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Microstructure simulation of grain growth in Cu through silicon vias using phase-field modeling

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ABSTRACT

A computationally-efficient 3D phase-field model for simulating grain growth in through silicon vias (TSVs) is presented. The model is capable of simulating grain growth in the cylindrical shape of a TSV. The results generated from the phase-field simulations are used in a finite element model with anisotropic elastic and isotropic plastic effects to investigate the large statistical distribution of Cu pumping (i.e. the irreversible thermal expansion of TSV) experimentally seen. The model thus allows to correlate the macroscopic plastic deformation with the grain size and grain orientations.

1. Introduction

Through silicon vias (TSVs) are a key part of 3D System in Package (SIP) devices, enabling the vertical interconnection of stacked dies. Most often they are filled with electro-plated Cu in polycrystalline form. Due to the large difference in coefficient of thermal expansion with Si, the exposure to high temperatures during subsequent processing steps causes irreversible (plastic) extrusion of the Cu, referred to as 'Cu pumping'. This results in a relatively high tensile stress inside the Cu at room temperature. The distribution of both Cu pumping and Cu stress values shows a large spread over TSVs of a single wafer [1–4]. For Cu pumping this spread is clearly correlated to variations in the Cu microstructure [5]. As potential reliability issues related to Cu pumping or Cu stress will first occur at the TSVs with the highest values for either, any model aiming to predict this behavior should include a statistical spread in addition to a median value. Therefore, variations in the Cu microstructure between TSVs and during exposure to the high BEOL processing temperatures (grain evolution [4,6]) must be taken into account.

Finite Element Models (FEM) for the study of reliability and failure mechanisms in TSVs encountered in literature assume homogeneous isotropic Cu properties [7–9]. We are developing a finite element model for the thermo-mechanical behavior of Cu TSVs incorporating Cu microstructure, in order to capture the resulting variations and build further understanding of the role of Cu microstructure. This paper presents a computationally-efficient model for simulating grain growth inside the TSV using the phase-field method.

Phase-field modeling is widely used to simulate grain-growth in heterogeneous materials on a mesoscale. This method allows to simulate the evolution of the polycrystalline structure in a Cu TSV and when coupled with a finite element model enables to include anisotropic properties as a function of grain orientation in the elasticity and plasticity models. In the phase-field method, different order parameters are assigned to the different grain orientations and grain boundaries are described as diffuse transitions in the values of these order parameters. Moreover, differential equations are derived from kinetic and thermodynamic principles, based on the assumption that a reduction in bulk energy, interfacial energy or elastic energy, is the driving force for grain evolution [10,11]. An important advantage of the phase-field method is that, thanks to the diffuse-interface description, there is no need to track the grain boundaries during microstructure evolution and

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therefore it is mathematically feasible to simulate the evolution of complex grain shapes and connected grain structures in 3D [10,11].

In this work a semi-implicit Fourier-spectral method is used to solve the differential equations. The implementation was adapted to treat the cylindrical shape of the TSVs. The time steps in the simulations are related to a physical time and temperature through the thermodynamic and kinetic properties of the material. The resulting grain structures were used in a finite element code, where the effect of anisotropic elasticity in the different grains in a TSV were analyzed as a function of the grain size.

The next section describes the theoretical background of the phase-field method with a focus on grain growth models. In the third section, we describe the modification made to the standard phase-field grain growth model in this work and show how it can be combined with a FEM to simulate grain growth and Cu pumping in a cylindrical TSV.

2. Phase-field method

The phase-field method provides a way to model the evolution of the grain structure and enables us to analyze the effect of anisotropy on microstructure evolution in materials. The phase-field method is widely used in various applications such as solidification, multiphase systems and electromagnetism. In this section, a standard model for grain growth in single phase materials is described. Readers are referred to [10,11] for a broader overview of the phase-field method for modeling microstructural evolution.

In polycrystalline materials, grains may continuously grow or shrink in time, under influence of an external load, such as pressure, or temperature.

According to Eq. (1) [9], the total free energy of a system, F, may consist of several contributions, namely the bulk chemical energy F_{bulk} (which defines the composition of equilibrium phases), interfacial energy F_{int} and elastic energy F_{el} (both affect the equilibrium phase and define the shape of grain boundaries):

$$F = F_{bulk} + F_{int} + F_{el} \tag{1}$$

In the grain growth model for single-phase materials, only the interfacial energy is considered.

In a phase-field model, interfaces are assumed to be diffuse, i.e. a narrow region with finite width over which the properties change continuously. By contrast, for sharp interfaces (used in other grain-growth methods such as Monte Carlo simulation), property changes are instant and sharp (Fig. 1). In phase-field

