Surface Structure Studies of Fluorite Oxides

Averyl Tan, Chris Stanek, Robin Grimes and Scott Owens

Department of Materials
Imperial College London

Atomic scale computer simulation is used to predict the energies and structures associated with surface hydroxide groups. The materials studied are tetragonal zirconia and cubic ceria and urania. Hydroxide equilibrium surface energies are predicted in addition to the energy to hydroxylate a previously dry surface. Results are predicted for (111), (110) and (100) surfaces and account is made for dipolar surface structures. Differences in structure and energy are apparent especially for the (111) surface, which in ZrO_2 will remain dry, but in UO_2 is completely covered by OH groups. For CeO_2 the (111) surface exhibits only a small driving force for hydroxylation. All other surfaces display a strong affinity for surface OH formation. Such effects will lead to different crystal morphologies.