Monte Carlo Simulation of Cu-Resistivity

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***Abstract*—We have developed an optimized model for electron behavior in Cu-line and we have implemented it using Monte Carlo method. Our model takes into account not only four normal scatterings but also the grain boundary scattering and the surface roughness scattering. The model has been tested with different line width and providing a good agreement with both calculated results and ITRS data.**

Keywords-Cu-resistivity; gain boundary scattering; Monte Carlo simutlation; surface roughness scattering;

I. INTRODUCTION

With the development of micro-electronic device, the interconnection is also scaling down continually. Recently the Cu interconnect is widely used by reason of its high conductivity. But research work indicates that when the size of Cu-line goes down to 130nm, the resistance increases rapidly with the decreasing dimension [1]. Normally the mean-free-path of electrons for Cu is about 39nm at room temperature [2]. And when the width of Cu-line is comparable with the electron mean-free-path, some scattering events become obvious, which used to be ignored for Cu-line. In this paper, we developed a Monte Carlo simulation for small-size Cu line considering size effect. Six scattering mechanisms are included, especially the grain boundary and surface roughness scattering. We analyze the relationship between resistivity and temperature as well as the line width and compare the results with ITRS data [3]. Meanwhile we evaluate the influence of each scattering respectively.

II. PHYSICAL MODEL AND THE SIMULATION METHOD

We developed a Monte Carlo program to simulate electrons behavior in copper. In order to describe the resistivity of Cu accuracy we consider size effect. The physical model of the program includes electron to electron scattering, plasma excimer scattering, acoustic and polar phonon scattering, grain boundary scattering and surface roughness scattering. For the electron to electron scattering [4], both the energy and the momentum changed, but the total of the whole system is constant. So usually it is less important than other scattering mechanism. But unlike in semiconductor, the density of electrons in metal is high. In this situation, we have to consider the scattering between electrons. The scattering is cause by the potential as in (1):

$$V(r) = \pm \frac{e^2}{4\pi\varepsilon_0\varepsilon r} e^{-\frac{r}{L_D}} \qquad (1)$$

Where e is the quantity of electricity, 1.6×10^{-19} C

$\varepsilon_0\varepsilon$ is dielectric constant, Here used ε_0

L_D is shielded length, 4.05×10^{-12} m

r is the distance between two electrons,

Plasma excimer scattering mechanism [5] is also one kind of carrier interaction. By reason of coulomb interaction between carriers, the local undulate of carrier density is not isolated. It causes oscillation of carrier density. It is similar to the lattice vibrant wave. The scattering cause by the periodic potential as in (2):

$$V(x,t) = \frac{e^2 n a_q}{\varepsilon_0 q}\left[e^{i(qx-\omega_q t)} - e^{-i(qx-\omega_q t)}\right] \qquad (2)$$

Where e is the quantity of electricity, 1.6×10^{-19} C

a_q is the amplitude of vibration,

ε_0 is dielectric constant in vacuum, ε_0

q is wave vector,

x is the electronic kinetic distance

$\hbar\omega_q$ is the energy of phonon. 60mev

t is the kinetic time

The metal also has phonon scattering [6-7]. Any potential which deviates from the ideal periodic potential will cause electron scattering. Both the acoustic and polar phonon scattering mechanism are caused by lattice vibration as in (3) and it is proportional to the sine function:

$$V(x,t)=A_+(q)e^{i(qx-\omega_q t)}+A_-(q)e^{-i(qx-\omega_q t)} \qquad (3)$$

Where e is the quantity of electricity , 1.6×10^{-19} C

A is the amplitude of vibration,

When the size is small enough, we have to consider the grain boundary scattering [8]. The grain boundary becomes an obstruction for electrons. It will become notable when the line width scaling closes to the electron mean-free-path. We choose a δ Function to simulate this potential as shown in Fig. 1 and can be calculated as in (4):

$$P=A\sum_i^n \delta(x-x_i) \qquad (4)$$

Where A is altitude of potential 0.1eV

x_i is the length of grain See in Figure 1.

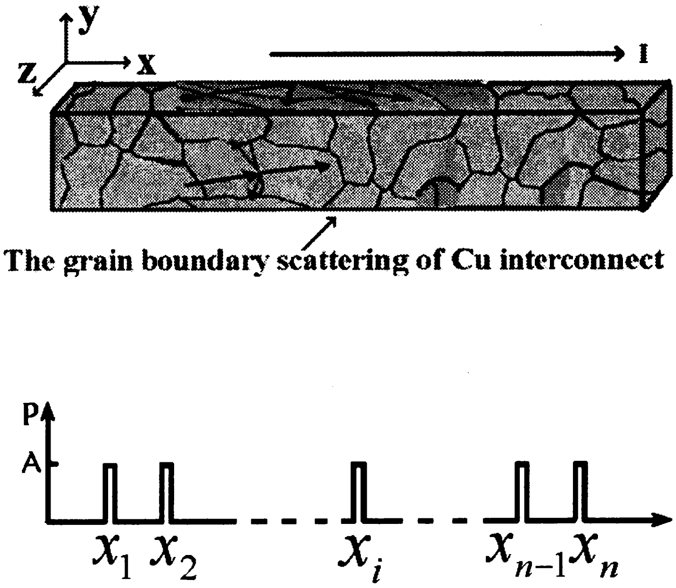

Figure 1. The sketch map and potiental of grain boundary

And the surface of copper interconnect is affected obviously by roughness [9] as shown in Fig. 2. It will scatter the electron and change its momentum. In our model we use summation of several Gaussian distributions (5) to describe the surface roughness

$$\sum_i^n \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu_i)^2}{2\sigma^2}} \qquad (5)$$

