Combined level set and ab-initio modeling of grain structure and texture evolution during self-annealing in thin Cu films

Håkan Hallberg
Division of Solid Mechanics
Lund University
P.O. Box 118, SE-221 00, Lund, Sweden

Pär A. T. Olsson
Materials Science and Applied Mathematics
Malmö University
SE-205 06 Malmö, Sweden

Electrical wiring in integrated circuits is commonly achieved by deposition of thin Cu films. Such electroplated films are metastable directly following the deposition and significant changes may occur in the material due to self-annealing, even at room temperature. The process causes substantial changes, for example, in terms of crystallographic texture, grain size and grain size distribution. Due to the extensive alterations of the microstructure also bulk thermomechanical and electrical properties of the film change. Self-annealing in thin Cu films has been investigated for several years but there is still, however, some dispute on the origins of the process and on the actual mechanisms which are involved. While quite substantial experimental research has been conducted on the subject, considerably less work has been published related to numerical modeling approaches to further investigate microstructure evolution during self-annealing in thin Cu films. Such numerical modeling is in focus of the present study.

In the present work, microstructure evolution in thin Cu films during room temperature self-annealing is investigated by means of a mesoscale level set model. The model is formulated such that the relative, or collective, influence of anisotropic grain boundary energy, mobility and heterogeneously distributed stored energy can be investigated. Ab-initio density functional theory (DFT) calculations are also performed to provide input to the mesoscale model in terms of the variation of grain boundary energy for different grain boundary configurations. The stability of the predominant (111) fiber texture in the as-deposited state is studied as well as the stability of some special low-Σ grain boundaries. Further, the numerical model allows tracing of the grain size distribution and any triggering and evolution of abnormal grain growth during self-annealing.

It is found that abnormal grain growth depends mainly on stored energy variations, whereas anisotropic grain boundary energy or mobility is insufficient to trigger abnormal growth in the model. However, texture dependent grain boundary properties contribute to an increased content of low-Σ boundaries in the annealed microstructure. Texture evolution is also caused by stored energy variations, since the coexisting (111) and (001) texture components in the as-deposited state evolve into a (001)-dominated texture after sufficient annealing time. Further, it is found that whereas stored energy variations promote the stability of the (001) texture component, anisotropic grain boundary energy and mobility tend to work the other way and stabilize the (111) component at the expense of (001) grains.