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Novel Microdoped Al Alloys for Highly Reliable Thin Film Interconnects

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Abstract

The theoretical computational model, based on empirical data, was suggested to fined out the elements-additives, which would be able to increase grain boundary electromigration and corrosion resistance of Al thin film interconnects.

Summary

Corrosion and electromigration, which are known to be the main reasons for metallization failures in semiconductor devices, under low temperatures, basically, occur at grain boundaries (GBs) and are controlled by GB diffusion.

The intergranular adsorption (IA) in metals and alloys causes changes in chemical composition, diffusion permeability and cohesive durability of grain boundaries (GB). IA has influence on the chemical reactions ability of GBs and, hence, can cardinally change such characteristics of polycristals, as resistance to creep, inergranular embrittlement and cracking along GBs, GB corrosion. So, the investigation of IA effects is of great interest for development of rational microdoping,preventing these processes. As concerned Al interconnects, for their doping up to now additives were chosen empirically, and these elements (e.g. Cu, Si, Mg, V, etc.) either act non-effectively, or change to the worse some physical/technological interconnects' characteristics. No detailed studies have been made to predict dopants, the most effectively acting against EM and not affecting any other properties of thin films.

In present paper we consider the changes of chemical composition and diffusion permeability of GBs in thin metal films after IA of different microadditives, which, the first, are adsorption-active as regards GBs, and, consequently, strongly segregate at GBs to a high concentration even if their concentration in a grain body is of 10^{-5} - 10^{-7} at.% level, and, the second, are more inert, than the matrix metal, in reactions with the oxidants or, on the contrary, are active in reactions with substrate's/sublayer's materials forming along GBs inert compounds, which act as so-called "intrinsic" diffusion barriers. Because of their very low concentration in grain bodies such impurities do not affect any other physical characteristics of thin films.

The model was suggested to evaluate the equilibrium enrichment of GBs in thin metal films with impurities due to IA, which leads to alterations of GB energy γ , self diffusion coefficient

D of base metal along GB and chemical activity of GB in reactions with different components of surroundings.

In our model there were applied: the "liquid" model of GB to estimate the free energy difference ΔG associated with transfer of dissolved impurity atom from the grain bulk to high angle GB - such estimation was shown, the first, to be the most conservative one and, the second, to give more realistic values in comparison with the "elastic" model estimation; half-empirical thermodynamic model connecting the decrease of D with the decrease of γ during IA; the value of electronegativity of GB as a measure of its chemical activity.

The suggested model takes into account the effect of "exhaustion" of grain bulk with weak soluble impurities during IA in fine grained films - this results in the dependence of all IA-provoked effects on the grain size.

The calculations of the influence of different additives on the characteristics of GBs in aluminum (79 additives) - the most widely used metal as material for interconnects - with different grain sizes have been carried out. The microadditives, the most effectively reducing D and altering the GB chemical activity in reactions with silicon, oxygen and chlorine, have been revealed.

To calculate the changes of GB characteristics during IA the computer program DIARA (Diffusion-Intergranular Adsorption-Reaction Activity) have been created, which enables us to predict the "useful" IA-active dopants for any matrix metals.