



Neutron total scattering and reverse Monte Carlo Modelling of SrTiO₃

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Neutron total scattering contains two kinds of scattering. One is Bragg scattering in which the position of Bragg peaks can give a good determination of the lattice parameters and the intensities of Bragg peaks contain the information of the average positions of atoms. The other is diffuse scattering, which contains information of oscillations of the atoms from their mean positions. Thus the neutron total scattering patterns are able to contain simultaneous information about long-range and short-range of atomic structure. Strontium titanate in its tetragonal and cubic phases has been studied using Reverse Monte Carlo modelling of neutron total scattering data. In Rietveld analysis, neighboring octahedra in a (001) layer rotate around [001] in the opposite sense, with the octahedra in adjacent (001) layers rotating in opposite direction in tetragonal phase. In RMC model, the calculated actual distribution of oxygen atoms in both phases is around their mean positions. The movement of Sr²⁺ is circumscribed in the interstice formed by the surrounding eight TiO₆ octahedra. Local structures remain fairly constant and are relatively insensitive to the phase transition