Where μ_i is random number, 0.4nm

σ decides the shape of Gauss function. 1.5nm

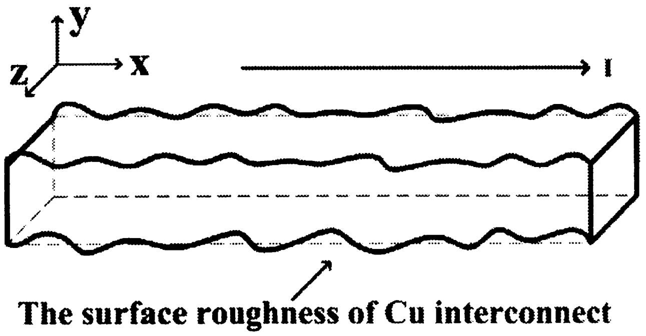

Figure 2. Comparison of simulated and calculated resistivity as temperature changing.

As we know the microscope movement of electron can be described to a series of alternant free flight and random scattering under electric field. Monte Carlo method cope this situation with random number sequence. It simulates single particle and is used to solve the transport problem by simulation electron free flight and scattering.

III. RESULTS AND DISCUSSION

The bulk Cu is simulated and compared with the experimental data. The simulated bulk Cu resistivity with various temperatures compared with the calculation results shown in Fig. 3.

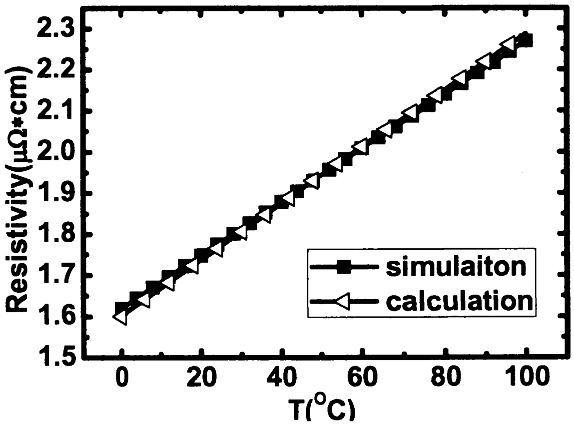

Figure 3. Comparison of simulated and calculated resistivity as temperature changing.

The calculation results are determined from the linear relation (6):

$$\rho/\rho_0 = 1 + \alpha(T - T_0) \qquad (6)$$

α is slope, 0.004

ρ_0 is room temperature value. 1.7 μ Ω *cm

From the figure, it can be seen good agreement is achieved by our simulation method. We discuss the influence of each scattering mechanism below. From Fig. 4, we can find that the polar phonon and plasma excimer scattering mechanisms impose more important impact. And the acoustic phonon almost has no influence. After adding the grain boundary and surface roughness scattering mechanisms, we reduce the width of Cu-line continually.

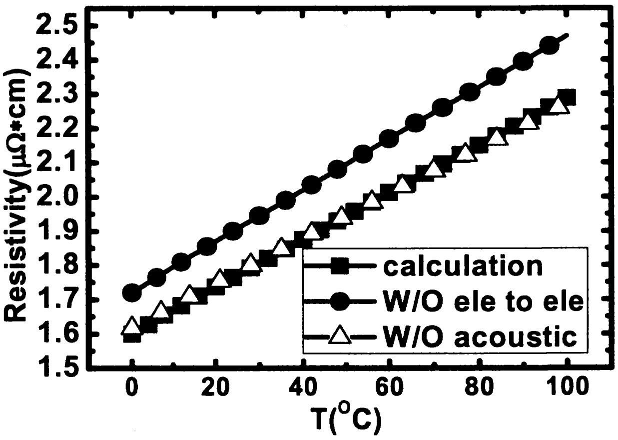

Fig. 4(a) The effect of electron to electron and acoustic phonon scattering mechanism

