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In-situ probing and modeling atomic layer deposition processes on Ge surface YUANXIA ZHENG, SUNGWOOK HONG, Penn State Univ, BRUCE RAYNER, Kurt J. Lesker Comanpy, SUMAN DATTA, ADRI VAN DUIN, ROMAN ENGEL-HERBERT, Penn State Univ — Germanium (Ge) is a promising CMOS compatible channel material with a low effective-mass of holes. One of the major challenges in developing Ge-FETs is integrating a high-quality gate-stack on Ge. A direct high-k dielectric deposition like HfO_2 on Ge has resulted in poor electrical characteristics of the semiconductor-dielectric interface.[1] GeO_2/Ge interface has been found low in interface-trap density, but its quality rapidly degraded when scaling down to ultrathin GeO_2.[2] Takagi *et al* showed that such interface quality can be preserved using an ultrathin Al_2O_3 layer on GeO_2/Ge, but the detailed mechanism has not been addressed and remained elusive.[3] In this work, we studied this problem by combining (a) *in-situ* spectroscopic ellipsometry for real-time monitoring of atomic-layer-deposition (ALD) processes on Ge, (b) *ex-situ* X-ray photoelectron spectroscopy (XPS) to probe the interface chemistry, and (c) reactive force field (ReaxFF) simulations to directly model the growth kinetics and interface formation. A strong surface-chemistry dependence (hydrogenated Ge vs oxidized Ge) has been found in the Al_2O_3-ALD nucleation (Trimethylaluminum+H_2O), which is well reproduced by ReaxFF simulation. Furthermore, both experiments and simulations revealed that the Al_2O_3 capping on GeO_2/Ge interface prevents oxygen diffusion into Ge, and therefore stabilizes the interface. [1] Appl. Phys. Lett. 87, 032107 (2005). [2] J. Appl. Phys. 106, 104117 (2009). [3] 2012 Symp. VLSI Technol. 2011–2012 (2012).

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