A COMPUTATIONAL FRAMEWORK FOR MODELING GRAIN STRUCTURE DEVELOPMENT IN THREE DIMENSIONS

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ABSTRACT

An approach to simulating the evolution of multiple-interface systems in three dimensions is presented, with a focus on grain the formation and evolution of grain structures. The approach is based on splitting the overall task into two pieces: calculating the speeds of all the interfaces in the system based on simulations of the underlying physics, and storing and updating the structural representation of the system based upon the computed rates of change. The representation and update part of the approach uses a multiple-material, level-set method with a finite element representation of the level set scalar fields. The method is implemented in a software framework, called the parallel level-set environment for nanoscale topography evolution (PLENTE), which can be used to complement discrete atomistic simulations and to link them to continuum simulations. To simulate a particular unit operation's effect on a grain structure, a computational model of the operation that can predict interface speeds is implemented as a "process model".

Three microelectronics-focused process models are presented in this thesis, in order of increasing separation from the representation task. The first process model is of the self-annealing observed in copper interconnects, using a curvature driven grain boundary migration mechanism. Using this process model to drive PLENTE shows an initial splitting of copper grain size distributions, as different grains fall into either growing or shrinking categories. Grain sizes then return to a monomodal distribution with a higher

average grain size, as seen in the literature. The second process model is a ballistic transport and reaction model that is used to simulate PVD, CVD, and RIE. For a simulation of tantalum oxide PVD, kinetic lattice Monte Carlo results are used as a starting structure. The grain structure of the films that develop compare well with micrographs of reactively sputtered Ta_xO_{1-x} films. Film density is then studied as a function of CVD precursor reactivity, showing a positive correlation, in qualitative agreement with experiment. The ballistic transport and reaction model is then used to simulate reactive ion etching using a two-species (reactive neutrals and energetic ions) model, in a porous substrate. Etches are seen to interact with the pore structure of the substrate. Finally, a process model that computes strain energy-driven grain boundary migration rates is presented. `PLENTE` is used to create a solid model of the system to be studied, and then thermomechanical computations are performed using a commercial finite element simulation package (Comsol Multiphysics). Studies on interconnect structures indicate, for the system studied, curvature driven grain boundary migration rates are larger than strain energy driven migration rates, at least initially. This research demonstrates a method to study the evolution of interconnect structures, but much more work needs to be done to achieve quantitative comparisons with experiment. Future work would include addressing both the need for better experimental information on grain structures, as well as improved implementation of PLENTE to reduce computational demands.