Compact and Efficient Monte Carlo Method to Reproduce Size Effect on Resistivity in Sub-0.1μm Metallic Interconnects

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***Abstract*—We present a compact and efficient Monte Carlo method to reproduce a size effect on resistivity in sub-0.1μm metallic interconnects. Implementation of our method is easy and our method is also not CPU-intensive thanks to its compactness and simplicity. In our method, the geometric effect of the size effect can be taken into account since surface scattering and grain boundary scattering, which are causes of the size effect on resistivity, are treated as real space interaction. We found that in rectangular metallic wires, mean free path of electrons around the corners of wires decreases owing to multiple surface scatterings and drift velocity around the corners is degraded. In very narrow and thin wires, this velocity degradation due to multiple surface scatterings is dominant and enhances the size effect of resistivity.**

Keywords-Monte Carlo Method; Interconnects; Size Effect; Resistivity;

I. INTRODUCTION

Recently, the size effect on resistivity in copper interconnects has emerged as a serious problem in development of the sub-0.1μm generation because it causes interconnect resistance to increase as scaling progresses [1]. Therefore, understanding of physical mechanisms and accurate prediction of the size effect on resistivity are required. Steinhögl *et al.* provided a compact analytical expression to predict the size effect considering surface scattering and grain boundary scattering [2] and their model is widely used. However, Wada *et al.* pointed out that Steinhögl's model was not good for very thin and narrow wires and measured resistivity was higher than in the model [3]. They also suggested that the difference between the measured values and the model was caused by surface scattering at the corners of the wire and the geometric effect was very important although Steinhögl's model took little account of it. Wang *et al.* developed a semiclassical Monte Carlo (MC) transport simulator considering various scattering mechanisms, including phonon scattering, electron-electron scattering, plasmon scattering, surface roughness scattering and grain boundary scattering, to analyze the size effect [4]. Their approach is high precise from the viewpoint of transport mechanisms in metal and it can straightforwardly take into account the geometric effect however, it is so complicated that the implementation of the method is difficult and the simulation itself is very CPU-intensive.

In this paper, we present a compact and efficient semiclassical MC method to reproduce the size effect on resistivity of sub-0.1μm metallic interconnects. Our simulation method is not CPU-intensive and easily applied for simulating various materials thanks to its compactness and simplicity. In our method a surface scattering and a grain boundary scattering is treated as real space interaction, therefore, a precise geometric effect on resistivity can also be incorporated in our method. It is shown by the MC simulator that corner scatterings limit the resistivity of the metal for very narrow and thin wires.

II. SIMULATION MODEL AND METHODOLOGY

A. Simulation Model to Reproduce Bulk Resistivity

Firstly, we present a compact MC method to reproduce resistivity and electronic mean free path of bulk metal. Our simulation model is based on Sommerfeld's theory of electronic transport in metals [5]. Fig. 1 shows a schematic representation

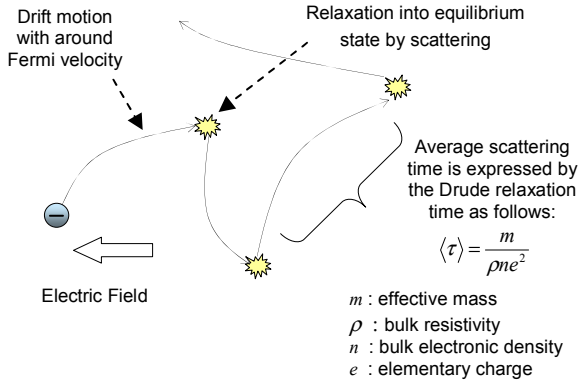

Figure 1. Schematic representation of the proposed compact MC method to reproduce resistivity and mean free path of a bulk metal. Electrons are accelerated by external field during Drude's relaxation time and they reach equilibrium state once they are scattered.

