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Cross-Sectional Characterization of $SrTiO_3$/Si(001) Interfaces using Aberration-Corrected STEM

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$SrTiO_3$ (STO) is the only perovskite oxide that can be epitaxially grown directly on Si making it an excellent intermediate layer for the integration of other functional perovskite oxides on Si. STO grows such that there is a 45° relative rotation with the underlying Si resulting in a small lattice mismatch of 1.7%, with the STO under compression [1]. To date, the exact atomic structure of the interface is still not settled and this study can shed more light about the physical structure of the STO/Si(001) interface. In this work, 5 monolayers of single-crystal STO were grown directly on Si(001) by molecular beam epitaxy (MBE) with a variant of the Motorola-developed process. After cleaning and desorbing the native oxide layer, a half monolayer of Sr was deposited at 550 °C on a clean Si(001) surface with 2×1 reconstruction. Sr and Ti were then co-deposited at 200 ℃ to the desired thickness with oxygen ramping. The STO layer was then crystallized by annealing for 5 minutes under vacuum at 550 °C [2]. Samples for TEM observation were prepared via standard cross-section method with ion milling. Aberration-corrected STEM images to characterize the interface were recorded with a JEOL ARM 200F operated at 200 keV.

Figures 1(a) and (b) are BF and HAADF STEM images showing the sample structure with a thin STO film on top of Si substrate. The projection orientation is [100] for the STO layer and [110] for the Si. A short STO section of different <110> orientation, as arrowed in figure 1(a), as well as slight crystal rotations are visible. These defects may be formed to release strain within the STO layer because of the lattice mismatch with Si. A vertical offset in the STO layer can also be observed, as arrowed in figure 1(b), with a magnified image of the marked area in figure 1(c). The line profile shown in figure 1(d) indicates that an Sr atom column is adjacent to a Ti atom column to the right of the arrow. In figure 2, two different Si terminating surfaces are observed at the interface. Half Si dimers are visible at the STO/Si interface in figures 2(a) and (b). Figure 2(e) is the line profile after Gaussian blur of figure 2(b) showing Si dimers in the substrate and a half dimer at the interface with adjacent Ti. The distance between the Si dimer and the first Ti atom column is ~0.384 nm. On the other hand, full Si dimers are visible continuously from the substrate to the interface in figures 2(c) and (d). The same result can be seen in the line profile, as shown in figure 2(f) after Gaussian blur. The distance between the last Si dimer and the first Ti atom column is ~0.386 nm [3].

References:
[1] J.H. Hao, *et al., Appl. Phys. Lett.* 87 (2005) 131908.
[2] L. Ji, *et al., Nat. Nanotechnol.* 10 (2015) 84.
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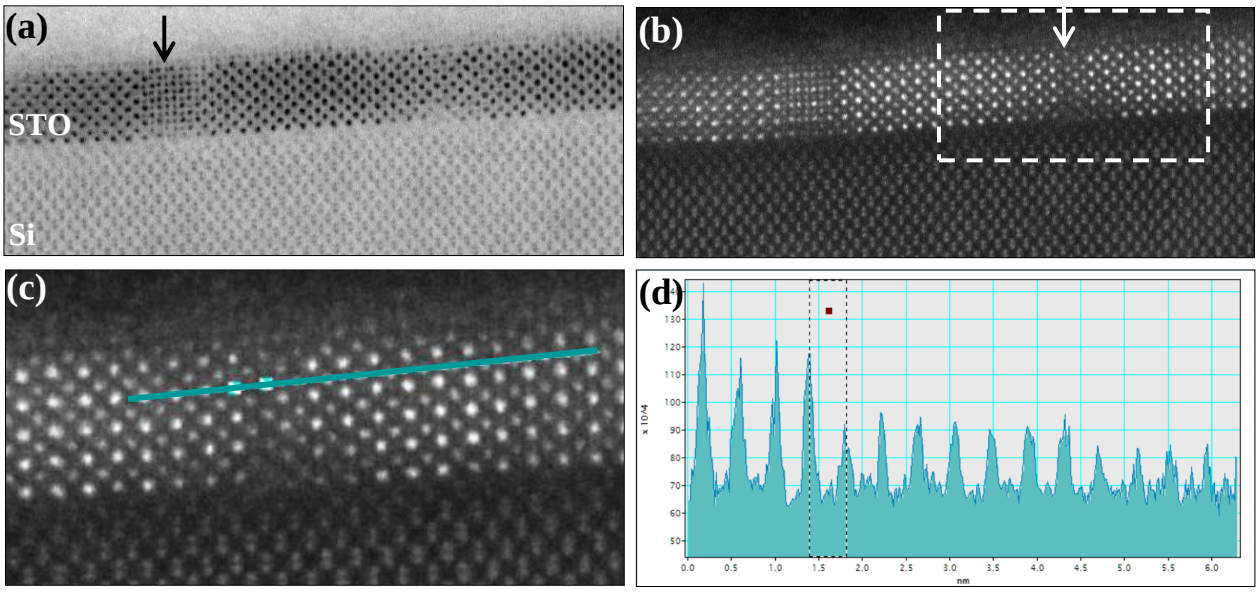

