# Simulation of three Dimensional Grain growth for Cu-interconnects

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***Abstract*—The temporal evolution and morphology of three-dimensional (3-D) grain growth in Cu interconnect are simulated by phase-field model techniques. In the simulation, a new local free energy density function is proposed in which the field variables can be reduced from 200 to 20. By restraining the grain orientations in the side face of interconnect, the model is applicable to simulating the microstructure evolution of polycrystalline Cu-lines in addition to the conventional 2-D or 3-D grain topology. The dependence of grain size on the line width is analyzed systematically. With the obtained topology of Cu grains and morphology of the line boundary, the resistivity of Cu interconnects is estimated by conventional Monte Carlo simulation which are tested with different experimental data. These results are important for evaluation and optimization the Cu interconnect process.**

***Keywords-Cu-interconnects; phase field method; grain growth; Cu-resistivity.***

## I. INTRODUCTION

The ITRS predicts that industrial interconnects width will be 36 nm in 2012 [1]. When the interconnect dimensions are of the order of the electron mean free path in Cu (about 39nm), its resistivity increases drastically due to the additional scatterings mainly from surface and grain boundaries which used to be ignored for bulk Cu [2] [3][4]. As the grain boundaries regions and outside roughness of the line are crucial to estimating the resistivity of Cu-line, the identification of Cu grains and its surface topology are important to the optimization of Cu scattering properties.

In recent years, several techniques for the computer simulation of grain growth have been developed, among which Monte Carlo Potts models [5] and phase-field approaches [6][7] are most versatile and mature for simulating coarsening phenomena, particularly in the presence of multiple phases or gradients of concentration, stress or temperature. However, the Potts model assumes that grain boundaries are sharp, while the phase-field model describe the diffuse grain boundaries which are more accordant with physical fact. In both Monte Carlo Potts and phase-field models, the kinetics and topology of coarsening are found to depend on the number of unique grain 'orientations' available to label the individual grains in the simulation cell. When this number of possible grain orientations is less than the total number of grains in the simulation cell, there is a high probability of grains coalescence, which has never been observed in polycrystalline specimens [8]. Thus, in the case of the phase-field model, a lot of phase field variables are needed to suppress this phenomenon. However, the time cost of the simulation increases linearly with the number of phase field variables, Q, and large Q will make this method hard to handle large simulation cell，especially for 3-D simulation.

In this paper, we present a modification to the phase-field method by proposing a new expression for the total free energy of a polycrystalline microstructure, with which the number of field variables is reduced greatly. Using this method, we analyze the dependence of grain size on the line width systematically. Based on the simulated microstructure, Cu-interconnects resistivities of different width are simulated using existing Monte Carlo method and good agreements with experimental data are achieved.

## II. MODEL AND THE SIMULATION METHOD

Grain growth is a process in which the average grain size of a single-phase polycrystalline material increases as a function of time, driven by the reduction in the total free energy of the microstructure [6]. Usually, the simulated polycrystalline region is mapped to a simulation cell and discretized using certain grid. In the phase-field model developed by Chen [6], each grid is specified by field variables $\eta_i(r, t)$ (i=1,2,…,Q) defined at a given time t at each position r. These field variables are continuous variables ranging from -1.0 to 1.0 and each parameter represents a certain grain orientation, thus Q field variables give Q possible orientations. For example, $\eta_1(r, t)=1.0$ means the material at position r at a given time t has an orientation labeled as 1. At the grain boundary region between orientation *i* and *j*, both variables will have absolute values intermediate between 0.0 and 1.0 as shown in Fig.1(a). Inspired by the diffuse interface theory, Chen [6] proposed the following expression for the total free energy of a polycrystalline microstructure by:

$$F(t)=\int\left[f(\{\eta_i(\mathrm{r},t)\})+\sum_{i=1}^{Q}\frac{\kappa_i}{2}\nabla\eta_i(\mathrm{r},t)^2\right]d\mathrm{r} \qquad (1)$$

where $\eta_i$ are field variables, Q is the number of field variables, $\kappa_i$ are the gradient energy coefficients, and *f* is the local free energy density function defined as

$$f(\{\eta_i\})=\sum_{i=1}^{Q}\left(-\frac{\alpha}{2}\eta_i^2+\frac{\beta}{4}\eta_i^4\right)+\gamma\sum_{i=1}^{Q}\sum_{j>i}^{Q}\eta_i^2\eta_j^2 \qquad (2)$$

