Simulation of Texture Development Caused Stress Build-Up in Electroplated Copper Lines

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1. Introduction

The technology process of metal layers produces large residual stresses. These stresses are built during the process itself or thereafter. The residual stresses determine the mechanical properties of the metal structures and of the whole package. In the case of interconnects' reliability the residual stresses play a significant role in the electromigration behavior. The stress distribution acts as an additional material transport force and causes anisotropy in self-diffusion and electromigration [1,10].

Due to its lower resistivity and improved electromigration resistance copper has replaced aluminum as material for advanced interconnects in multilevel integrated circuits.
Compared with physical vapor deposition (PVD) and chemical vapor deposition (CVD), electroplating of copper has shown superior ability to fill submicron trenches and vias of dual damascene architectures.
Copper interconnects posses a characteristic microstructure, i.e., a network of grain boundaries circumscribing grains with their distinctive lattice orientations, which can be influenced by process conditions.
Experimental and theoretical investigations have shown that the metal microstructure during its evolution produces significant microstrains [8,12,13]. The distribution of the stress which arises due to these microstrains strongly depends on the grain morphology.
Different aspects of the connection between microstructure and stress have been investigated in the last 30 years. The focus was mostly on some specific grain-grain boundary configurations in early or mature stages of microstructure evolution [8]. As a result we have numerous models derived on the basis of continuum mechanics, which are applicable only for highly simplified situations.
On the other side a group of researchers, mostly mathematicians, has developed complex models for describing morphology of the microstructural evolution, a development which culminates in muli-level set models of grain evolution. Such models can to a high degree reproduce the realistic grain boundary network, but they do not include stress.
The goal of this work is the integration of microstructure models which describe strain development due to grain dynamics with the macroscopic mechanical problem.
The solution of a mechanical problem will provide a distribution of the mechanical stress in tensor form, which can further be used for electromigration reliability analysis and the assessment of general mechanical properties of the whole package [9,10].

2. Theoretical Background

The mechanical stress in metal layers has several sources.
Thermal stresses are always present, but they alone can by far not be the sole explanation for the huge stress gradients which have been experimentally observed. Careful analysis of the material behavior has determined other possible sources of the stress [4,8].
Basically, residual stresses develop due to the microstructure evolution during metal layer deposition processes and days and months aftermath [8]. Metal films applied in modern interconnect technology are complex polycrystalline structures.
The development of the polycrystalline film structure depends on the properties of the underlying layer and process parameters. For example, process conditions which support high adatom mobility during material deposition will also enhance creation of crystalline domains with a significant size. Extremely low adatom mobility will produce amorphous films.
Also widely applied is annealing of already deposited metal layers, which is motivated by the fact that an increased temperature induces an additional microstructure transformation and possibly more desirable mechanical properties.

There are numerous microstructural sources of intrinsic stress described in the literature such as grain boundary coalescence in the early stage of the film growth, inter-grains misfit stresses, grain growth, and annihilation of excess vacancies [7,8].
A crucial issue for modeling and simulation of mechanical behavior of the metal films is describing the grain growth and connecting this growth to the microstructural stress build up.

In this work we use predictions of a level set based simulation [5,6] to obtain the grain size distribution from the bottom to the top of a polycrystalline film for different stages of a texture evolution. Relying on the obtained grain size distribution, models for the calculation of microstructural stress caused by effects of grain boundary area reduction, adjacent grains coalescence, and excess vacancy annihilation are applied. The resulting stress is on microscopic scale isotropic and can be expressed by the following formula

$$\sigma_{res} = -\frac{2E}{1-\upsilon}\left(\frac{1}{L}-\frac{1}{L_0}\right)\Delta a + \frac{4E\Omega}{L(1-\upsilon)}\sqrt{\frac{D_V t_0}{\pi}}\left(C_{bulk}-C_{gb}\right). \quad (1)$$

