# Geometric Phase Analysis of the lattice distortion in $SrTiO_{3-x}:N_y$ single crystal and defects produced by microwave $NH_3$ plasma.

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Perovskite oxides have been the subject of intense research regarding their ferroelectric and dielectric properties. In particular, strontium titanate ($SrTiO_3$) is the foundation of the emerging field of oxides electronics [1,2]. Phenomena like 2D-Electron Gas or resistivity switching have been recently discovered upon material doping or fine compositional tuning in these perovskite materials.

The flexibility of the perovskite structure makes possible the substitution of the cationic position (Sr, Ti) as well as the anionic position (O). One method to introduce N into $SrTiO_3$ (STO) perovskite structure is by mean of microwave induced $NH_3$ plasma procedure. This is a two-step treatment where modifications of the chemical composition are used to change the electronic structure and properties [3]. The process consists in the formation of oxygen vacancies, and a second step of the anionic substitution $N^{-3} \rightarrow O^{-2}$. Substitution of $O^{2-}$ with $N^{3-}$ in perovskites is possible due to the similar ion size of both elements. However, due to the charge compensating mechanism complete anionic substitution of $O^{-2}$ by $N^{-3}$ keeping the perovskite structure cannot be realized without the presence of anionic vacancies. The concentration of vacancies collapses in dislocations, stacking faults and new structures or superstructures. Therefore, it is extremely demanding the careful characterization of defects produced during the ammonia plasma treatment.

Several questions arise in this work such as the defect types, how the lattice distortion is around the defect, the local change in composition, and where the N is inserted in the structure. The composition changes around the defects can be better studied by Z-contrast image and mapped with sub-nanometer spatial resolution utilizing electron energy loss spectroscopy (EELS) in scanning transmission electron microscopy. In one hand, STEM-EELS analysis shows an excess of Ti and N ion in the defect. On the other hand, Z-contrast STEM images show an interchange of Ti and Sr planes or depending on the region, an excess of Ti in the defect.

To analyse the local distortion around defects the Geometric Phase Analysis (GPA) method is used. This method calculates the local lattice distortion matrix $\boldsymbol{e(r)}$ with respect to displacement field $\boldsymbol{u(r)}$ [4], obtained from the phase images matrix. This matrix is then separated into the symmetric strain matrix, $\boldsymbol{\varepsilon(r)}$ and the rotation matrix, $\boldsymbol{\omega(r)}$. Strain is defined with respect to the undistorted lattice in the same sample, which is taken as a reference lattice. Figure 1 shows STEM-HAADF image of the [110] zone axis with defects along <001> direction. Figure 2a represents the GPA analysis in the calculation of the strain matrix component $\boldsymbol{\varepsilon_{xx}(r)}$ which is the one changing around the defects. A line profile of $\boldsymbol{\varepsilon_{xx}(r)}$ across the defect is shown in Figure 2b, where a positive variation is seen at the left side of the defect, representing a tensile strain of the lattice, and a negative variation at the right side, showing a compressive strain of the lattice.

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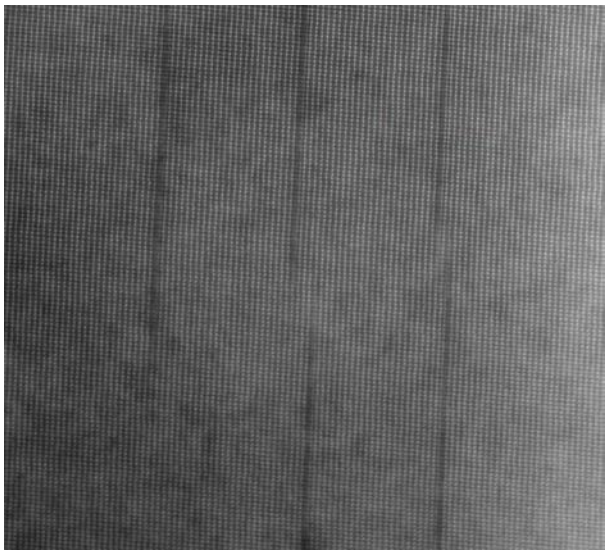

***Figure 1***: Z contrast STEM image of the [110] zone axis with defects along <001> direction.

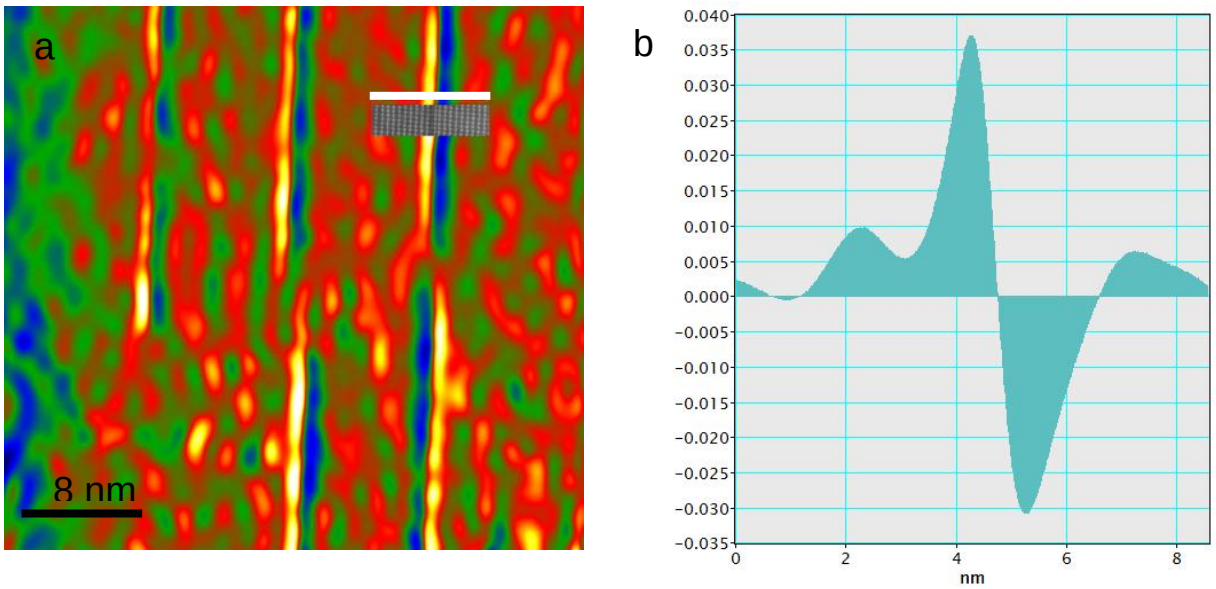


***Figure 2***: (a) Strain matrix component $\varepsilon_{xx}(r)$ of image in Figure 1, with the Z contrast STEM image region inserted. (b) Line profile $\varepsilon_{xx}(r)$ across the defect.