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where $\alpha$, $\beta$, and $\gamma$ are phenomenological parameters. The most important requirement for the phenomenological parameters is that Eqn. (2) can provide 2Q degenerate minima. When $\alpha=\beta>0$ and $\gamma>\beta/2$, the minima locates wherever one field parameters takes on the value of unity and others are zeros. Using Chen's method, the time evolution of the average grain area <A> during a 2-D simulation on 256×256 simple-square grid is plotted in Fig.2(a). It can be found that the grains grow much faster when Q=10 than the case of Q=100, reflecting the fact that the probability of coalescence is higher [6][8]. It's apparent that Q is at least 100 to obtain non-coalescence grain growth for 2D simulation. For 3D simulation, more than 200 field variables are required [8], which makes this method unable to handle large simulation cell.

To solve this problem, we propose a new free energy density function in present work as follows:

$$f(\{\eta_i\}) = \sum_{i=1}^{Q}(-\frac{\alpha}{2}\eta_i^2 + \frac{\beta}{4}\eta_i^4) + \gamma\sum_{i=1}^{Q}\sum_{j>i}^{Q}\sum_{k>j}^{Q}\eta_i^2\eta_j^2\eta_k^2 \quad (3)$$

where $\alpha$, $\beta$, and $\gamma$ are phenomenological parameters. When $\alpha=\beta>0$ and $\gamma>\beta/2$, the minima locates wherever two of the field parameters takes on the value of unity and others are zeros. Compared with Eqn.(2) [6], this function provides Q×(Q-1)/2 degenerate minima which means that less Q can produce comparative minima. To illustrate this, the field variables value of a one-dimensional simulation grid is shown in Fig.1 (b) as a function of the position $x$. Two grain boundaries are shown at $x$=0 and $x$=15. Around the $x$=0 boundary, four field variables ($\eta_1$, $\eta_2$, $\eta_3$, $\eta_4$) are all changed between 0.0 and 1.0, while around the $x$=15 boundary only 2 field variables ($\eta_1$, $\eta_3$) are changed. Thus, there will be two different grain boundaries' energies in our method. This is consonant with the experimental result given by [9] where the grain boundaries' energy in Cu-line can be roughly divided into two classes, thus our method is more reliable to simulate the grain growth of Cu-line.

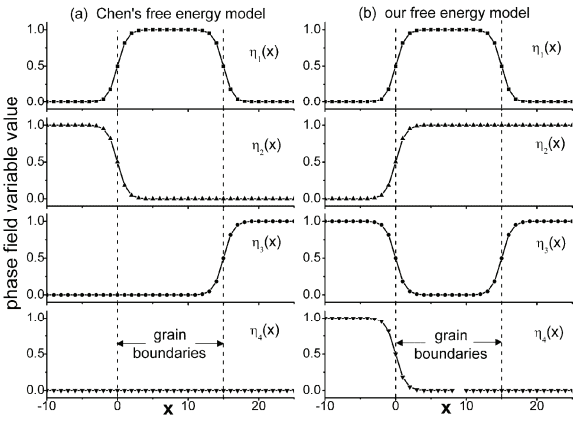


Figure 1. The values of the phase field variable as a function of the position $x$. In (a) the orientation of the grain between $x$=0 and $x$=15 is specified by one field variable $\eta_1$, while In (b) the orientation of the center grain is specified by a pair of field variables ($\eta_1$, $\eta_2$). Around the grain boundaries at $x$=0 and $x$=15, several field variables have a smooth variation between 0 and 1.

