Impact of Line-Edge Roughness on Electrical Resistivity in Decananoscale Copper Wires: A Monte Carlo Study

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***Abstract*—We present impact of Line-Edge Roughness (LER) and Line-Width-Roughness (LWR) on electrical resistivity in decananoscale copper wires utilizing a semi-classical Monte Carlo (MC) simulation. Effects of LER/LWR on electron transport are considered as a geometric effect within the framework of classical physics. Dependence of the resistivity on parameters characterizing LER has been analyzed in detail. We show that mean free path (MFP) of electrons plays a key role in resistivity degradation due to LER/LWR: When the MFP is shorter than wavelength of LER, the degradation takes place due to LWR rather than LER itself (LWR mode) and control of correlation between line-edges is important to suppress the degradation due to the LER. In contrast, when the MFP is longer than wavelength of LER, degradation of resistivity takes place due to LER (LER mode). In the LER mode, control of the correlation between line-edge is not effective and the amplitude should be decreased to suppress the degradation.**

Keywords-Monte Carlo method; copper; interconnect; size effect; electrical resistivity and resistance; line-edge roughness (LER); line-width roughness (LWR); mean free path; scattering;

I. INTRODUCTION

It is pointed out that Line-Edge Roughness (LER) and/or Line-Width Roughness (LWR) give rise to degradation of electrical resistivity in deeply scaled copper wires and they enhance the size effect on electrical resistivity [1]. To suppress the resistivity degradation due to LER/LWR, precise understanding of degradation mechanisms is required. And numerical tools to estimate the degradation are also required from the viewpoint of development efficiency. So far, an analytical model as described in Ref. 2 is proposed to estimate resistivity of wires with LER/LWR. The model introduces the local resistance which is a function of local wire width and calculates total resistance by integrating it along the long-direction of the wires. It is considered that this approximation is valid only when the length-scale of LER longer than mean free path (MFP) of electron [2]. However, the details of relationship between wavelength of the LER and MFP are not fully investigated yet, and we consider that a proper method to investigate them is a semi-classical Monte Carlo (MC) method [3,4] where microscopic carrier scatterings are considered explicitly and MFP of electron in the material is simulated properly.

In this paper, we present the degradation of electrical resistivity in decananoscale copper wires utilizing the semi-classical Monte Carlo simulation, especially focusing on the relationship between wavelength of the LER and MFP. Dependence of resistivity on parameters characterizing LER/LWR such as amplitude and correlation between line-edges is also presented. We found that when the MFP is longer than wavelength of LER, degradation of resistivity takes place due to LER. In contrast, when MFP is shorter than wavelength of LER, the degradation takes place due to LWR rather than LER itself. In the latter case, the correlation between line-edges becomes the most important parameter to suppress the degradation of electrical resistivity due to the LER/LWR.

II. SIMULATION MODEL AND METHODOLOGY

Figure 1 shows a schematic diagram of the simulation model. A scattering inside copper wires to reproduce bulk resistivity and interface scattering to reproduce the size effect are taken into account with a phenomenological manner [4]. In this study, the interface scattering is assumed to be perfectly diffusive (probability for specular scattering is zero). This assumption is proper for copper wires [4]. Electrons in the wires drift with around Fermi velocity and their drift motions are disturbed by the scatterings. We assume that material inside wires is a crystal copper. Resistivity of the copper is assumed to be 1.7 μΩcm and MFP of the simulated electrons for the copper is about 40 nm at room temperature (RT).

In this study, the effect of the LER/LWR on carrier transport is considered as a geometric effect within the framework of classical physics. We prepare 3-dimensional

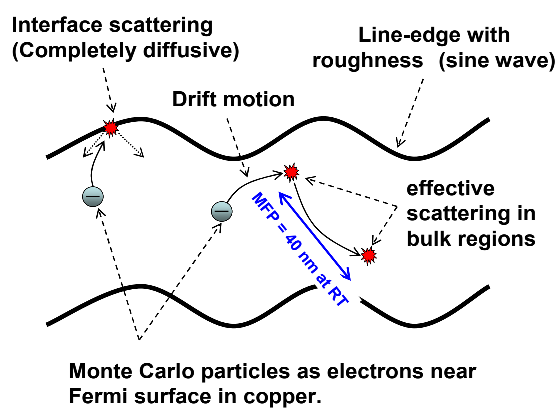

Figure 1. Schematic diagram of our Monte Carlo simulator.

