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Measuring the Cation and Oxygen Atomic Column Displacement at Picometer Precision

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The multifaceted magnetic, electrical, and structural functionalities of perovskite oxides critically depend on distortions of their crystal lattice [1]. These distortions include the displacement of cations, deformation of oxygen octahedra (BO_6, where B is a transition metal atom), and collective tilts of the octahedral network. Atomistic understanding of these distortions and elucidation of their influence on the final properties requires imaging and measuring of atomic positions for both cations and oxygen.

In this work, we present imaging and quantification procedures on a routine basis for perovskite oxides at picometer precision, from series data acquisition, multi-frame image alignment, to final image quantification. For the data acquisition, three scanning modes have been implemented in the multi-frame images acquisition, i.e. conventional raster, orthogonal, and rotation scan [2, 3]. The image stacks were then aligned by rigid and non-rigid registration (NRR) methods [4–6]. The final aligned images were analyzed using the oxygen-octahedra picker software [7]. To evaluate the measurement precision and the noise level (by including different numbers of averaged frames) influences on the atomic column center detection, we measure the Ti–Sr and Ti–O atomic column distances on ADF and ABF images, respectively. The measurements precision was defined as the standard deviation of the measured distances. As shown in Fig. 1, in general, the statistical precision improves when increasing the number of averaged frames. Experimentally, we demonstrate that under a daily reproducible working condition (sample drift and slight sample contamination present), one can achieve 3 pm and 4 pm precision for ADF and ABF images, respectively [7]. With NRR alignment, the measurement precision is further improved. Fig. 2 shows the details of the measurement precision on rigidly and non-rigidly aligned images. Finally, the application of the picometer precision measurement at hetero-structure interfaces will be discussed [8].

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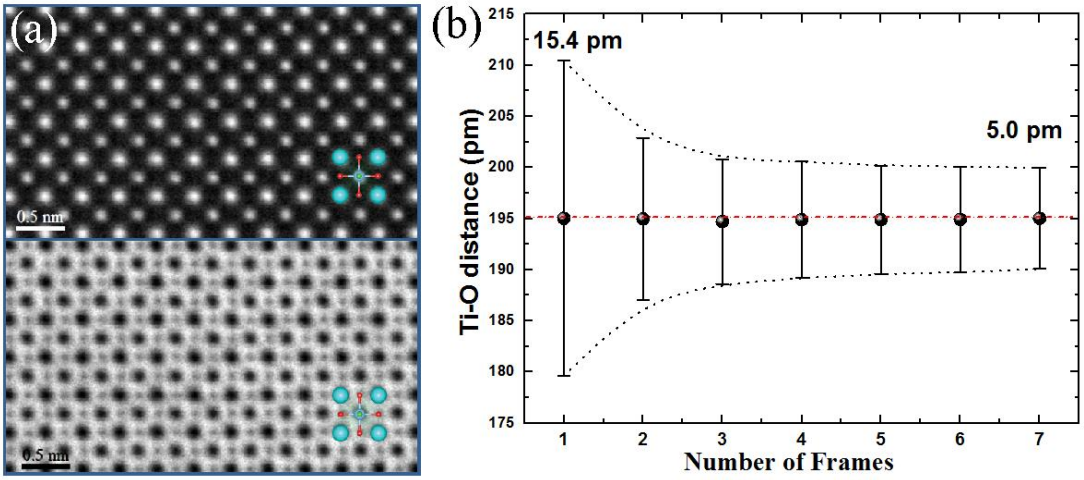

Figure 1. (a) Simultaneously acquired ADF and ABF images of $SrTiO_3$ along the [001] zone axis. (b) Influence of the number of averaged frames on the statistical precision. The solid sphere gives the averaged value (the red dash-dotted line shows the theoretical Ti–O distance of $SrTiO_3$ along the [001] projection), and the error bars show standard deviations.

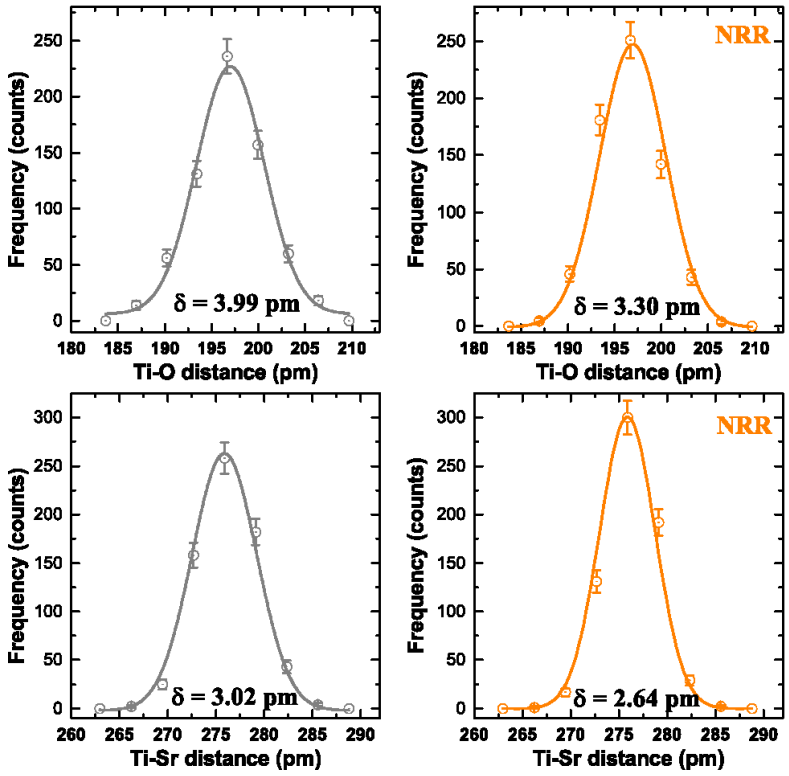

Figure 2. Histograms of the measured Ti–Sr and Ti–O atomic column distances for ADF and ABF images, respectively. Gray and orange represent the measurement performed on the rigidly and non-rigidly aligned image series. The statistics are based on 168 TiO_6 octahedra (12 u.c. x 14 u.c.) measurements. 7 frames were acquired with a short dwell time (2 µs per pixel), the frames were then aligned by rigid and NRR methods.

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