of our simulation model. There are two important assumptions. The first is that only electrons near the Fermi surface contribute to the electric current. The conductive electrons move around inside the wires with about the Fermi velocity. So, we simulate only electrons near the Fermi surface. The second assumption is that when electrons are accelerated by an external field and become energetic, they loose their energy by a scattering in the Drude relaxation time [5] and immediately reach a state of equilibrium. We simulate these dynamics by an ensemble MC method as described in [6]. Our method is equivalent to solving the Boltzmann transport equation with constant relaxation time approximation and can reproduce correct mean free path of electrons and resistivity of the bulk metal with only a few well-known parameters, which are the electronic effective mass m, the resistivity ρ and the electronic density n of the bulk metals. Therefore, we can easily apply this method for simulating various materials, copper, aluminum, tungsten and so on, which are generally used for interconnect material. In addition, this method is not CPU-intensive because of its simplicity.

B. *Surface Scattering and Grain Boundary Scattering*

To reproduce the size effect on resistivity, modeling of surface scattering and grain boundary scattering are required [2]. Both the scatterings are treated as real space interaction to incorporate the geometric effect precisely.

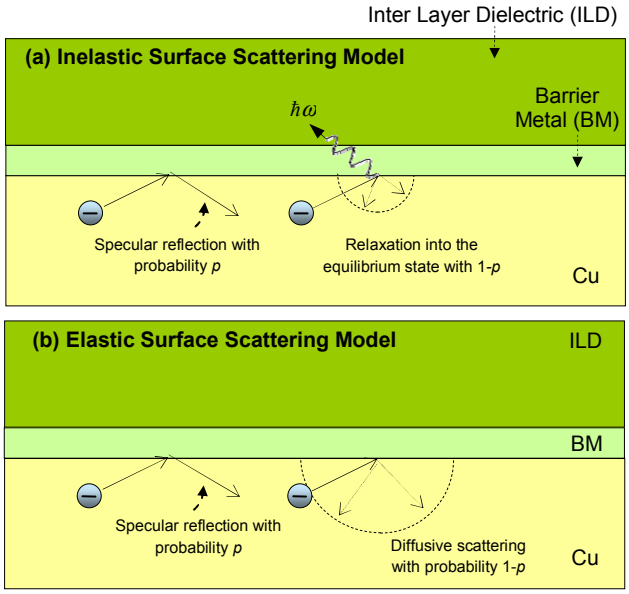

Figure 2. Schematic representation of surface scattering models for Cu interconnects. Scatterings are treated as real space interaction to incorporate the geometric effect on resistivity.

For the surface scattering model, two phenomenological scattering models are examined. The first one is an inelastic surface scattering model shown in Fig. 2(a) and the second one is an elastic surface scattering model shown in Fig. 2(b). In the inelastic surface scattering model, once electrons reach an interface between a conductive metal and a barrier metal, they are specularly reflected with probability p or they reach a state of equilibrium by a certain scattering mechanism with probability 1-p. In this model, we consider that an origin of the inelastic scattering is a phonon or plasmon in the barrier metal or near the interface. Because mean free path in the barrier metal is generally shorter than in the conductive metal, electrons injected into the barrier metal are immediately scattered and reflected to a conductive metal. On the other hand, in the elastic model, electrons are specularly reflected with probability p or diffusively reflected with probability 1-p, where electrons' energy is conserved although their momentum is randomized. This model is sometimes employed for a surface roughness scattering model at interface between silicon and silicon dioxide in MC simulation [7].

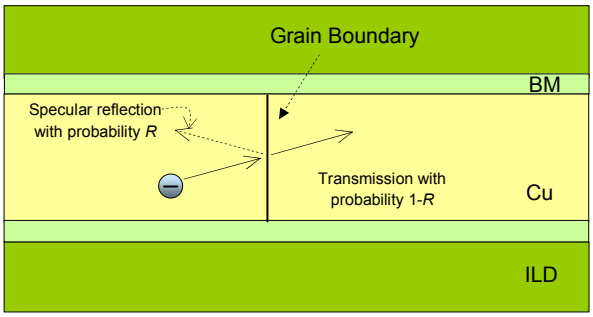

Figure 3. Schematic representation of grain boundary scattering model. Electrons that reach the grain boundary are elastically reflected with probability R or transmit the boundary with 1-R.

