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Probing the Local Lattice Distortions in Doped $SrTiO_3$ Using Quantitative STEM

Salva Salmani-Rezaie[1], Honggyu Kim[1], Kaveh Ahadi[1] and Susanne Stemmer[1*]

[1.] Materials Department, University of California, Santa Barbara, CA, USA.
* Corresponding author: stemmer@mrl.ucsb.edu

$SrTiO_3$ is a cubic perovskite material that has been widely investigated because of its high electron mobility, superconductivity, and high permittivity. Undoped $SrTiO_3$ is a conventional band insulator. It can be doped by substitution of trivalent rare-earth elements (*R*), such as La or Sm, on the Sr^{2+} site. Each *R* ion donates one electron to the conduction band of $SrTiO_3$. In general, local lattice distortions around individual dopant atoms are believed to influence transport properties and their role as dopant atoms. For example, among the possible rare earth dopants, differences exist in ionic radius and other properties, such as number of unpaired f-electrons. Therefore, revealing the effect of individual dopants on the lattice could impact the understanding of the unique transport properties of $SrTiO_3$.

In this study, we investigate Sm-doped $SrTiO_3$ films grown by molecular beam epitaxy (MBE) on (001) $SrTiO_3$ single crystals. The carrier concentration, and thus the Sm concentration, was determined by the Hall effect and, for the samples investigated here, was about 2% and 3%, respectively. An undoped $SrTiO_3$ was used as a calibration sample to establish experimental noise and uncertainty. Plan-view TEM samples were prepared by mechanical polishing using a 1.5° wedge angle. HAADF-STEM images were recorded using an FEI Titan S/TEM operating at 300 keV with a semi-convergence angle of 9.6 mrad. To improve the signal to noise ratio and minimize scan distortion, 20 fast-scan images were recorded, cross-correlated and then averaged. The position of every atomic column was determined by fitting to subsequent 2D Gaussian function to obtain sub-pixel resolution. The atomic column intensities were measured by utilizing quantitative STEM (QSTEM) technique. Previously, this technique has been applied to detect the dopant atom and determine its 3D configuration in the Gd-doped SrTiO3 [1, 2]. In this work, we apply the same technique to determine the location of the Sm dopant atoms. Furthermore, we investigate the local lattice distortion induced by Sm dopants. Our study shows that Sm dopants cause the displacement of Ti atoms from their ideal positions. The number of distorted columns in the images correlates with the dopant concentration.

Figure 1(a) shows a representative image of a Sm-doped $SrTiO_3$ film recorded along [001]. Intensity maps of the Sr-Sm and Ti-O columns [Figs. 1(b,c)] are extracted from Fig. 1(a). The spread of data points of undoped $SrTiO_3$ was used to approximate the experimental error function for the column intensity. Sr columns with intensity values above the experimental cutoff contain Sm dopants. The Sr column labeled in Fig. 1(b) with high intensity and uniform $I_{Ti\text{-}O}$ in Fig. 1(c) defines the column with Sm dopant. Figure 2 shows I_{sr} as a function of the $I_{Ti\text{-}O}$ for 2% and 3% Sm-doped $SrTiO_3$. The data for a small region of undoped $SrTiO_3$ is presented in Fig. 2(a). The experimental error function is determined by the standard deviation of the difference between experimental data points and the linear data fit. With increasing the amount of Sm doping, more points lie above the experimental cutoff region [Figs. 2(b,c)]. To study the effect of the Sm dopant on local structural distortion, the displacement vector corresponding to the Ti column was calculated. The displacement is calculated as the difference between its actual atom position obtained by Gaussian peak fitting and the center of mass of surrounding four Sr (Sm) atoms. Figures 3(a-c) show the displacement vector for the samples. By increasing the dopant concentration, an increasing degree of local column displacement can be detected. This can also be seen in the contour plot of the

displacement vectors [Figs. 3(d-f)]. We will discuss the role of the local structural distortion in the properties of doped $SrTiO_3$ [3].

References:

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[2] J Zhang et al., Sci. Rep. **5** (2015), p. 12419.
[3] The authors acknowledge support by the U.S. Department of Energy (Grant No. DEFG02-2ER45994).

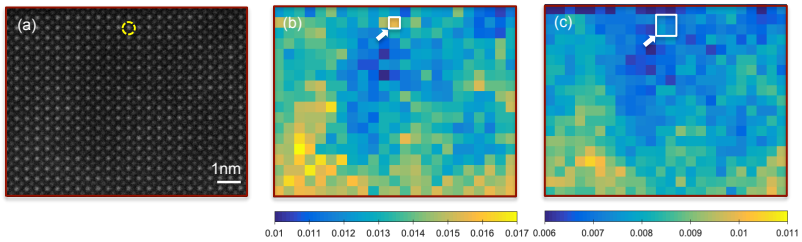

Figure 1. (a) HAADF-STEM image of Sm-doped $SrTiO_3$. (b) I_{Sr} and (c) $I_{Sn\text{-}O}$ maps from the image shown in (a).

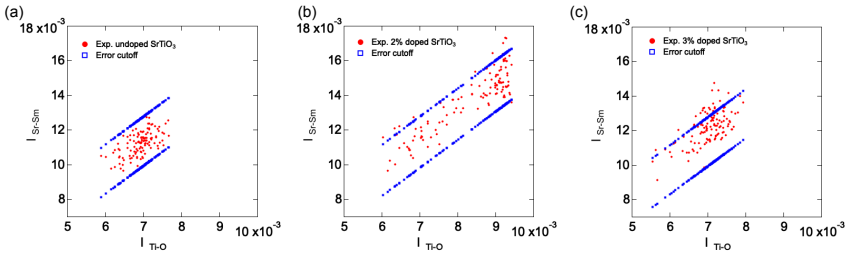

Figure 2. Sr column intensity as a function of the Ti-O intensity for (a) undoped (b) 2% Sm-doped and (c) 3% Sm-doped $SrTiO_3$.

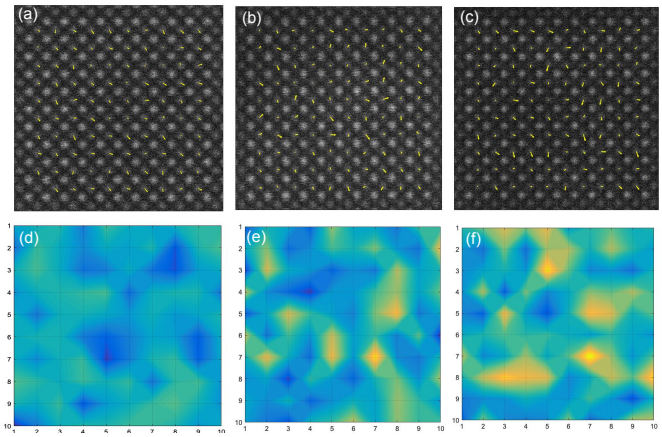

Figure 3. Displacement vectors and contour plots of (a,d) undoped (b,e) 2% Sm-doped and (c,f) 3% Sm-doped $SrTiO_3$.

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