

Abstract Submitted
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Theoretical investigation of phase transitions in hafnia XUHUI LUO, A.A. DEMKOV, Department of Physics, UT Austin — Transition metal (TM) oxides find applications in ceramics, catalysis and semiconductor technology. In particular, hafnium dioxide or hafnia will succeed silica as a gate dielectric in advanced CMOS devices. However, the thermodynamics properties of thin TM oxide films are not well understood, despite their technological importance. Studying the details of phase transitions in hafnia experimentally is difficult due to their extremely high temperature. We have studied theoretically the phase transitions in hafnia using density functional theory. First we investigate the stability of the cubic phase of hafnia and find it unstable (transforming without a barrier to a tetragonal phase *via* a soft-phonon mode) in agreement with experiment. However, for low symmetry structures the full phonon mode analysis is rather complicated and other means of generating phase transition pathways need to be employed. We use the nudged elastic band method (NEBM) to find the transition path and estimate the energy barrier along it. In the case of the cubic to tetragonal phase transition NEBM finds the same soft-mode path and no barrier in agreement with the previous calculations. Using NEBM we are able to identify the pathway for the tetragonal to monoclinic phase transition, and find a 0.2 eV barrier. This work is supported by the National Science Foundation under contract DMR-0606464.

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