For the grain boundary scattering, phenomenological transmission/reflection model is used in the same way in Ref. [2]. In this model, electrons are specularly and elastically reflected at the grain boundary with probability R or transmit with probability of 1-R (Fig. 3).

C. *Simulated Structure*

Fig. 4 shows a simulated interconnect structure and a snapshot of simulated electrons. We focus on rectangular wires in this paper. The bamboo structure shown in Fig. 4 is employed as grain distribution. Average grain size is assumed to be equal to the wire width. This assumption is appropriate for sub-0.1μm copper wires fabricated by the damascene process [2]. Lattice temperature is assumed to be 300K.

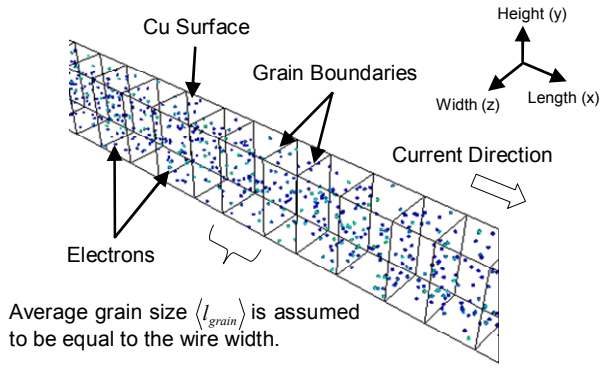

Figure 4. A snapshot of an ensemble MC simulation for a rectangular Cu interconnect. Electrons are scattered not only in bulk region but also at a surface and grain boundaries. An average grain size is assumed to be equal to the wire width.

III. RESULTS AND DISCUSSIONS

A. Comparison with Experimental Results and Performance

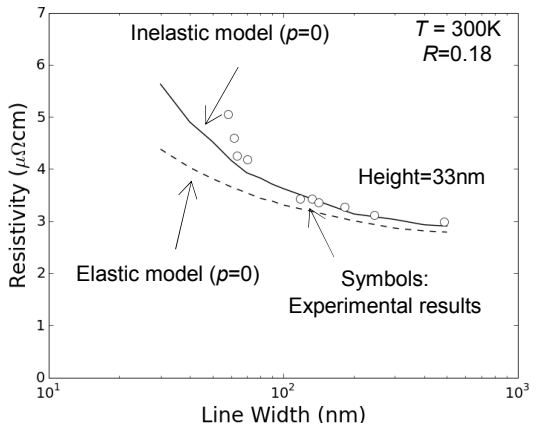

Figure 5. Relationship between wire width and resistivity obtained by MC simulations and experiments. Inelastic surface scattering is better to reproduce the size effect.

Fig. 5 shows the relationship between wire width and resistivity obtained by the proposed method and experimental results. Open symbols show experimental results [3], and solid and dashed line show MC results with the elastic surface scattering model and the inelastic surface scattering model, respectively. MC with the elastic surface scattering underestimates resistivity entirely even if the surface scattering parameter p is set to zero. On the other hand, MC results with the inelastic surface scattering model (p=0) are in good agreement with experimental data except for the narrow region below 50 nm. We consider that discrepancy between MC results with the inelastic model and experimental results below 50 nm arises from approximation for grain distribution and variability of experimental data. The effect of more complicate and realistic grain distribution on resistivity is under investigation and will be discussed elsewhere. The fact that

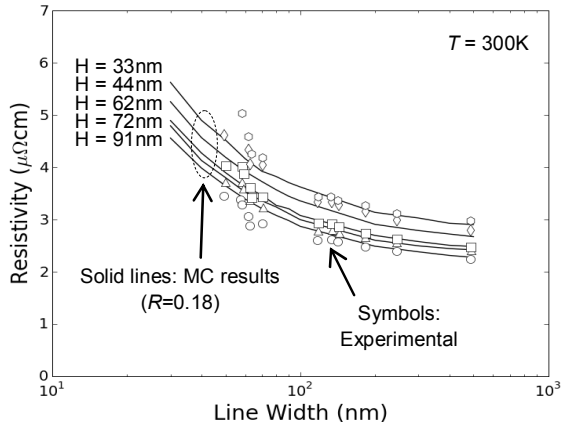

Figure 6. Relationship between wire width and resistivity obtained by MC simulations and experiments for several values of the wire height. MC results show good agreement with experimental ones.

