Electron Density in Cubic $SrTiO_3$ from γ–ray Diffraction

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The electron density and atomic displacements in the prototype perovskite $SrTiO_3$ have been studied using extensive and accurate γ-ray diffraction data (λ = 0.0392 Å) at room temperature. The 6 strongest structure factors have been determined under extinction-free conditions by means of an extended-face thin-crystal plate in Laue geometry, so that the lowest I_{obs}/I_{kin} ratio was 0.98 for the full data set. The maximum thermal diffuse scattering contribution was only 3% at $\sin\theta/\lambda = 1.72$ Å^{-1}.

The thermal displacement parameters are in good agreement with lattice dynamical calculations as well as with neutron diffraction results. Contrary to simple expectation, anharmonic motion effects are negligible for all atoms. This finding is consistent with a previous γ-ray study which revealed $SrTiO_3$ as a harmonic system at T_c + 5 K [1], *i.e.* very close to the antiferrodistortive phase transition.

The charge density was modeled using *VALRAY*. The population of the 3*d* subshell on Ti is found to be 0.200(45) |e|, *i.e.* close to zero, in agreement with the observed magnetic behaviour. The electronic properties at the bond critical points indicate ionic Ti-O and Sr-O interactions of different strength which is corroborated by the net charges of the atomic basins: q(Sr) = 1.18 |e|, q(Ti) = 3.10 |e| and q(O) = –1.42 |e|.

[1] Jauch W., Palmer A., *Phys. Rev. B*, 1999, **60**, 590.

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