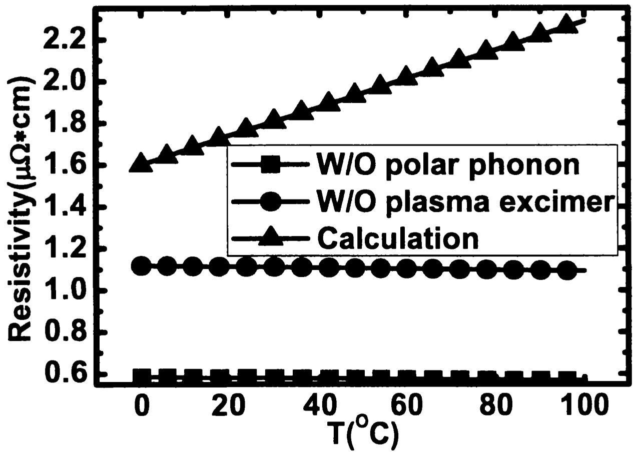

Fig. 4(b) The effect of polar phonon and plasma excimer scattering mechanism

Figure 4. The effect of electron to electron and acoustic phonon scattering mechanism

The relationship between resistivity with line width is shown in Fig. 5. The simulation is verified by comparing the results to the experimental data [3] and the model is based on Fuchs-Sondheimer model [10]. And we show this relationship by a histogram in Fig. 6. If we increase the line width, the influence of these mechanisms diminishes. It will totally disappear until the line width goes to 180nm. Then we evaluate the scattering mechanism's influence in Fig. 7. From this figure, we find that when we ignore grain boundary and surface roughness scattering mechanisms, the line resistivity becomes irrelevant with the line width. Then there is no difference between bulk and line.

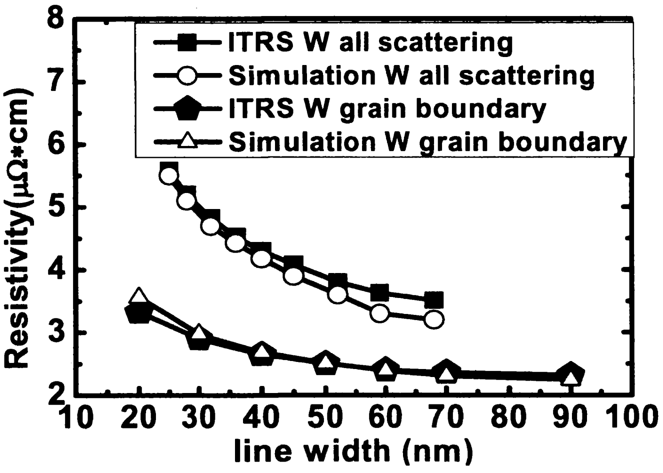

Figure 5. Relationship between resistivity and line width(compared with ITRS data[3])

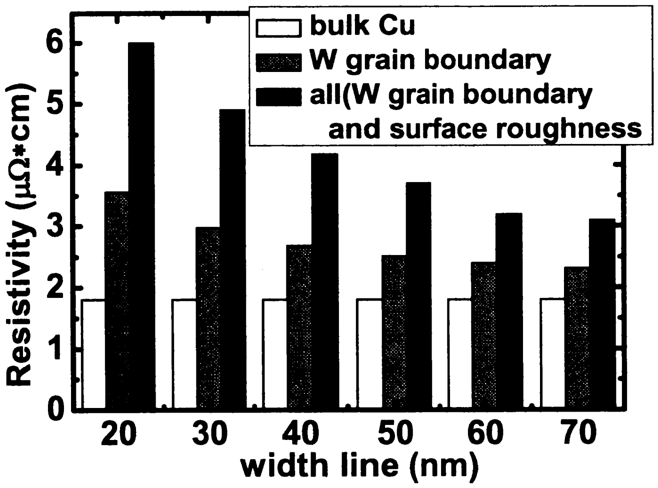

Figure 6. The sketch map of relationship between resistivity with width

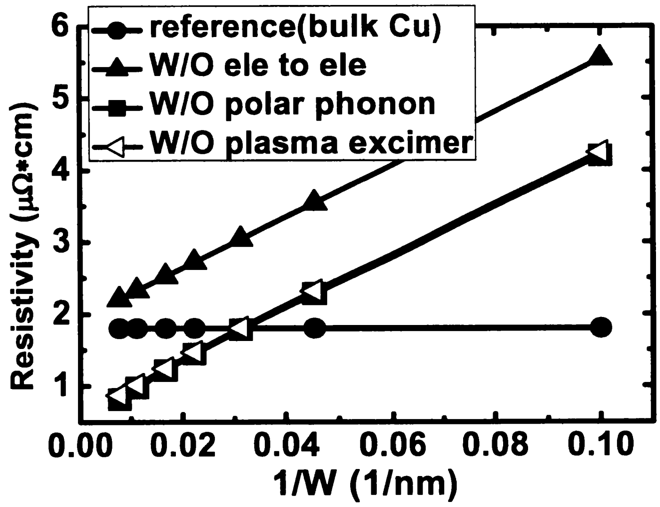

Figure 7. The influence to resistivity of each scattering mechanism

IV. CONCLUSIONS

In our work, we developed a model with six scattering mechanisms to simulate small size Cu-line by Monte Carlo method. Good agreement can be obtained between simulating results and the experimental results. The results can help to optimize the characteristics of Cu interconnection.

ACKNOWLEDGMENT

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