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(3D) structures explicitly with LER/LWR. Electrons are scattered at the curved interfaces and their state are randomized. In addition, we use a 3D drift current continuity equation for steady state in order to consider the effect of non-uniformity of electric field due to the LER/LWR on electrical resistivity

$$\nabla \cdot (\sigma(x,y,z)\mathbf{E}(x,y,z)) = 0,$$

where $\sigma(x,y,z)$ and $\mathbf{E}(x,y,z)$ represent electrical conductivity distribution and electric field distribution, respectively. This equation is often used in conventional TCAD tools to estimate current density and electric field distribution inside metallic wires. Our simulation procedure using above equation is as follows: First, we obtain initial electric field distribution by solving the continuity equation where electric conductivity distribution is uniform and constant. Then we simulate particle movement under the electric field and obtain conductivity distribution $\sigma_{MC}(x,y,z)$ inside the wire. Afterward, we update electric field through the continuity equation with $\sigma_{MC}(x,y,z)$ and simulate particle movement under the updated field and obtain terminal current. Finally, we obtain effective electrical resistivity of wires with LER by the following equation

$$\rho_{eff.} = \frac{V_{app}}{I_{MC}} \cdot \frac{\overline{w} \cdot h}{L},$$

where V_{app}, I_{MC}, $\overline{w}$, h, and L represent applied voltage, mean terminal current obtained by MC simulation, mean wire width, wire height, and wire length, respectively.

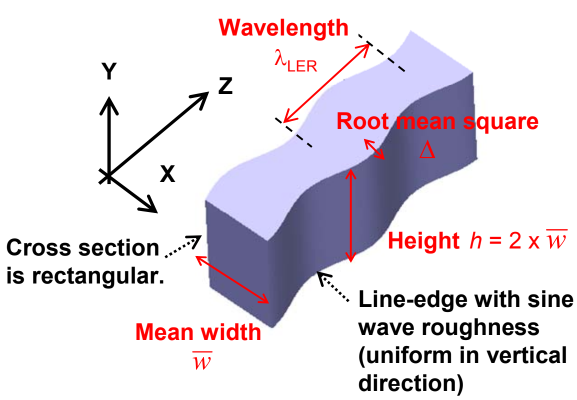


Figure 2. Simulated structure and geometric parameters.

Figure 2 shows a simulated structure and its geometric parameters. We assume that waveform of LER is sine wave and ignore grain boundary (GB) and scatterings by GB in order to clarify the degradation mechanism due to LER/LWR. The parameters characterizing the LER are wavelength (λ_{LER}), amplitude (root mean square, Δ), and average width ($\overline{w}$). We assume that the aspect ratio is constant and its value is 2. The length of wires is 60 nm, and periodic boundary condition is applied for MC particles and Dirichlet's boundary condition is applied for field equations. And we introduce the correlation between line-edges δ as a parameters, which is an important one represents the amplitude of LWR [5]. The definition and the relationship between the correlation δ and LWR are shown in Figure 3[1]. We assume that lattice temperature is 300 K.

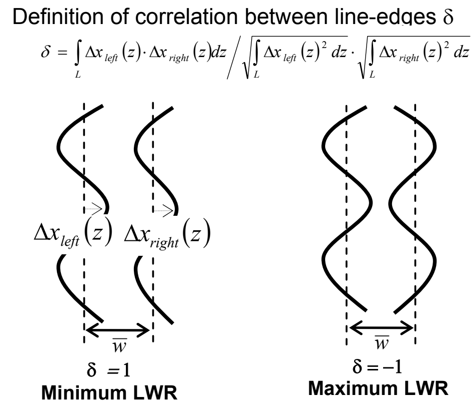


Figure 3. Definition of correlation between line-edges and relationship between the correlation and LWR.

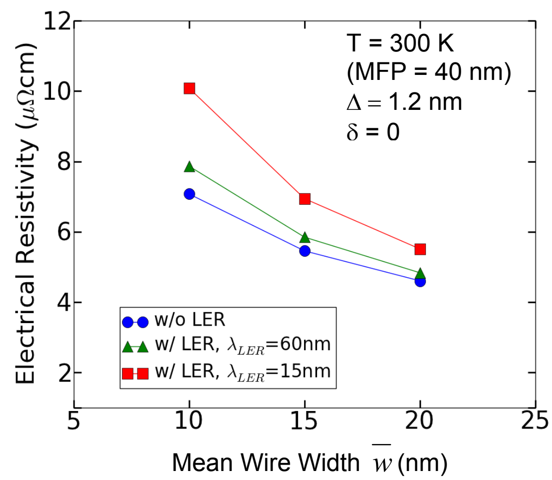


Figure 4. Simulation results of size effect on resistivity of the wires w/ and w/o LER.

