MICROSTRUCTURE EVOLUTION IN CU THIN FILMS, INVESTIGATED BY *AB-INITIO* AND LEVEL SET MODELING

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Summary The microstructure of Cu thin films may evolve significantly from the as-deposited state by self-annealing, also at room temperature. These microstructure alterations are of importance as they have a profound impact on both electrical and mechanical film properties. In the present study, the microstructure developments during self-annealing are studied by means of combining *ab-initio* and mesoscale level set modeling. This allows investigation of relative and combined effects of anisotropic grain boundary energy, mobility and stored energy distribution on the evolution of both grain structure and texture. Variation of grain boundary energy is evaluated by density functional theory calculations and is used as input for the mesoscale level set model. Based on the numerical simulations, observations are made related to, for example, the stability of the (111) texture which is dominant in the as-deposited state, to the prerequisites for abnormal grain growth and to the influence of stored energy heterogeneities.

MODELING OF SELF-ANNEALING IN CU THIN FILMS

Background

Electrical wiring in integrated circuits is commonly achieved by deposition of thin Cu films. These electroplated films are, however, metastable directly following the deposition and significant changes may occur in the material due to self-annealing. This process can continue for hours or days after deposition, also at room temperature. The process causes substantial changes to the microstructure. 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. The phenomena has been in focus for numerous experimental investigations, but considerably less attention has been given to numerical modeling approaches which permit further studying of the microstructure evolution during self-annealing in thin Cu films. Such numerical modeling is in focus of the present study.

Modeling framework

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. This allows very accurate representation of the grain boundary network in the polycrystalline microstructure. The model is formulated in such way that the relative, or collective, influence of anisotropic grain boundary energy, mobility and heterogeneously distributed stored energy can be investigated. Related research has also been presented previously in [1-3]. The consideration of anisotropic grain boundary properties is achieved by allowing misorientation-dependent grain boundary quantities to be evaluated locally in the microstructure with high precision. *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.

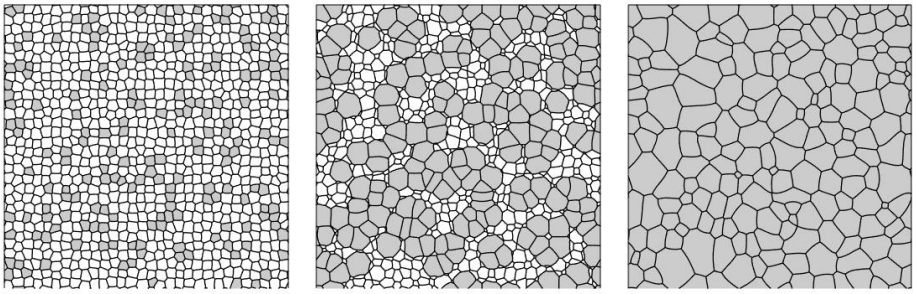

Figure 1: Abnormal growth, from left to right, of (001) grains (gray) at the expense of the (111) texture component (white). The abnormal growth of (001) grains is triggered by a lower stored energy content in this texture component.

CONCLUSIONS

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A mesoscale level set model of microstructure evolution in polycrystalline materials is established. Using results from *ab-initio* DFT calculations, the level set model is shown to be a competent tool for tracing microstructure evolution during room temperature self-annealing in Cu thin films.

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, cf. Figure 1. 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.

References

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