

Lanthanum distribution in highly La-doped SrTiO₃ crystals

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Our interdisciplinary investigation has shown the heterogeneity of dopant distribution in lanthanum-doped strontium titanate (LSTO) single crystals with a five wt % doping level of La. Using the X-ray diffraction analysis and pycnometric density measurement; we have described a discrepancy between the theoretical density and experimentally determined value. The origin of this behavior could be either the creation of the voids in the matrix or the intergrowth of secondary phases with La surplus in the crystal. Transmission Electron Microscopy (TEM), Energy-dispersive X-ray Spectroscopy (EDX), and Selected Area Diffraction (SAD) microscopic investigation have confirmed the second hypothesis, namely that in different regions of LSTO, the local concentration of La shows a substantial variation in the micro- and nanoscopic scale. To study the influence of the La dopants on the electronic structure and, therefore, on the electrical conductivity, we have used the Local Conductivity Atomic Force Microscopy (LCAFM) method as a local electrical probe to map the electrical conductivity in-plane of the La-doped crystal's surface. The LCAFM conductivity maps reveal heterogeneous conductivity (here in the form of the bands with higher conductivity than the surroundings) related to band-like inhomogeneities of the La distribution. Using LCAFM measurements with atomic resolution obtained between the conducting and nonconducting regions, we analyze the spreading (spatial expansion) of doping on the undoped or low-doped part of the STO crystal. The found limitation of the doping effect of La on the dielectric part of the STO crystal to 4-5 lattice constants is in good correlation with *ab initio* studies from the literature and our recent work [1].

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References

1. Pilch M.M., Rodenbücher C., Krok F., Szot K., "Heterogeneity in La Distribution in Highly La-Doped SrTiO₃ Crystals", *Crystals* 13 (2023) 1552. <https://doi.org/10.3390/cryst13111552>