Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Transition temperature of martensitic transformations in hafnia and zirconia XUHUI LUO, UT Austin, A.A. DEMKOV, UT Ausitn — Transition metal oxides find applications in ceramics, catalysis and semiconductor technology. In particular, hafnium dioxide or hafnia will succeed silica as a gate dielectric in advanced transistors. However, thermodynamic properties of thin hafnia films are not well understood, despite their technological importance. We use density functional theory to investigate the tetragonal to monoclinic phase transition in hafnia and zirconia. We find that unlike the case of the cubic to tetragonal transition, this phase transition is not driven by a soft mode. We use transition state theory to identify the minimum energy path (MEP) employing first principle calculations for hafnia and zirconia, sow that both transformations are martensitic, and obtain the transition barriers. Martensitic transformations include both the internal coordinate transformation and deformation of the cell lattice vectors ("strain and shuffle"), therefore the potential energy surface and MEP are function not only of the internal atomic coordinates but also of the unit cell lattice vectors. Considering the simplest case of uniform strain the transition temperatures we then relate the barrier height to the transition temperature. As a self-consistency check, assuming the equality of thermodynamics potentials of the tetragonal and monoclinic phases during the transition, and using the difference in the internal energy calculated from first principles we estimate the entropy change associated with the transition which is found in good agreement with that calculated form the phonon spectra.

Alex Demkov
UT Austin

Date submitted: 29 Nov 2007 Electronic form version 1.4