

ATOMIC LAYER DEPOSITON OF HIGH-K DIELECTRICS FOR METAL-OXIDE-SEMICONDUCTOR DEVICES

You-Sheng Lin, Ragesh Puthenkovilakam, and Jane P. Chang

Department of Chemical Engineering
University of California
Los Angeles, CA 90095

The need to replace SiO₂ by a higher dielectric constant material in fabricating smaller and faster metal-oxide-semiconductor transistors is well recognized by the National Technology Roadmap for Semiconductors. Atomic layer deposition of ZrO₂ and HfO₂ is investigated in this study to replace SiO₂ as the gate dielectric material in metal-oxide-semiconductor devices. Complementary analytical techniques including x-ray photoemission spectroscopy (XPS), spectroscopic ellipsometry, medium energy ion scattering (MEIS), electron energy loss spectroscopy (EELS), high resolution transmission electron microscopy (HRTEM), and extended x-ray absorption fine structure (EXAFS) analyses are used to characterize the interface of the high-k dielectrics and silicon and to aid the understanding of the resulting device performance.^{1,2,3}

Metal alkoxide and oxygen were used sequentially to deposit these high-k dielectric materials, which were determined to be stoichiometric, amorphous, smooth, uniform, and highly conformal by the above mentioned techniques. The interfacial layer was determined to be metal silicate, with graded metal concentration towards the interface. The thermal stability of these samples depended strongly on the deposition conditions and the annealing chemistry. The as-deposited ZrO₂ and HfO₂ were thermally stable up to 880°C and 950°C, respectively. Post-deposition annealing in oxygen or ammonia improved the thermal stability of as-deposited ZrO₂ and HfO₂ to 925°C and 1100°C, likely due to the oxidation/nitridation of the interface. The dielectric constants of ZrO₂ and HfO₂ were 18 and 21, respectively, with very small hysteresis and low interface state densities. Upon oxygen or ammonia annealing, the formation of SiO_x and SiH_xN_yO_z at the interface reduced the overall dielectric constants. The as-deposited films had an equivalent oxide thickness (EOT) of ~1.3 nm and leakage current levels that were several orders of magnitude lower than that of SiO₂ at the same EOT. The I-V curve can be fitted to a Schottky emission mechanism at low potential field and a Poole-Frenkel conduction mechanism at high potential field. Both the Schottky and Poole-Frenkel emissions stemmed from lowering a Coulombic potential barrier for free-carrier generation out of a defect center or trap under an applied electric field.

We also investigated the electronic and dielectric properties of cubic-zirconium oxide using density functional theory as implemented in the CAMbridge Serial Total Energy Package (CASTEP),⁴ an ab initio quantum mechanical code that performs the total energy pseudo potential calculations in the framework of density functional theory. The results showed that tetrahedrally coordinated Zr atoms yielded the largest interface band gap and therefore are most preferable for device applications while 6 and 7 fold coordinated Zr at the interface introduced too many gap states at the interface

reducing the effective interface band gap. The 8-fold Zr at the interface showed intermediate characteristics with a band gap comparable to that of an Si/SiO₂ interface. These calculations thus provide insight of interfacial engineering and in passivating interfacial states.

References:

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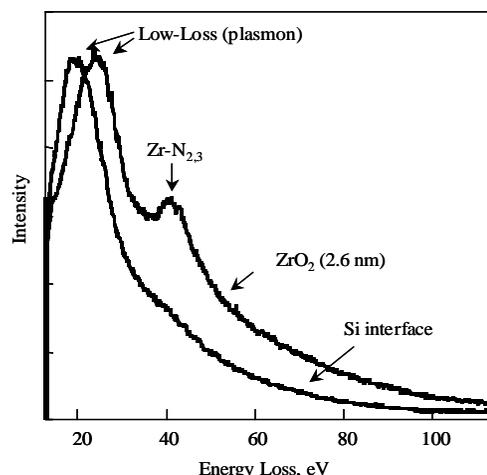


Figure 1: Electron energy loss spectra of the ZrO₂/Si structure: bulk versus interface.

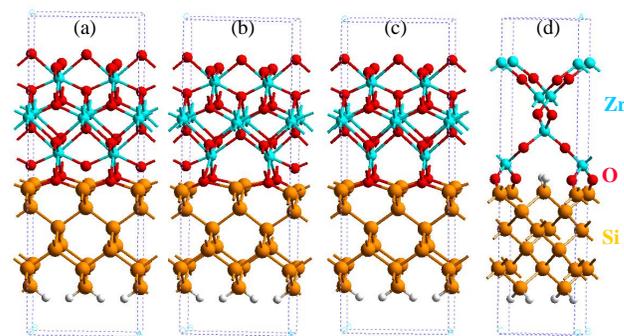


Figure 2: Model interfaces: (a) 8-fold coordinated Zr, (b) 7-fold coordinated Zr, (c) 6-fold coordinated Zr, and (d) 4-fold coordinated Zr, at the ZrO₂/Si interface.

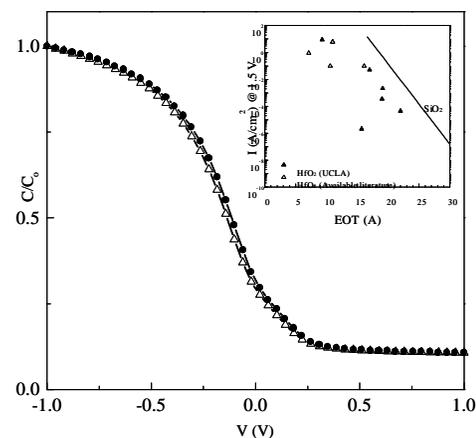


Figure 3: C-V and I-V responses of the HfO₂ dielectric thin film in a MOS capacitor.