as structural and thermal disorder contributions in the experimental EXAFS data.

At the next step, the structural models obtained by RMC were used to simulate the Cu K-edge XANES spectra, in which the temperature effect is the most pronounced. XANES calculations were performed by ab initio FEFF [3] and FDMNES [4] codes. The simulated XANES spectra are in good agreement with the experiment and reproduce the main temperature-dependent XANES features. It is important to note that the use of equilibrium atomic positions obtained from diffraction does not allow one to achieve good agreement with the experiment even when temperature dependence of the unit cell parameters is considered.

References

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