The final set kinetic equations is given by [6]:

$$\frac{d\eta_i(r,t)}{dt} = -L_i\frac{\partial F(t)}{\partial \eta_i(r,t)} = -L_i(\frac{\partial f(\{\eta_i\})}{\partial \eta_i(r,t)} - \kappa_i\nabla^2\eta_i(r,t)) \quad (4)$$
$$(i = 1,2,\cdots,Q)$$

where $L_i$ are kinetic rate coefficients related to the grain-boundary mobility, and the Laplacian operator in Eqn. (3) is discretized as:

$$\nabla^2\eta_i(r,t) = \frac{1}{(\Delta x)^2}\sum_i(\eta_i(r_i,t) - \eta_i(r,t)) \quad (5)$$

where the index $i$ runs over all first-nearest-neighbor sites ri for site r. Usually, each field variables are initiated to a small random value -0.001<$\eta_i$<0.001 because there is no grain at first. Then, at each step, Eqn. (5) is calculated and the result is used to calculate Eqn. (4). The field variables values are updated and the time evolution of the microstructure is obtained. To verify that much less Q is needed using Eqn. (3), we had simulated the evolution of a 256×256 simple-square grid. Follow the assumption that $\alpha=\beta=\gamma$=1.0, $\Delta x$=2.0, $\kappa_i$=2.0 and $L_i$=1.0 for all $i$ [6], 6000 simulation steps are run and the obtained average grain area <A> for different Q is shown in Fig. 2(b). It is clear that the grains growth rate converges rapidly for Q as small as 15. The linear dependence of the average grain area on time also agrees with most of the previous simulation results [5][6].

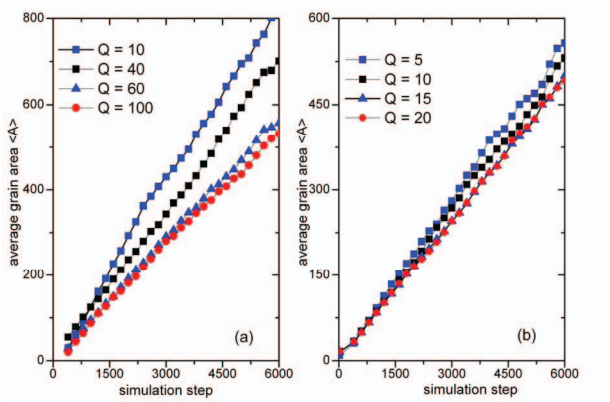


Figure 2. Evolution of the average grain area during a 2-D simulation with various $Q$. (a) is the result of Chen's method and (b) is the result of our proposed method. In both simulations, periodical boundary condition is used.

## III. RESULT AND DISCUSSION

To further verify our method, the distribution of the grain size in this 2D simulation is compared with Chen's results in Fig.3. The similar distribution found here means that our method is acceptable.

To verify 3-D simulation ability of our method, temporal evolution of a 128×64×56 cell is simulated and shown in Fig.4. As we can see, the average grain size increases with simulation time and small grains are gradually disappear due to boundary migration. Two different grain boundaries mentioned in section II are both shown, and it is easy to find that the mobility of the two boundaries is different.

Traditionally, periodical boundary condition is used to calculate Eqn. (5) because the average grains size is much smaller than the simulation cell. However, as the grain growth

of Cu interconnects is confined to several tens nanometer and the final average grain size is comparable with the line size [10], the traditional periodical boundary condition becomes inapplicable.

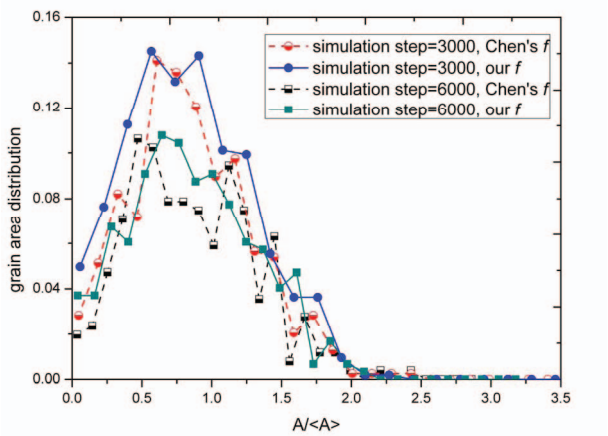


Figure 3. The distribution of grain sizes simulated with our and Chen's method, using periodical boundary condition.

