

Spin-resolved atomic orbital model refinement for combined charge and spin density analysis: application to the $YTiO_3$ perovskite

A new crystallographic method is proposed in order to obtain a spin-resolved atomic orbital model fitted against X-ray and polarized neutron diffraction data. This atomic orbital model will be applied to the $YTiO_3$ perovskite crystal, using high energy (short wavelength) SR and polarized neutrons diffraction data .The resulting experimental wavefunction gives radial extension, orientation and population of outer atomic orbitals for each atom and shows *ad orbital ordering* . The interaction term between Ti^{3+} , Y^{3+} cations and O^{2-} ligands will be discussed. The spin resolved electron density obtained by means of this orbital model will be compared to that obtained by the usual multipole model previously published

Keywords: synchrotron radiation and polarized neutrons diffraction; perovskite; spin density; charge density; $YTiO_3$; experimental orbital model