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The electronic structure of $\text{ZrO}_2/\text{Si}(111)$

Zirconium and some of its alloys, oxides and nitrides are known for their anti-corrosive and excellent wear resistant character under a variety of extreme conditions. For example the nuclear industry employs Zr-based materials due to their low neutron absorption character, mechanical strength, toughness, and ability to withstand harsh environmental conditions such as high temperatures and intense radiation. ZrO_2 has also been singled-out as a candidate material for inert matrix fuels to be used in Generation IV nuclear reactors. The formation of ZrO_2 under different growth conditions leads to variations in electronic properties and crystal structure and hence macroscopic physical properties. Control of growth may enable tuning the electronic and structural properties of this material for specific applications. The current preliminary study investigates the effect of deposition conditions on the electronic and crystal structure of atomic layer deposition grown ZrO_2 films on silicon, using synchrotron-based high resolution photoemission, TEM, SIMS, and glancing angle x-ray diffraction. The precursors used in the deposition were ZrCl_4 and H_2O using two growth temperatures of 200°C and 300°C . Additionally, ZrO_2 films were subjected to rapid thermal annealing at 600°C to investigate the effect on the valence electronic structure upon crystallization. Results are related to the detailed electronic structure of ZrO_2 thin films and bulk material.

Primary authors: Dr STAMPFL, Anton (Australian Nuclear Science and Technology Organisation); CLEMENTS, Richard; Dr MURISON, Julie (ANSTO); TRIANI, Gerry (ANSTO); Dr PI, Tun-Wen (National Synchrotron Radiation Research Center)

Presenter: Dr STAMPFL, Anton (Australian Nuclear Science and Technology Organisation)

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