MC with the inelastic model is in good agreement with the experimental results indicates that a scattering at interface between copper and barrier metal is an inelastic process rather than an elastic process. Fig. 6 shows the relationship between wire width and resistivity obtained by the MC method with the inelastic surface scattering (p=0) model and experimental results for several values of wire height. Solid lines show simulation results and open symbols show experimental data [3]. Simulation results using the inelastic surface model show good agreement with experimental ones for various wire size.

Computational time per point on a typical workstation is around several minutes even though the simulation program is written in an interpreted language Python [8]. Our MC method is very effective from the viewpoint of both accuracy and computational time.

B. Geometrical Effect on Resistivity in Rectangular Wire

In order to analyze the influence of the surface scattering on the size effect in rectangular wires, we calculate averaged drift velocity distributions inside the wires. The grain boundary scattering is artificially ignored here to clarify the surface scattering effects. Fig. 7 shows the drift velocity distributions in the cross-section of the wire and projection of electronic trajectories during 1 ps (solid lines). Around each line-edge of the wires, degradation of drift velocity by surface scatterings is observed as dark regions of the figure. In addition, velocity around the corners is more degraded (darker region). This is caused by multiple surface scatterings at the corners as shown in Fig. 7(d). They reduce the effective mean free path of electron near the corners and degrade the velocity.

Fig. 8 shows comparison with an analytical model [2] and MC results. Solid lines show results by analytical model and open circles show MC results. In the analytical model, parameter for surface scattering p [2] is set to zero and grain boundary scattering parameter R is set to 0.18, which are the same values as in our simulation. Difference between them increases with decreasing lateral and vertical dimensions of wires. This trend is explained as follows; in very narrow and thin rectangular wires, the multiple surface scatterings around the corners are dominant and the drift velocity inside the wires is strongly degraded and the size effect is enhanced. This causes increase in difference between our model and the analytical model in thinner and narrower region. It is important to consider this kind of geometric effect for accurate prediction of the size effect on resistivity in sub-0.1μm interconnects.

IV. SUMMARY

We developed a compact and efficient Monte Carlo method to reproduce the size effect on resistivity in sub-0.1μm metallic interconnects. Using the inelastic surface scattering model, good agreement with experimental results is obtained. Our method is effective from the viewpoint of computational time thanks to its compactness and simplicity. A surface scattering is treated as real space interaction and a geometric effect on resistivity is incorporated in our method. The consideration of the geometric effect is important for accurate prediction of the size effect. In rectangular wires, the multiple surface scatterings around the corners of the wires degrade drift

