

RMC analysis of EXAFS spectra of metal ions in aqueous solutions

Alexei Kuzmin¹, Aleksandr Kalinko², László Pusztai³

¹Institute of Solid State Physics, University of Latvia, Latvia

²Universität Paderborn, Naturwissenschaftliche Fakultät, Department Chemie, Germany

³Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Konkoly-Thege M. út 29-33, 1121 Budapest, Hungary
e-mail: a.kuzmin@cfi.lu.lv

Local environment of metal ions in aqueous solutions has been studied for a long time by X-ray and neutron scattering. X-ray absorption spectroscopy is a complementary technique which is well suited to address this issue due to element and short range order sensitivity. Several approaches are commonly employed to extract the structural information from the extended X-ray absorption fine structure (EXAFS) above the absorption edge of an element. The first coordination shell around metal ions can be easily analysed using conventional method based on the best-fit of EXAFS using some analytical (often Gaussian) distribution model for interatomic distances. However, in spite of structural disorder in solution, the EXAFS spectra of metal ions often contain high frequency contributions due to so-called multiple-scattering (MS) effects caused by high-order distribution functions or outer hydration shells. The analysis of these contributions is a complicated task and requires the use of constraints for structural parameters or advanced simulation methods such as molecular dynamics or reverse Monte Carlo (RMC) simulations. In this study, we demonstrate the use of the RMC method based on evolutionary algorithm [1] for the analysis of EXAFS spectra of several (Cu^{2+} , Zn^{2+} , Rb^+ , Cs^+) metal ions in aqueous solutions.

References

[1] J. Timoshenko, A. Kuzmin, and J Purans, J. Phys.: Condens. Matter **26** (2014) 055401