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Study of Sub-atomic Channeling in $SrTiO_3$ Crystal Along <100> Direction Using *Multislice* Simulations

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With aberration correction to the lenses, transmission electron microscopes (TEMs), the field of analytical scanning TEM (STEM) reached a new realm in resolution [1]. Imaging atomic columns in the crystals sub-Å apart and even individual atoms has been achieved [2, 3]. Atomic-resolution spectroscopy followed the atomic-scale imaging [4]. These advances in the STEM instrument enable researchers to pursue new challenges, offering a window into sub-atomic physics and materials science, which were not considered doable before. For example, Muller et al. [5] reported that it is possible to measure sub-atomic electrical fields inside the crystals using the aberration-corrected STEM. Additionally, Jeong et al. [6] reported that it is possible to probe core electronic orbitals of the atoms.

Here, inspired by recent advances in the experimental sub-atomic measurements using the aberration-corrected analytical STEM, we present a study of electron probe propagation in the crystalline material at sub-atomic length scale. We found an existence of sub-atomic channeling with unique characteristics and a formation of a helicon-type spiraling beams, showing that there is a rich sub-atomic science to be explored using the available aberration-corrected analytical STEMs. This study focuses on the understanding of the STEM probe propagation through a perovskite $SrTiO_3$ crystal along the <100> crystallographic direction with three distinct atomic columns [7].

The propagation of the aberration-corrected STEM probe in the $SrTiO_3$ was studied as a function of the distance of the probe from the atomic column at sub-atomic distances. This simulations were carried out using the *Multislice* method as implemented by the TEMSIM code [8]. The beam propagation simulations are performed at different crystal temperatures and at different STEM probe convergence angles (10 to 50 mrad), and beam energies (80 to 300 keV).

As can be seen from Fig. 1, when the probe is located exactly on top of the atomic columns, for instance Sr and Ti/O, the expected on-column channeling is observed. However, when the probe is slightly off from the atomic column, at a distance smaller than the size of the atomic dimensions, the on-column channeling disappears; instead, the propagating beam oscillates back and forth around the center of the atomic column, like a pendulum, which is the 'sub-atomic' channeling. Additionally, when the probe is present in certain locations, i.e., very close to the O column, the propagating probe form a helicon-type spiraling beam, circulating around the O column (Fig. 2). We also studied STEM probe parameters, which can be used to control the intensity of these helicon-type beams [9].

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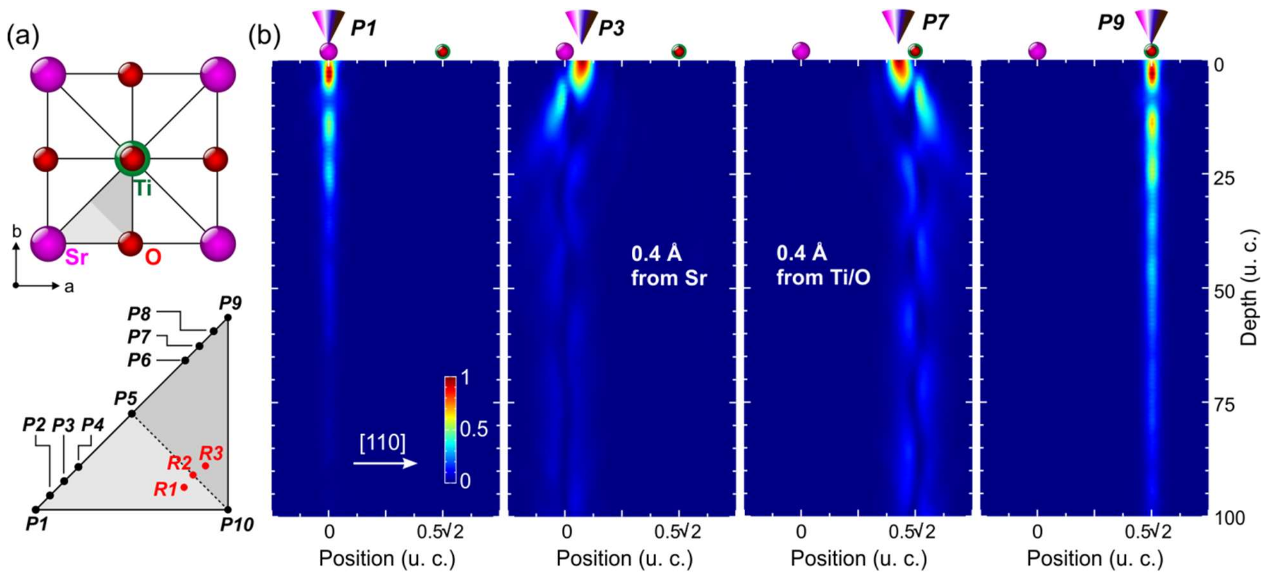

Figure 1. (a) Schematic illustration of a $SrTiO_3$ unit cell viewed along the <100> direction. STEM probe positions (P1-P10 and R1-R3) studied in this work are shown. (b) Examples of two-dimensional beam intensity depth profiles of a simulated STEM probe when the probe moves from Sr to Ti/O atomic columns with sub-atomic steps.

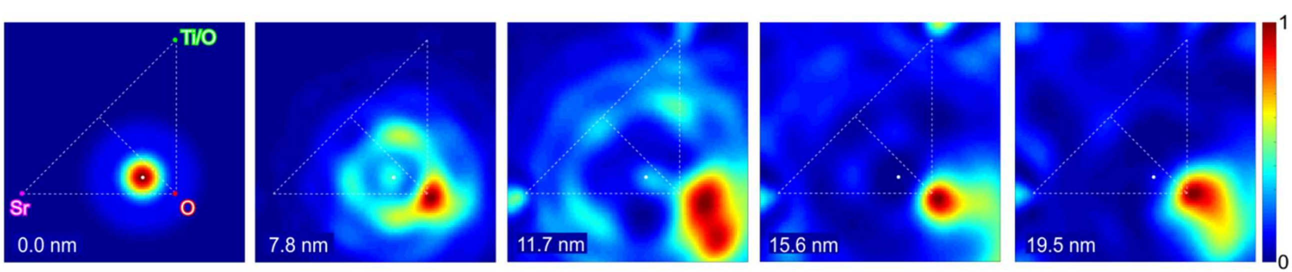

Figure 2. Beam propagation through the $SrTiO_3$ crystal viewed along the <100> direction showing formation of the helicon-type beam. Here the STEM probe is located at the asymmetric position around O atomic column.

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