The first term in this equation represents stresses developed due to the grain growth [7]. L is the current grain diameter

and L_0 is the grain diameter from the previous growth phase. Δa is the excess volume per unit area of a grain boundary which has a value in the order of an atomic diameter. The second term of (1) is related to the annihilation of vacancies at the grain boundaries. The annihilation sites are transformed into the gaps between the grains which are closed by straining of the grains. D_V is the bulk vacancy diffusivity, C_{bulk} is the vacancy concentration inside the grain, and C_{gb} in the grain boundary (Figure 1). t_0 is the average time needed for grain bulk - grain boundary system to reach these vacancy concentrations. E and ν are Young's modulus and Poisson's ratio of copper, respectively. Residuum stresses described by (1) are used to set the overall, (macroscopic) stress equilibrium problem.
The solution of this equilibrium problem under consideration of interface conditions to the surrounding layers yields the anisotropic stress distribution (σ_{ij}). The stress-dependent dynamics of the grain growth is given by [4]

$$\frac{\partial L}{\partial t} = \frac{D^* \Omega}{k_B T \delta} \Delta p \,, \tag{2}$$

here Ω is the atomic volume, δ is the average jump distance in the grain boundary, T is the temperature, k_B is the Boltzmann constant, and Δp is the pressure difference which drives the migration of the grain boundary.
The hydrostatic pressure p is defined as

$$p = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \,. \tag{3}$$

D^* is the effective diffusivity [4,6]

$$D^* = \delta^2 \alpha \exp(-\frac{\Delta H}{k_B T}) \,, \tag{4}$$

where α is the atomic frequency and ΔH is the activation energy for the boundary migration.
In the first phase of the deposition process, islands with varying crystal orientation are formed, which grow isotropically (Fig. 2). In the course of further deposition these islands start to coalescence, which forces the islands to grow in the height instead in a direction parallel to the substrate surface (Fig 3). The islands are consequentially transformed from an island shape to a grain-like shape.
The orientation of the crystal structure in a single grain (e.g. perpendicular to the substrate surface) is independent of the neighboring grains, since due to the structure of the underlayers, it is not possible to evolve a perfect crystal structure in the first atom layers [4,13].

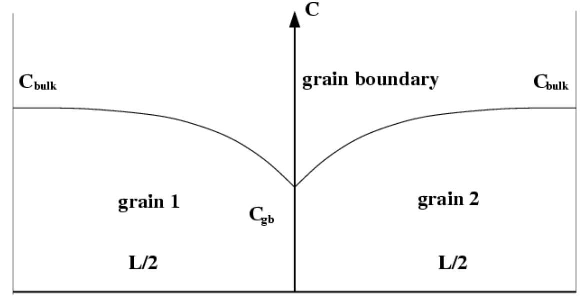

Fig. 1: Model used for calculation of stresses generated from vacancy annihilation at grain boundaries. For simplicity an analytical solution of the one-dimensional diffusion problem is applied [7].

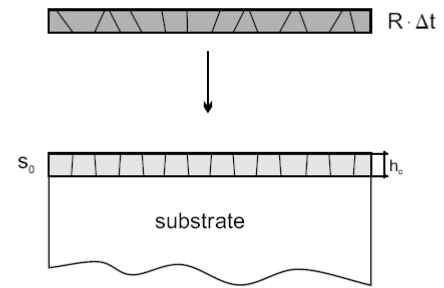

Fig. 2: Initial mode. R is the deposition rate and h_c film thickness immediate after grain formation.

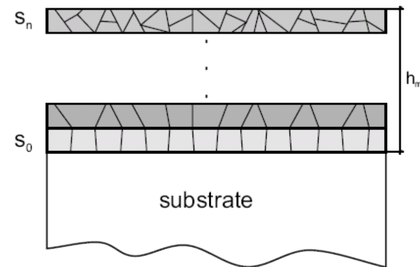

Fig. 3: Grains formed in the initial mode continue development in transient mode.