III. SIMULATION RESULTS AND DISSCUSSION

Figure 4 shows simulation results of electrical resistivity of the wires without (w/o) and with (w/) LER/LWR as a function of mean wire width. The root mean square and the correlation between line-edges are assumed to be constant (Δ = 1.2 nm, δ = 0). It is observed that the degradation due to LER/LWR increases with decreasing mean wire width and also observed that the shorter wavelength has the larger impact on resistivity. Figures 5, 6, and 7 show the relationship between LER parameters and electrical resistivity in the case with $\overline{w}$ = 20 nm, 15 nm, and 10 nm, respectively. In the shorter wavelength, the correlation between line-edges has negligible effect on resistivity degradation in all the conditions. On the other hand, the degradation in the cases with longer wavelength

[1] The sign is opposite to that in Ref. [3] due to a slight difference of the definition.

depends on the correlation between line-edges, and the dependence become stronger according to scaling down of the wire width.

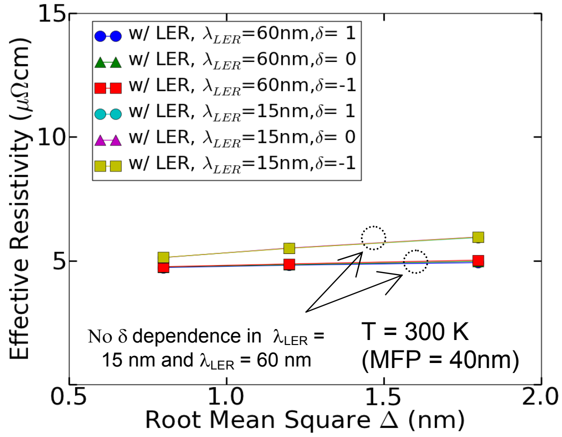


Figure 5. Simulation results of dependence of resistivity on LER parameters in the wires with $\overline{w}$ = 20 nm.

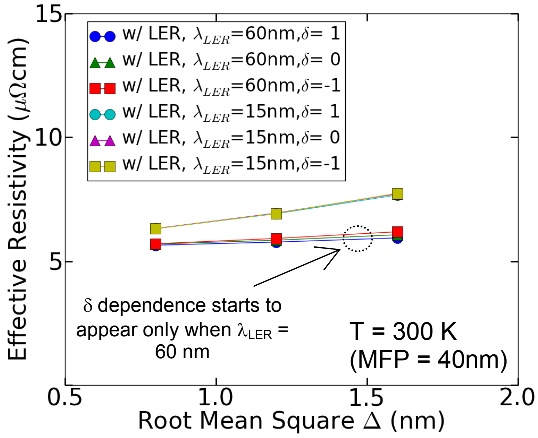


Figure 6. Simulation results of dependence of resistivity on LER parameters in the wires with $\overline{w}$ =15 nm.

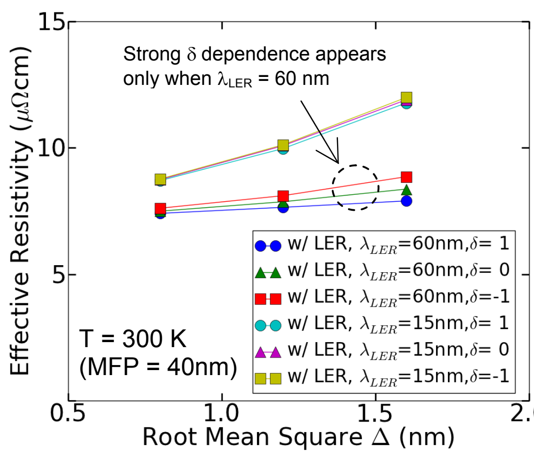
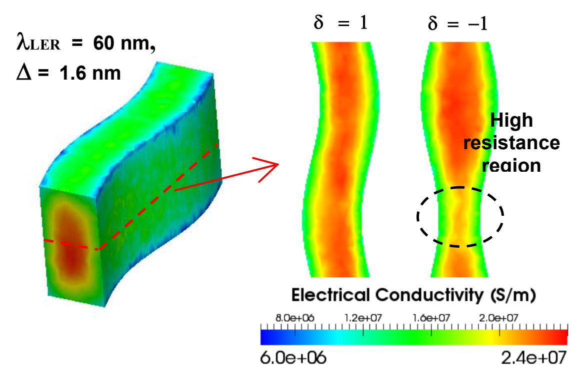
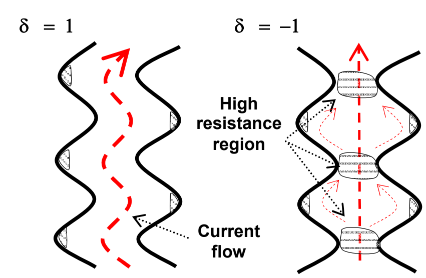


Figure 7. Simulation results of depenence of resistivity on LER parameters in the wires with $\overline{w}$ = 10 nm.