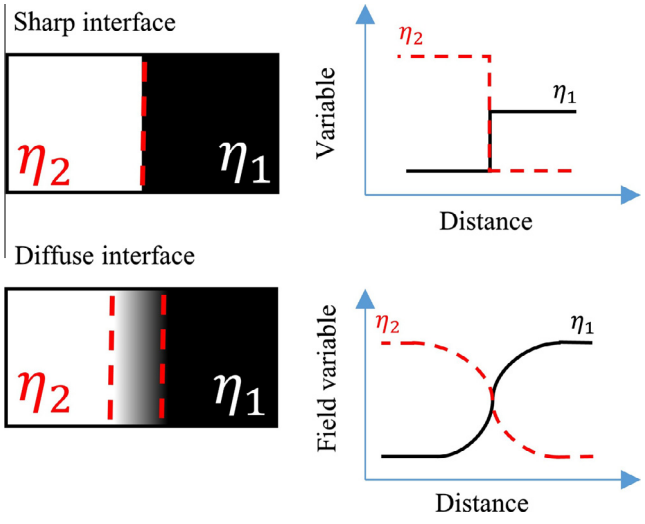

Fig. 1. Sharp interface (top) and diffuse interface (bottom) representation, for defining grain boundaries.

models for grain growth, grains with different crystal orientations are represented using order parameters, $\eta_i(r, t)$. These are continuous functions of space r and time t. Within each grain only one of the order parameters, the one representing the crystal orientation of that grain equals 1 and the others are zero; across the grain boundaries, the values of the order parameters gradually change between 0 and 1 [12].

The free energy is a function of all order parameters representing the different grain orientations and their gradients. It has the following form [9]:

$$F(\eta_1, \eta_2, \ldots, \eta_P) = \int_V \left[f_0(\eta_1, \eta_2, \ldots \eta_P) + \frac{\kappa}{2} \sum_k (\vec{\nabla}\eta_k)^2 \right] d\vec{r} \tag{2}$$

where $f_0(\eta_1, \eta_2, \ldots)$ is called the local free energy density (J/m^3) and $\left(\frac{\kappa}{2}\sum_k(\vec{\nabla}\eta_k)^2\right)$ is the gradient free energy density which is responsible for the diffuse-interface characteristics. κ is a positive coefficient related to the interface thickness l and energy γ (as $\sqrt{\kappa} \propto \gamma, l$). For polycrystalline materials, the local free energy density as a function of the set of order parameters (η_i), is defined as in Eq. (3) [13]:

$$f_0(\eta_1, \eta_2, \ldots) = \sum_{k=1}^{P} \left(-\frac{\alpha}{2}\eta_k^2 + \frac{\beta}{4}\eta_k^4 \right) + \gamma \sum_{i=1}^{p} \sum_{j \neq i}^{p} \eta_i^2 \eta_j^2 \tag{3}$$

It has degenerate minima at $(\eta_1, \ldots, \eta_i, \ldots) = (1, 0, \ldots, 0)$, $(0, 1, 0, \ldots), \ldots, (0, \ldots, 1, \ldots, 0)$, corresponding to the different crystal orientations of the grains.

Time-dependent Ginzburg–Landau equations are solved to determine the time evolution of the order parameters (i.e. the grain structure in the considered case of grain growth) [12,13]:

$$\frac{\partial \eta_k(\vec{r}, t)}{\partial t} = -L_k \frac{\delta F}{\delta \eta_k(\vec{r}, t)} = -L_k \left[\frac{\partial f_0}{\partial \eta_k} - \kappa \vec{\nabla} \cdot \vec{\nabla} \eta_k \right] \tag{4}$$

$$\frac{\partial \eta_k(\vec{r}, t)}{\partial t} = -L_k \left(-\alpha \eta_k + \beta \eta_k^3 + 2\gamma \eta_k \sum_{j \neq k}^{p} \eta_j^2 - \kappa \nabla^2 \eta_k \right) \tag{5}$$

Eq. (5) is calculated for every orientation in the phase-field system, which can be computationally intensive when we deal with a large number of order parameters.

For the numerical solution, differential Eq. (5) can be transformed into algebraic Eq. (6) in Fourier space. The method requires a uniform 2D or 3D equally spaced grid and periodic boundary conditions.

$$-\left(\frac{L\kappa\Delta t}{(\Delta x)^2}\right)\tilde{\eta}_{s-1}^{n+1} + \left(1 + L\kappa\Delta t(g_1^2 + g_2^2) + 2\frac{L\kappa\Delta t}{(\Delta x)^2}\right)\tilde{\eta}_s^{n+1} - \left(\frac{L\kappa\Delta t}{(\Delta x)^2}\right)\tilde{\eta}_{s+1}^{n+1} = \tilde{\eta}_s^n - L\Delta t\left(\widetilde{\frac{\partial f_0}{\partial \eta}}\right)_s^n \tag{6}$$

In this equation $\tilde{\eta}_{r,s}^n$ are the Fourier transforms of the order parameters at time step n and grid point (r, s). Δx is the distance between neighboring grid points, Δt is the time between the evaluated time steps and κ and L as mentioned earlier are material constants and impact the interface energy and thickness ($\gamma = \frac{4\sqrt{2}}{3}\sqrt{\kappa\Delta f}$) [12,14]. After solving (6), an inverse Fourier transform is taken from the $\tilde{\eta}_{r,s}^{n+1}$ to obtain η_{s-1}^{n+1} in real space. It is important to choose an optimal grid spacing (Δx), between grid points, namely fine enough to resolve the diffuse interface profile, and large enough to limit the computation time and memory usage. This semi-implicit Fourier-spectral method enables use of a larger time step, as compared to a standard finite difference discretization. The periodic boundary conditions may limit the applicability of the method.