586c Grain Focused Simulation of Zirconia Cvd

Max Bloomfield, Zhe Song, Bridget R. Rogers, and Timothy S. Cale

We applied our grain-focused simulation environment called PLENTE (Parallel Levelset Environment for Nanoscale Topography Evolution [1]) to improve our understanding of CVD zirconia films. We focus on CVD from zirconium t-butoxide (ZBT) onto hydrogen-terminated silicon (H-Si) surfaces, under well defined conditions [2]. We begin our simulations from AFM data obtained on the films during the nucleation stage. Simulated deposition proceeds from this initial nucleation stage using a simple chemistry model and low pressure transport model [3], incorporating principles of reaction kinetics modeling. PLENTE retains grain-structural information throughout the deposition simulation. In-situ ellipsometry observations show that the incubation behavior for this system is a strong function of temperature. Atomic force microscopy (AFM) data from the films during the pre-coalescence stage of deposition, as well as comparisons against behavior for the same precursor on different substrates, suggest that nucleation is ongoing the pre-coalescence stage of deposition. We compare simulated film microstructure, both before and after simulated coalescence, to ellipsometric data and AFM and transmission electron micrographs to determine which nucleation model best reproduces experimentally observed film characteristics. Different nucleation models used in PLENTE will result in different properties of our simulated films; e.g., void fraction and island size distributions. Specific nucleation models we consider are: 1) hydroxyl groups act as traps, and 2) homogeneous nucleation due to interactions of mobile adsorbed species.

1. “A computational framework for modeling grain structure evolution in three-dimensions”, Max O. Bloomfield, David F. Richards, Timothy S. Cale, Phil. Mag 83(31-34), 3549-3568 (2003). 2. Z. Song and B.R. Rogers, “In-situ Ellipsometric Study of The Initial Deposition of ZrO2 on H-Si and Native Silicon Oxide Surfaces by HV-CVD”, JVST A 23(1), 165-176 (2005). 3. “Formation and Evolution of Grain Structure in Thin Films”, Max O. Bloomfield and Timothy S. Cale, Micro. Eng. 76(1-4), 195-204 (2004).