Structural Evolution of TiO_2 during Stoichiometry Restoration after Ion-Beam Modification

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Titanium dioxide (TiO_2) is a technologically important transition metal oxide extensively used in catalysis, sensing, and oxide electronics. Beyond its applications, TiO_2 serves as a model material for studying defect formation, irradiation effects, and ion-driven structural transformations. Its surfaces exhibit moderate chemical reactivity and a pronounced ability to sustain ionic migration, making TiO_2 particularly suitable for investigating ion-beam induced reduction, defect engineering, and subsequent redox-driven structural evolution.

In this presentation, we report on TiO_2 surface modification induced by 2 keV Ar^+ ion irradiation at moderate fluences up to 10^{17} ions/cm^2. The resulting structural and electronic changes were investigated using local-conductivity atomic force microscopy (LC-AFM) and in situ electron diffraction techniques (μLEED/LEEM) and X-ray photoelectron spectroscopy (XPS). Ion irradiation produces a strongly reduced near-surface region extending up to several tens of nanometers.

Subsequently, we track the structural and electronic evolution of the irradiated crystal during annealing in ultra-high vacuum. We demonstrate that thermal reoxidation of the ion-beam modified surface occurs already below 400 ºC, at temperatures significantly lower than predicted by classical bulk point-defect diffusion models. Quantitative analysis indicates effective diffusion coefficients several orders of magnitude higher than bulk values.

The obtained results will be discussed in the framework of enhanced oxygen transport mediated by irradiation-activated extended defects, including dislocation networks and crystallographic shear planes, which serve as highly efficient ion-migration pathways. These defect structures couple ionic motion with electronic conduction and promote an insulator-metal-like transition under moderate thermal conditions.