As expected, above results arise from the following reasons: When λ_{LER} = 60 nm, the value of which longer than MFP, the resistivity degradation is controlled by LWR rather than LER itself (LWR mode). Figure 8 (a) shows electrical conductivity distribution inside the wires with $\overline{w}$ = 15 nm. When $\delta = 1$ (left in Figure 8 (a)), it is observed that electrical conductivity distribution responds along the curved interfaces and electric current flows along shape of interfaces, and degradation becomes relatively weak. When $\delta = -1$, the LER forms bottleneck regions in the wires. Since their cross-sectional areas are small and conductivity around them is lower than the other regions, they limit flow of electric current, and consequently total resistance and effective resistivity increases. On the other hand, when λ_{LER} = 15 nm, the resistivity degradation takes place due to LER rather than LWR (LER mode). Figure 9 (a) shows electrical conductivity inside the wires with λ_{LER} = 15 nm. In this case, conductivity distributions do not respond to the shape of interfaces because electron drift motion around the convex regions is limited by cascade interface scatterings (CIS) and the effective MFP around the convex regions becomes short. These regions behave as dead layers for electrical conduction (Figure 9 (b)). As a result, effective wire width decreases and effective resistivity is higher than that of wires with λ_{LER} = 60 nm and dependence of resistivity on δ becomes very weak. MC transport simulation can treat these behaviors quite naturally.

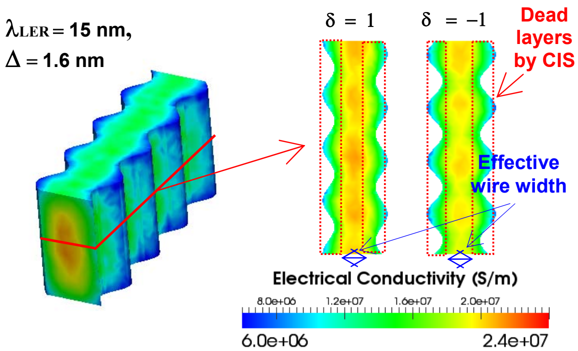


(a) Electrical conductivity distribution inside wires with $\overline{w}$ = 15 nm.

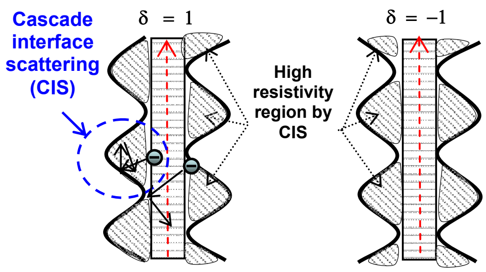


(b) Degradation mechanism: LWR mode

Figure 8. (a) Electrical conductivity distribution inside wires with $\overline{w}$ = 15 nm and (b) degradation mechanisms due to LER with λ_{LER} = 60 nm.



(a) Electrical conductivity distribution inside wires with $\overline{w}$ = 15 nm.



(b) Degradation mechanism: LER mode

Figure 9. (a) Electrical conductivity distribution inside wires and (b) degradation mechanisms due to LER with λ_{LER} = 15 nm.

In wires with more realistic structures, power spectrum of LER is generally Gaussian distribution-like, and grain boundaries exist. In the case of copper wires, they are fabricated by damascene process generally and mean grain size is approximately proportional to the mean wire width [5,6]. Therefore, grain boundaries may limit MFP of electrons in realistic decananoscale and nanoscale copper wires. And also, basically MFP depends on temperature, material and structure. Effects of grains, temperature, material and structure, and their interactions on electron transport in deeply scaled metallic wires are now under investigation by our Monte Carlo simulator and will be presented elsewhere.

IV. SUMMARY

We have clarified impact of LER on electrical resistivity and relationship between mean free path and wavelength of LER in decananoscale copper wires with sine wave LER utilizing a semi-classical Monte Carlo simulation. When wavelength of the LER is longer than mean free path of electrons, resistivity degradation takes place due to LWR rather than LER itself (LWR mode) and the degradation can be suppressed by the control of the correlation between line-edges. On the other hand, when wavelength of the LER is shorter than mean free path, the degradation takes place due to LER itself (LER mode) and impact on resistivity is stronger than that of LWR mode. In this case, the control of the correlation is not effective to suppress the degradation due to LER and decreasing the amplitude is the only method to suppress the degradation. We consider that Monte Carlo simulation can be a useful tool for optimizing electrical resistance in deeply scaled metallic wires with LER/LWR.

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