## Materials Science & Engineering Doctoral Defense

Phase-field Modeling of Electromigration-induced

Defects' Evolution in Interconnects Films

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## **Abstract**

Electromigration, the net atomic diffusion associated with the momentum transfer from electrons moving through a material, is a major cause of device and component failure in microelectronics. The deleterious effects from electromigration rise with increased current density, a parameter that will only continue to increase as our electronic devices get smaller and more compact. Understanding the dynamic diffusional pathways and mechanisms of these electromigration-induced and propagated defects can further our attempts at mitigating these failure modes. This dissertation provides insight into the relationships between these defects and parameters of electric field strength, grain boundary misorientation, grain size, void size, eigenstrain, varied atomic mobilities, and microstructure. First, an existing phase-field model was modified to investigate the various defect modes associated with electromigration in an equiaxed non-columnar microstructure. Of specific interest was the effect of grain boundary misalignment with respect to current flow and the mechanisms responsible for the changes in defect kinetics. Grain size, magnitude of externally applied electric field, and the utilization of locally distinct atomic mobilities were other parameters investigated. Networks of randomly distributed grains, a common microstructure of interconnects, were simulated in both 2- and 3dimensions displaying the effects of 3-D capillarity on diffusional dynamics. Also, a numerical model was developed to study the effect of electromigration on void migration and coalescence. Void migration rates were found to be slowed from compressive forces and the nature of the deformation concurrent with migration was examined through the lens of chemical potential. Void migration was also validated with previously reported theoretical explanations. Void coalescence and void budding were investigated and found to be dependent on the magnitude of interfacial energy and electric field strength. A grasp on the mechanistic pathways of electromigration-induced defect evolution is imperative to the development of reliable electronics, especially as electronic devices continue to miniaturize. This dissertation displays a working understanding of the mechanistic pathways interconnects can fail due to electromigration, as well as provide direction for future research and understanding.