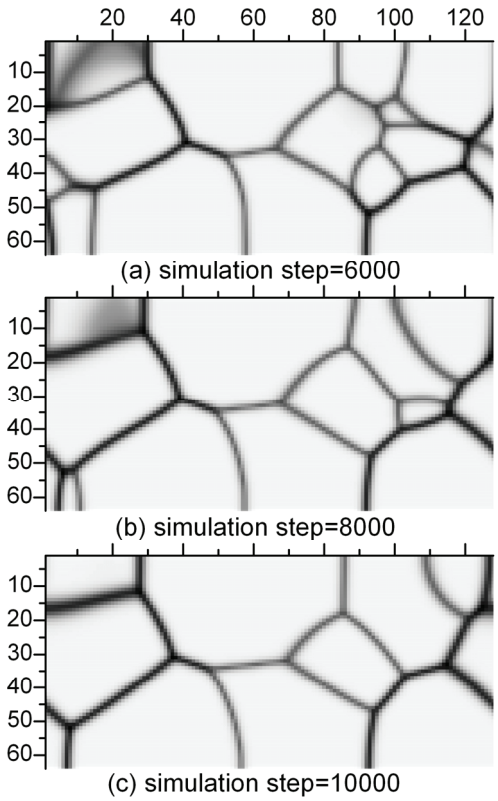


Figure 4. Microstructure evolution in the plane of z=28 for a 128×64×56 simple-cubic grid. Two different grain boundaries are shown and a more physical Cu grain growth is given.

It is known that a strong <111> texture can be observed along the surface or the diffusion barrier/metallic film interfaces, this texture has lower strain and surface energies [11][12]. In present work, we add an additional layer of grids around the simulation cell. In these layers, half of the phase variables are set to 0.1 so that adjacent grains incline to certain orientations. Under this boundary condition, the microstructure evolutions of various Cu lines are simulated and the average grain sizes are obtained after 10000 simulation steps. The simulation results are compared with experimental data given by V.Carreau [10] in Fig. 5(a). It is clearly shown that, the obtained average grain size is confined by the line width for line widths below 700 nm. The good agreement demonstrates the reliability of this work.

To demonstrate the validity of this work further, we predicted the average grain size of different line width from 20nm to 40nm and the results are shown in Fig. 5(b). The obtained microstructures of these Cu lines are employed in a Monte Carlo program to calculate the resistivity. The simulation results are compared with the experimental resistivity of different Cu lines with the same size presented by IMEC [13] in Table I. The good agreement shows that our method can predict the resistivity of Cu line well.

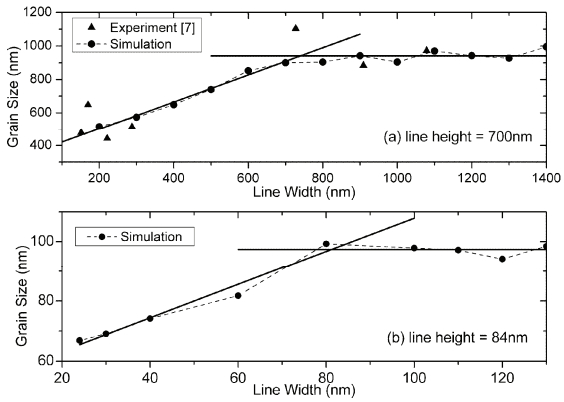


Figure 5. (a) Correlation between the line width and the average grain size at line eight = 700nm. The results are compared with experimental data [10]. (b) The predicted correlation between the line width and the average grain size at line height = 84nm.

TABLE I. RESISTIVITY OF CU-LINE WITH DIFFERENT WIDTH

| **Line width** | ***20nm*** | ***25nm*** | ***30nm*** | ***40nm*** |
|---|---|---|---|---|
| Experiment(μΩ·cm) [13] | 5-5.6 | 5-5.5 | 4.1-4.6 | 3.6-3.9 |
| Simulation(μΩ·cm) | 5.47 | 5.12 | 4.36 | 3.90 |

## IV. CONCLUSIONS

Phase-field model techniques are used to simulate the evolution of Cu interconnect. In the simulation, a new local free energy density function is proposed in which the field variables can be reduced greatly. By restraining the grain orientations in the side face of interconnect, the model is applicable to simulating the microstructure evolution of poly-crystalline Cu lines. These modifications have greatly cut down the number of the field variables needed and also improved the simulation efficiency a lot. The obtained average grain sizes and resistivity of different Cu lines are compared with experimental data and show good agreement.

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