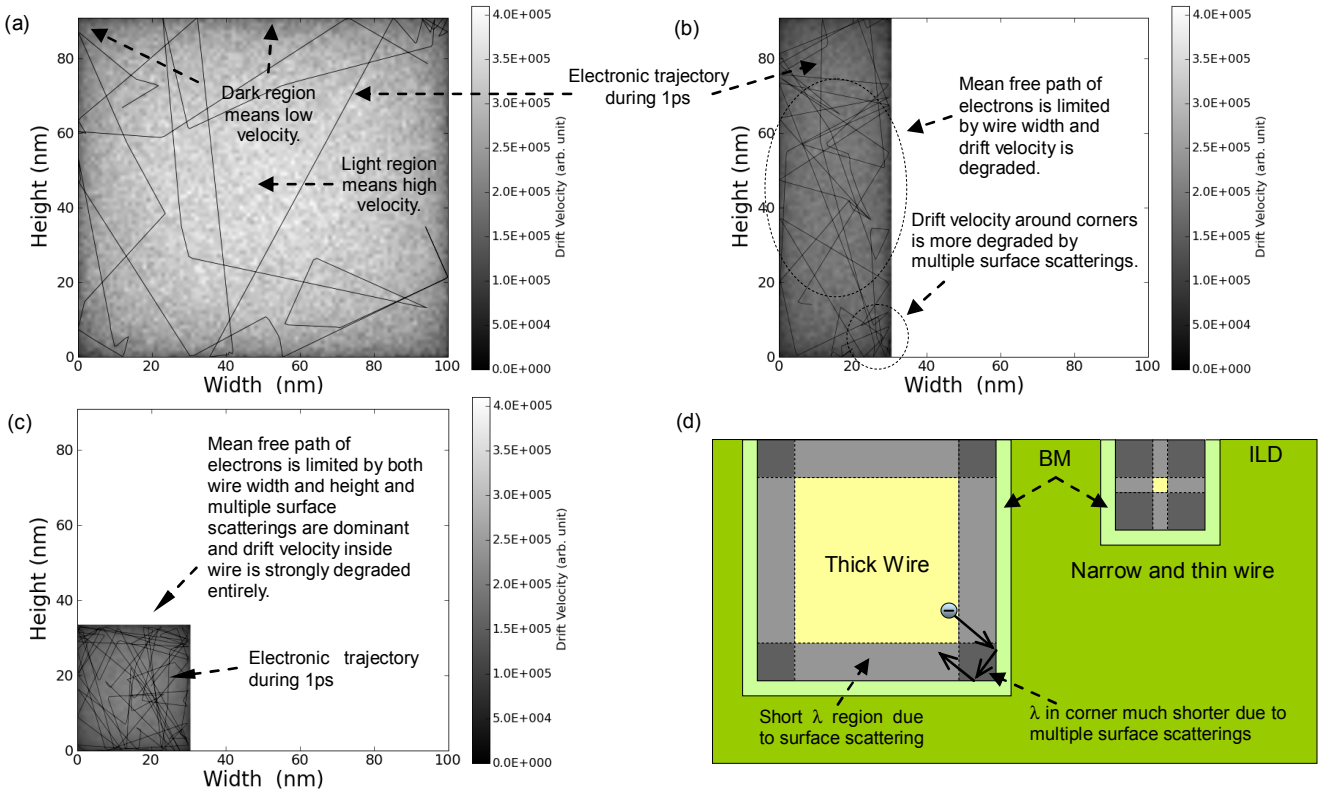

Figure 7. (a), (b) and (c) show averaged drift velocity distributions and solid lines are electronic trajectories during 1ps in Cu wires simulated by the proposed MC method. Grain boundary scattering is artificially ignored to clarify the effect of surface scattering. Lighter regions mean higher velocity and darker regions mean lower velocity. (d) is explanation for velocity degradation caused by scaling. In narrower and thinner wires, multiple surface scatterings are dominant and drift velocity throughout the wire is strongly degraded and increase of resistivity is enhanced.

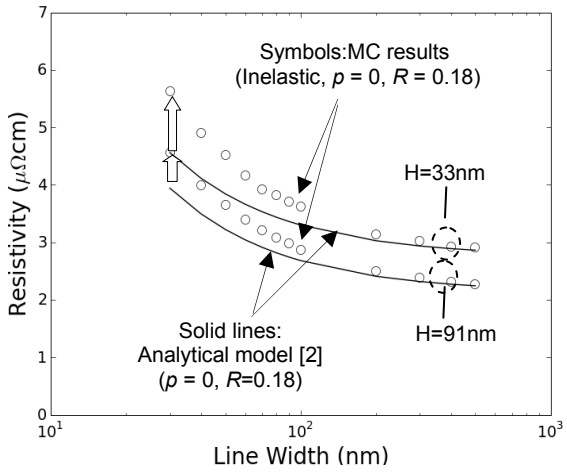

Figure 8. Comparison with analytical model [2] and our Monte Carlo results. Difference between them increases with decreasing lateral and vertical dimension of wires due to multiple surface scatterings around the corners.

velocity around there and in sub-0.1μm metallic interconnects the corner effect is dominant and enhances the size effect.

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