Seeing atomic defects

Benchmark oxide

- TiO₂ remains a model oxide for many surface science studies, particularly for Scanning Probe Microscopy (SPM).
- Statistical analysis reveals three types of defect contrast – can we prove these are linked to characteristic defects on the surface?

nc-AFM

- Even in UHV, residual adsorbates can be seen on the surface after a few hours.
- Rows match TiO₂ (110) surface, but what about the atoms, defects and adsorbates?

Methods

- Experimental feedback loop on frequency change, while topography and current is measured.
- First principles simulations, with multiple scattering theory for tunneling.
- Identification of surface species provided by AFM.
- Three modes observed.

Simultaneous STM/AFM

- Registry between STM and AFM images is very sensitive to the type of tip – STM and AFM images can be in- and out-of-phase.
- Powerful tool for understanding contrast and studying further defects or adsorbates.

Hydrogen manipulation

- Subsurface hydrogen invisible in AFM, but seen in STM.
- Combined STM/AFM records manipulation of H from surface to subsurface site.