Multi-level set simulation calibrated to minimum and maximum grain size, average grain growth velocity, and film deposition rate is used to obtain the initial grain size distribution [5,6]. This grain size distribution $L(x,z,y,t)$ is the basis for a direct calculation of the initial stress (1). The stress calculation can also be performed by using (1) as residuum stress in the overall mechanical equilibrium problem ($\nabla \tilde{\sigma} = 0$). Using (3) the hydrostatic pressure distribution is calculated and used to determine grain growth in the next time step (2). The whole procedure is continued until $L(x,z,y,t)$ and $\tilde{\sigma}(x,z,y,t)$ reach a stationary distribution.

3. Simulation Results

As a basis for our theoretical and investigation we use a copper layer electroplated at room temperature on the top of a SiO_2 layer as presented in experimental studies [2,3]. Before electroplating of copper, 80 nm of TaN and a copper seed layer were PVD deposited. These layers are necessary for making an optimal electrical contact [2,3].

Microstructural and textural analyses are commonly carried out using FIB imaging, XRD pole figures, and EBSD (electron backscatter diffraction). EBSD is a SEM–based technique which provides microstructural information with high spatial resolution. Among many other representations, pole figures, color coded orientation maps, grain size distribution, and misorientations' distribution can be derived from experimental data [11].

A comprehensive analysis of experimental data enables us to reconstruct the complete history of grain evolution starting with the plating process itself and continuing hours after the complete film is formed.

Comparison and study of experimental data with results of multi-level set simulation of the grain evolution [5,6] allows us to model not only the three-dimensional grain size distribution but also the dynamics which leads to this distribution.

Normally, the microstructural evolution of the copper films is investigated at three different stages:

a) as-plated,
b) after days at room temperature,
c) after annealing in forming gas.

Since all main features of recrystallization, take place already at room temperature we confine our analysis of the microstructure (grain) evolution to stages a) and b).

During these stages the microstructure develops from a network of 0.1 µm diameter grains to a polycrystalline structure with 1.0 µm diameter grains which span the whole cross-section of the copper interconnect line [3].

Figure 4 displays the simulated slice of a copper film with compressive and tensile pressure distribution. The film is deposited in z direction. According to the level set simulation [5,6] and SEM pictures, grains develop column or V–shapes perpendicular to the surface. The increase of the tensile stress in vertical direction is caused by lateral grain growth, reducing the grain boundary areas, and consequently densification of the material. This is also the explanation why peak values of the tensile and compressive pressure develop in the planes parallel to $x\,y$ plane.

Generally it can not be ruled out that the TaN and the copper seed underlayers develop a microstructure which also contributes to the overall stress distribution. However, due to small thickness of these layers (80 nm) compared to 1.0 µm copper film thickness, we assume that this contribution is negligible. An important issue is that a microstructure of a TaN -type thin interlayer influences the microstructure of the subsequently electroplated metal film in the early stage of grain nucleation but this is handled elsewhere [12].

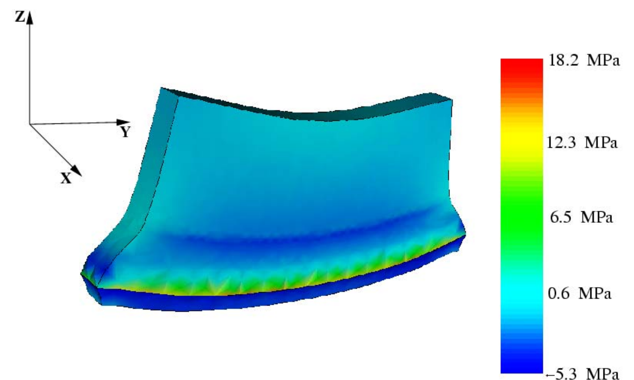

Fig.4: Stress distribution in a slice of copper film deposited in z-direction on TaN/SiO_2 layer. A belt of high tensile stress is built-up perpendicular to the deposition direction.

The vacancy redistribution introduced with the second term of the stress expression (1) has shown to have only minor impact vertical grain growth.

