

## Literature Digest Vol. 5: February 2003

### Devices – High k materials

*“Band offsets and Schottky barrier heights of high k dielectric constant oxides”*

P.W. Peacock, J. Robertson

J. Appl. Phys. 92 (2002) 412

The local density functional pseudopotential method is used to calculate the electronic structure and band offsets of high k oxides on Si. The paper addresses the fact that high k dielectrics should act as barriers for to both electrons and holes. The simplest solution would be to choose oxides with very wide gaps. However, oxides with wide gaps tend to have small k values. Therefore one must align the gap of the dielectric with respect to the silicon substrate to prevent the transfer of electrons and holes. The authors calculate the offset of the conduction bands between the dielectric (which is treated as a wideband semiconductor) and the silicon substrate. The conduction band (CB) offset is defined as the energy difference between the conduction bands of the two materials with respect to vacuum. Materials with a CB offset of > 1 eV are suitable materials. The following materials fulfilled this condition: Al<sub>2</sub>O<sub>3</sub> (2.4 eV); Y<sub>2</sub>O<sub>3</sub> (2.2 eV); La<sub>2</sub>O<sub>3</sub> (2.3 eV); ZrO<sub>2</sub> (1.6 eV); HfO<sub>2</sub> (1.3 eV); BaZrO<sub>3</sub> (1.6 eV); LaAlO<sub>3</sub> (1.0 eV); ZrSiO<sub>4</sub> (1.3 eV).