Non-contact AFM observation of a new reconstruction on Zn-terminated polar ZnO(0001)

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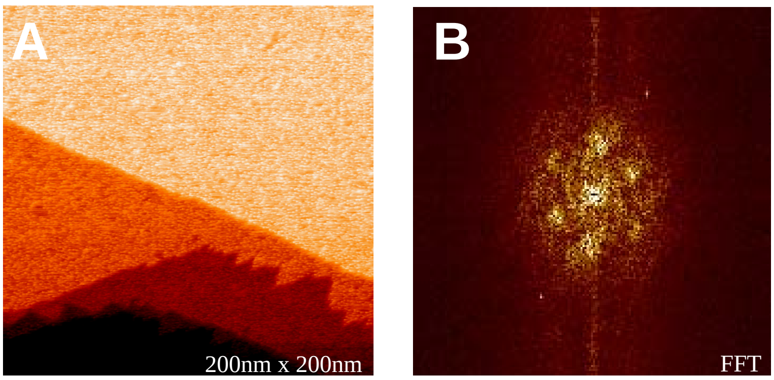
Zinc oxide (ZnO) is an important material used for instance in heterogeneous catalysis or as the active material in chemical sensors. Despite its widespread use in such important technologies, a full description of the structure of the ZnO surfaces in the clean state or the interaction with simple adsorbates is still a matter of considerable debate. Recent STM studies have led to a fairly good understanding of the non-polar faces of ZnO [1,2]. However, it was not possible to resolve directly the atomic-scale arrangement of atoms on the low-index polar ZnO(0001) surfaces. The inability to resolve the structure of this surface in atomic detail is normally ascribed to the poor conductivity of ZnO. Zinc Oxide has the hexagonal wurtzite structure, and the (1×1) terminated (0001)-Zn surface created when cutting the crystal perpendicular to the c-axis is polar and the resulting macroscopic dipole needs to be cancelled for the surface to be stable. The surface dipole can be compensated by removing approximately 25% of the surface charge, and in general three different mechanisms to achieve this are considered: 1) though creation of surface states, 2) through removal of surface atoms or 3) through adsorption.
Here we present new non-contact AFM studies of the polar Zn-terminated polar ZnO(0001) surface prepared by Ar^+ sputtering and annealed in an oxygen atmosphere. High-resolution AFM images (Figure A) of this surface reveal for the first time a hexagonal superstructure on this surface. The observed superstructure has little long range order, but organized in smaller domains the surface exhibits an apparent hexagonal pattern (Fourier transform in Figure B) with a periodicity larger than the interatomic distance of Zn on the unreconstructed ZnO(0001)-Zn face. We tentatively attribute the observed hexagonal superstructure to the formation of a reconstructed surface layer to cancel out the dipole of the polar surface.



[1] B. Meyer *et al. Angw. Chem. Int. Ed* **43** 6642-6645 (2004)
[2] O. Dulub *et al.*, Surf. Sci. **519**, 201-207 (2002)