The (001) Surface of SrTiO₃: a Grazing-Incidence X-Ray Diffraction Study

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The (001) surface of $SrTiO_3$ (STO) serves as a popular substrate for the epitaxial growth of perovskite thin films, and much work, using AFM, STM, TEM, electron diffraction, ion-scattering and theoretical simulation, has been performed in an effort to understand its atomic structure. In comparison, very little grazing-incidence X-ray diffraction (GIXD) data is available, and to date, no agreement exists as to the atomic arrangement. We have prepared a crystal surface with hydration/etching, and using AFM and X-ray photoemission spectroscopy, we could verify that the termination is purely TiO₂. We then performed GIXD at the Materials Science Beamline of the Swiss Light Source synchrotron. The use of a novel 366 x 157 element "pixel detector" capable of low-noise, single-photon counting, allowed us to efficiently collect diffraction data on the surface-sensitive "crystal-truncation-rods" in reciprocal space. The resulting data set, a total of 1840 points along 27 integral- and fractional-order rods, was fit to an atomic model which includes both (2x2) and (2x1) surface reconstructions. The result is a consistent description of the (001) STO-surface at the atomic level.

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