Structural and electronic properties of Fe-doped SrTiO\textsubscript{3} thin films revealing the importance of cation nonstoichiometry induced by pulsed laser deposition

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SrTiO\textsubscript{3} (STO) is one of the best investigated materials in solid state ionics and commonly used as a model material for perovskite-type oxides with large band gaps. The defect model of bulk SrTiO\textsubscript{3} is well understood and the conductivity of bulk samples can be tailored by acceptor or donor doping, e.g. with Fe\textsuperscript{3+} or Nb\textsuperscript{5+} on the Ti\textsuperscript{4+} site. However, the implications of cation nonstoichiometry are still not very well understood. Such a cation nonstoichiometry might become very relevant in thin films prepared by pulsed laser deposition (PLD) since an exact transfer of the target composition to the thin film is often not reached. This may be particularly important for low doped oxides.

In this study, the effect of cation nonstoichiometry on electronic properties in SrTiO\textsubscript{3} thin films is discussed and a model linking composition, structure and electrical conductivity is presented. Different kinds of 2 % Fe-doped SrTiO\textsubscript{3} thin films were prepared by modifying the target composition and the deposition parameters used for pulsed laser deposition (PLD). The composition of the thin films was measured by ICP-OES and a significant Sr deficiency was found for layers deposited from stoichiometric targets. Deposition from pellets with a Sr overstoichiometry, however, yielded stoichiometric thin films. Epitaxial thin films were analyzed by means of X-ray diffraction (reciprocal space mapping) and a shift in the out-of-plane lattice parameter was found depending on the concentration of Sr vacancies (see Fig. 1). The thin films deposited from a stoichiometric target exhibit conductivities close to the intrinsic conductivity of ultra-pure SrTiO\textsubscript{3}, despite Fe doping and cation nonstoichiometry. Deposition from a Sr overstoichiometric target, on the other hand, leads to thin films with a bulk-like conductivity (in accordance with doping). A model is presented which explains this unusual behavior. It is based on cation vacancies and antisite defects (Fe\textsuperscript{2+} on A sites). The validity of the model is tested by measuring the electrical behavior of nonstoichiometric bulk samples and comparing it with the thin film properties. This study also emphasizes that properties of slightly Fe-doped SrTiO\textsubscript{3} thin films strongly depend on the PLD process.