Fig. 1. (a) BF, and **(b)** HAADF, images showing a short section of different STO orientation (arrowed in the BF image) and a vertical offset in the STO unit cell (arrowed in the HAADF image); **(c)** Magnified image of area marked in (b); **(d)** Line profiles of (c) showing the vertical intensity offset.

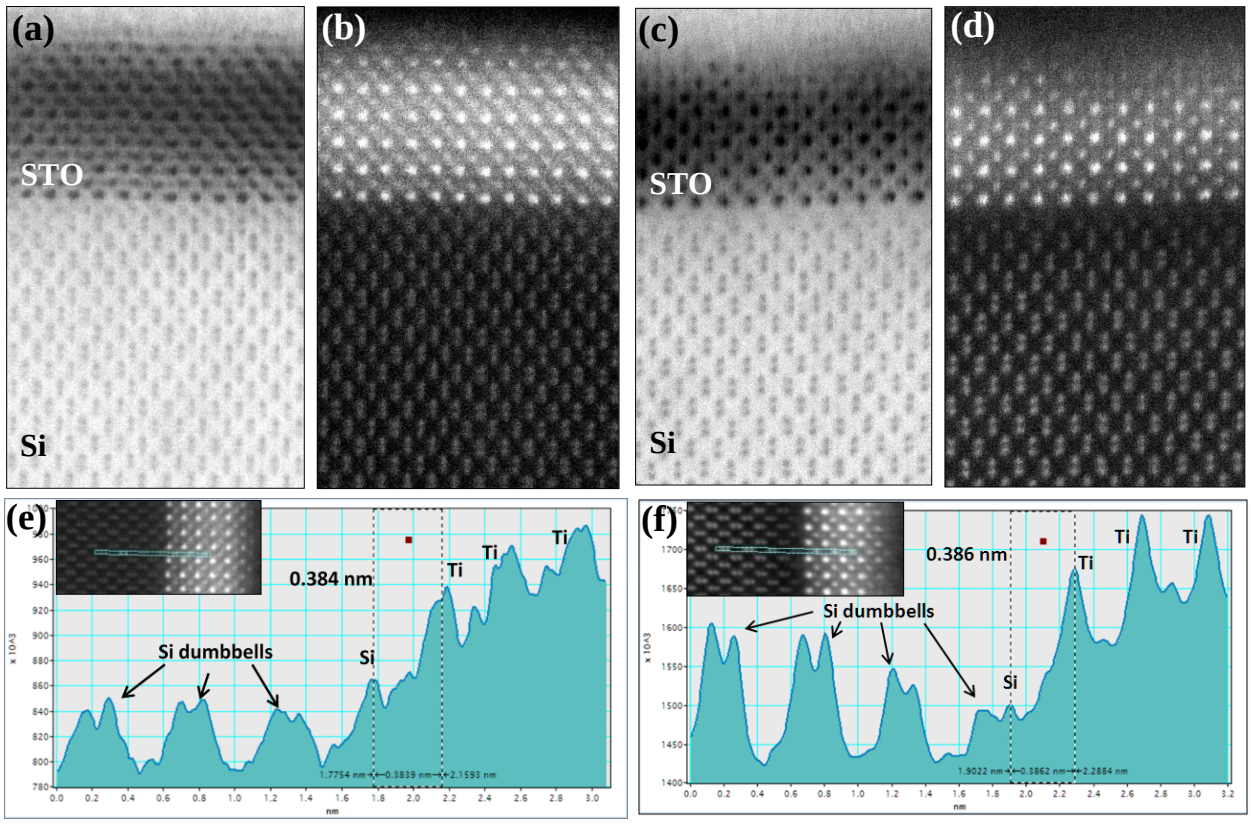

Fig. 2. (a) BF, and **(b)** HAADF, images of $SrTiO_3$/Si interface with half Si dimers. **(c)** BF, and **(d)** HAADF, images showing full Si dimers at the $SrTiO_3$/Si interface. **(e)** Line profile of (b) after Gaussian blur showing half Si dimer at the interface. **(f)** Line profile of (d) after Gaussian blur showing full Si dimer at the interface.

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