Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Combined theoretical and experimental study of thin hafnia films[1] XUHUI LUO, ALEXANDER A. DEMKOV, The University of Texas, DINA TRIYSO, PETER FEJES, RICH GREGORY, STEFAN ZOLLNER, Freescale Semiconductor, Inc. — Hafnia-based dielectric films have replaced silica as a gate dielectric in field effect transistors. We present a joint experimental and theoretical study of ultra thin hafnia films grown on Si (001) by atomic layer deposition. Using density functional theory we investigate the surface energy of monoclinic and tetragonal hafnia films in search for thermodynamic means of controlling the film microstructure. Our calculations of the surface phase diagram reveal that in the absence of hydrogen (111), and ($\bar{1}11$) are the lowest energy surface terminations of monoclinic hafnia under a wide range of chemical environment. On the other hand, the structural analysis, indicates films with thickness of 4 nm or less to be polycrystalline, predominantly monoclinic with the texture axis being the normal to the ($21\bar{1}$), ($11\bar{2}$). Our calculations suggest that under oxygen rich conditions the ($11\bar{2}$) termination can be stabilized. Furthermore, we discuss the effects of the hydroxylation on the thermodynamics of the hafnia film grown by ALD and provide a new perspective into the dynamics of the film growth.

[1]Supported in part by the NSF under grant DMR-0606464

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Date submitted: 21 Nov 2008 Electronic form version 1.4