Polar oxide surfaces and interfaces

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The question of the stability of polar interfaces is closely related to that of polar surfaces of ionic solids: the apparent presence of electric dipole moments in the unit cell perpendicular to the surface/interface leads to an electrostatic instability. These effects have been studied most extensively in compound semiconductors and more recently in the more ionic insulating oxides. The previously established view that polar oxide surfaces facet into neutral faces, while surface reconstructions stabilize the compound semiconductor polar surfaces, has been altered with discoveries of reconstruction stabilized polar oxide surfaces. We will briefly review the oxide surface faceting and reconstruction mechanisms to set the stage for our most recent work on hydrogen stabilization of unreconstructed polar surface [1], and in-situ ETEM studies on interactions of oxide surfaces with water [2], hydrogen and oxygen [3]. Our newest line of research is designed to explore if and how the oxide surface polarity can affect the epitaxial growth of polar oxide [4] and nitride [5] films with applications in spintronics and photonics. We combine HRTEM experiment and theory with density functional theory to elucidate the atomic and electronic structure of these novel polar interfaces and to develop fundamental understanding of polar interface stabilization mechanisms.

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[2] "Interaction of Oxide Surfaces with Water: Environmental Transmission Electron Microscopy of MgO Hydroxylation", M. Gajdardziska-Josifovska and R. Sharma, *Microscopy and Microanalysis* **11** (2005) 1-10.
[3] "Environmental Transmission Electron Microscopy Study of NiO(111) Polar Surface Oxidation and Reduction" M. Gajdardziska-Josifovska and R. Sharma, in preparation.
[4] "Polar Oxide Interface Stabilization by Formation of Metallic Nanocrystals" V. K. Lazarov, S. Chambers and M. Gardardziska-Josifovska, *Phys. Rev. Lett.* **90** (2003) 216108.
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