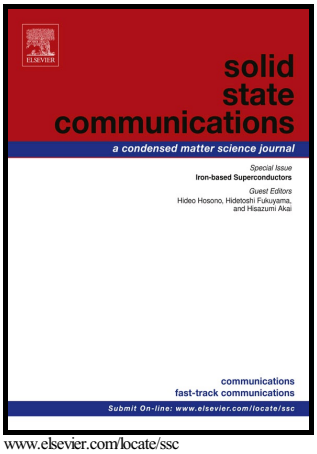

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Takamitsu Yamanaka., Muhtar, Takeyuki Suzuki

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Electron hybridization and anharmonic thermal vibration effect on structure transition of $SrTiO_3$ at high-pressure and low-temperature

Takamitsu Yamanaka[1,2], Muhtar [2], Takeyuki Suzuki[4]

[1]Department of Earth and Space Science, Graduate School of Osaka-University 1-1 Machikaneyama Toyonaka Osaka Japan, 560-0043

[2]Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China

[3]Carnegie Institution of Washington Geophysical Laboratory, 5251 Broad Branch Rd N.W. Washington DC 20015, USA

[4]Comprehensive Analysis Center, Institute of Science and Industrial Research, Osaka University 8-1 Mihogadake Ibaraki Osaka 567-0047

Abstract

We execute electron density analysis of $SrTiO_3$ at low temperatures up 80 K and high pressures up to 11.88 GPa using X-ray single-crystal diffraction and *ab initio* quantum chemical molecular orbital (MO) calculation. By changing pressures, the cubic $SrTiO_3$ with perovskite structure goes through a antiferroelastic distortion to tetragonal symmetry above the critical pressure P_c = 7 GPa with $c/a<1$ and decreasing with increasing pressure. On the other hand, by changing temperatures, the tetragonal distortion occurs below the critical temperature T_c = 105 K with $c/a>1$ and increasing with lowering temperature.

Difference Fourier (D-F) synthesis experimentally proves the residual electron densities $\Delta\rho(xyz)$ are associated with two different effects: electron hybridization bonding electron and anharmonic thermal vibration atoms. The *d-p-*π hybridization between Ti(3*d*) and O(2*p*) orbitals is confirmed in the residual electron density, which is deformed from the ideal spherical density conducted by the atomic scattering factor *fi* using Hartree-Fock (HF) approximation. MO calculation also reveals the electron hybridization. Anharmonic thermal vibration of atoms yields a large effect to the structure transition. Mulliken charges analysis of MO calculation indicates much smaller charges than their formal ionic charges. Their ionicity increases from cubic to tetragonal above P_c and below T_c.