First Principles Modelling of High-k Dielectric Films: Deposition and Thermal Stability

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As new material sets are introduced into silicon processing, and as Moore's law drives transistor dimensions towards atomic scales, new approaches are required to technology computer aided design (TCAD) for process and device simulation. A specific example for the changing requirements in TCAD arises when considering replacement gate oxides in future MOSFETs. Considerable interest is now being focussed on the search for gate oxides with a high dielectric constant (k) to eliminate large leakage currents and high electric fields across thin silicon dioxide layers. For the problem of integration of high-k dielectrics, conventional microelectronic TCAD tools are inappropriate for materials selection issues, such as the identification of film growth mechanisms or the chemical stability of gate stacks.

Fortunately, the methods of electronic structure theory can be used to predict material properties from first principles, and we are applying these methods to directly explore process development issues. First principles calculations are used to provide a reliable atomic-scale description of bulk and surface/interface properties. We here report the application of electronic structure methods to high-k materials that are being considered as replacement gate oxide layers. We address two issues central to the integration of such new materials into the CMOS process: deposition of thin films and thermodynamic stability.

Layers of alumina are routinely grown on silicon for electronics applications by atomic layer deposition (ALD) (using $AlMe_3$ and H_2O precursors), but the underlying reaction mechanisms are poorly understood. From periodic cell calculations on the model alumina surfaces alpha-(0 0 0 1) and gamma-(0 0 1), we elucidate reaction mechanisms and discuss consequences for film growth [1].

Zirconium and hafnium oxides are leading high-k candidates for the MOSFET gate insulating layer, and the corresponding silicates have also been proposed ($M_xSi_{1-x}O_4$, M= Zr, Hf). Relaxing structures from a bulk zircon-like model for these silicates, we compute the thermodynamic stability across the composition range $0<x<1$. We find that these 'solid solutions' are unstable and we predict whether decomposition occurs spontaneously or during a high-temperature anneal [2].

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[1] H.P.Pinto & S.D.Elliott, *Surface Science* (2003; in preparation). See also http://www.nmrc.ie/hike

[2] S. Monaghan, M.Eng.Sc. Thesis, University College Cork, submitted (2002).

Figure: Atomic-scale model of growth of alumina layers by ALD, showing precursor $[Al(CH_3)_3]$ adsorption onto a hydroxylated surface (Al=turquoise, O=red, C=grey, H=white).