A plane with high compressive pressure is visible at the boundary between the copper layer and, as assumed in the model, the microstructurally inactive underlayer (Figure 4). This compressive stress does not have origin in the microstructure evolution; it is a consequence of the fixed attachment of the copper layer to the underlayer.

The dependence of the microscopic strain on the maximum grain size reached at the end of recrystallization is presented in Figure 5. Maximum grain sizes are set in accordance to experimental observations [3].

A larger maximum grain size yields larger material densification which explains the shift of the profiles in the diagram (Figure 5) towards higher strain regions.

In Figure 5 we can also observe that the rate of densification (higher strain gradient) is higher in the lower part of the film area, which corresponds the experimentally observed fact [13] that most of the collapsing grains disappear in this region. In accordance, Figure 4 shows that the peak tensile stress belt is built in the lower part of the thin film slice.

Figure 6 shows the hydrostatic pressure versus as-plated grain size. The compressive pressure component possesses higher dynamics than the tensile component. This can be explained by the fact that the evolution of the tensile stress is directly connected to the grain growth and mechanisms which possibly induce compressive stress (such as vacancy redistribution between grain boundary and grain bulk) are not very pronounced.

Similar values of the stresses are obtained in [2] with corresponding process conditions.

The model has been implemented in in-house tool for simulation of microstructural stress evolution StrDep. The tool is capable of solving multi-physics equations by means of the finite element method. All simulations have been carried out on a high performance IBM-AIX cluster.

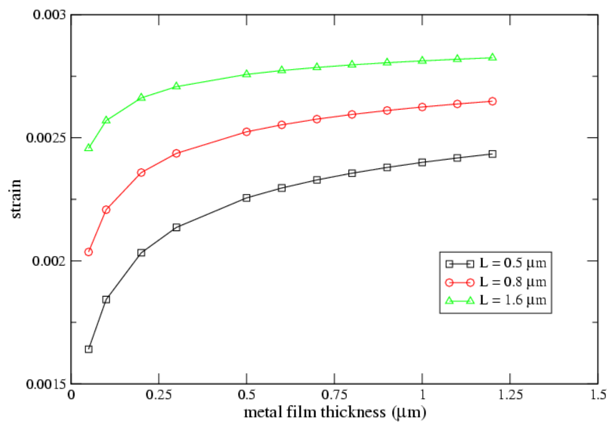

Fig. 5: Strain build-up versus thickness of metal film.

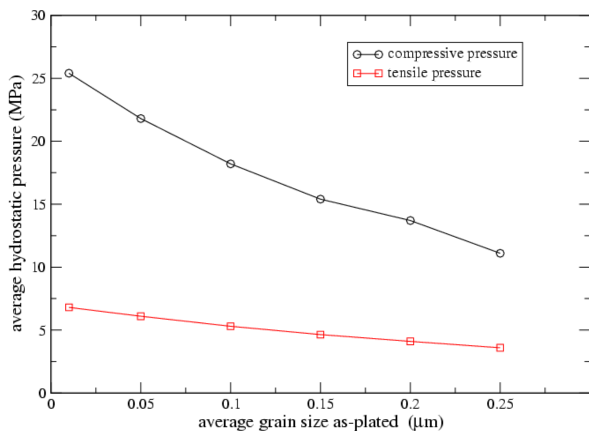

Fig.6: Compressive and tensile stress component development versus grain size.

4. Summary and Conclusion

We presented a simulation concept which connects microstructural mechanical properties of copper films to the overall stress distribution. The underlying model is designed by combining several earlier models which describe different microstructural contributions to stress build up.

The mechanical effects of surrounding layers are also included in our analysis. The analysis of the models and simulation results and their comparison to the relevant experimental results has been carried out.

The simulated stress distribution is comparable to the stresses measured after the deposition of copper films. The basic features of texture evolution seen in simulations are the same as those observed during measurements.

5. Acknowledgment

This work has been supported by the European Community with project PROMENADE, IST-2002-2.3.1.2.

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