

Probing structural distortions with new high-precision resonant X-ray diffraction approach

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The variability of X-ray photon energy at synchrotrons presents unique capabilities to increase the contrast for the characterization of subtle structure deviations. Within Resonant X-ray Diffraction (RXD), tuning independent scattering contributions of selected, resonantly scattering atoms in the unit cell can even promote a total destructive interference of allowed Bragg reflections for a majority of structures. At a certain photon energy the structure factor vanishes, resulting a high contrast several orders of magnitude upon change of structural parameters. This permits to elucidate structural details with very high accuracy. Diminutive deviations of the ideal structure will change this specific energy in the RXD spectra giving access to e.g. static as well as dynamic atomic displacements.

We used this enhanced RXD approach for the first time to determine the crystal structure of a recently found, crystalline phase of strontium titanate SrTiO₃ formed under the influence of an electric field [1]. A loss of inversion symmetry had been evident from the experimental detection of pyro- and piezoelectricity for this phase [2, 3], but standard methods had failed to obtain the structural parameters. The measurements were performed in the vicinity of the Sr-K absorption edge on reflections with exactly one odd Miller index. With high structural precision of 1 pm the polar character of the tetragonal phase was validated in terms of BaTiO₃-like, polar displacements of titanium and oxygen in opposed directions along the applied field.

[1] Hanzig, J. et al. (2013). Physical Review B 88, 024104.

[2] Hanzig, J. et al. (2015). New Journal of Physics 17, 023036.

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