Direct Projection Analysis of EXAFS Modulations

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EXAFS modulations have been analysed using a direct projection method known from structure determinations using photoelectron diffraction [1,2]. In this method experimental EXAFS modulations are projected onto calculated ones with just one singular neighbouring atom at a series of distances. Compared to the usual analysis with a Fourier transform of the EXAFS modulation function, the systematic errors in initial values for nearest neighbour distances are significantly reduced from 40 - 80 pm to 10 - 20 pm. This improvement results from the correct treatment of the energy dependence of the phase shift within the scattering process at the neighbouring atom. Tests of the method are presented with experimental EXAFS modulations from $SrTiO_3$ and $BaTiO_3$ single crystals as well as from a newly discovered $BaTiO_3$ derived quasicrystalline film on a Pt(111) substrate [3].

References:

[1] P. Hofmann and K.-M. Schindler, Phys. Rev. B **47**, 13941 (1993).

[2] P. Hofmann, K.-M. Schindler, S. Bao, A. M. Bradshaw, and D. P. Woodruff, Nature **368**, 131 (1994).

[3] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature **502**, 215 (2013).