Resistivity of thin Cu films with surface roughness

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We present an atomistic first-principles calculation of resistivity induced by atomically rough surfaces of thin Cu films. Our calculations show that the resistivity increases significantly due to surface roughness scattering and it is quite sensitive to both the amount and the nature of roughness. We determine the degree of specular scattering at rough surfaces by a parameter p which is obtained by fitting the *ab initio* data to the well-known Fuchs-Sondheimer model for surface scattering of thin metal films. In particular, we have obtained the $p=p(x)$ curve, where $(1-x)$ is the concentration of the rough sites on the Cu surface.

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I. INTRODUCTION

One of the key issues for integrated circuit technology is the increase in Cu interconnect resistivity with decreasing wire cross section,[1] a phenomenon typically referred to as “size effect.”[2] This effect severely impacts the time delay of the interconnects and thus represents a major challenge for the continuing evolution of the microelectronics devices. The size effect becomes appreciable when the interconnect linewidth approaches ~100 nm, namely, when it reaches two to three times the mean free path which is 39 nm for Cu at room temperature. The size effect becomes severe below 50 nm, giving rise to ~100% increase in the resistivity.[3–5]

Several scattering mechanisms contribute to the resistivity of Cu interconnect, and the problem of size effect is usually addressed by decomposing the total resistivity ρ into several contributions using the Matthiessen's rule,[6]

$$\rho = \rho_b + \rho_{\mathrm{im}} + \rho_s + \rho_g, \tag{1}$$

where ρ_b is the bulk or geometry independent resistivity which is largely determined by electron scattering from phonons; ρ_{im}, ρ_s, and ρ_g are resistivity components due to scattering by impurities, surface roughness, and grain boundaries, respectively. A number of experiments have been attempted to identify the influence of each scattering mechanism independently.[3,4,7–9] Surface scattering is considered to play a key role in the increase in resistivity of Cu thin films. Recently it is observed that for 250–75-nm-wide Cu lines, approximately 50% increase in resistivity is due to surface roughness scattering.[4] From a theoretical point of view, several models have been proposed in the literature[10–20] for each component of Eq. (1). A widely used semiclassical model for surface scattering is the Fuchs-Sondheimer (FS) model[10,11] where a phenomenological parameter p is used to characterize electron scattering at the surface: $p=1$ means perfectly specular scattering while $p=0$ means completely diffusive scattering. Other more advanced analytic models[16–20] have also been proposed in recent years in the general area of thin-film resistivity which take into account the quantum mechanical effects that may become prominent at very thin film thickness.

While the empirical and analytic models have provided useful knowledge on the influence of different scattering mechanisms in Cu interconnects and are appealing for their simplicity, there is a clear need that calls for more accurate quantitative methods to directly calculate the resistivity for realistic atomic configurations without employing any phenomenological parameter and without fitting to experimental data. Atomistic first-principles approaches can be very useful in this regard. Recently, several *ab initio* studies[21,22] of the resistance of Cu films and nanowires have been reported where a supercell approach was employed on periodic atomic structures. In an earlier study,[21] we have shown a 30%–40% reduction in the conductance of thin Cu films due to surface roughness and the reduction was attributed to the destruction of isotropic Fermi surface sheets by the atomic mounds. However, one limitation of the supercell approach is that it can be applied only to calculate the resistance, but not the resistivity. Besides, within this approach the roughness on the surface cannot be completely random due to the periodic atomic arrangements.

In this work, we use an *ab initio* technique[23] to investigate electron scattering by completely random surface roughness. We also treat the Cu film as a two-probe device of specific length l and thickness d rather than a periodic structure as in Ref. 21. By calculating the slope of film resistance R versus l for a given set of (d,x), where $(1-x)$ is the concentration of disorder on the Cu surfaces, we obtain resistivity of the rough films as a function of (d,x) for a wide range of values of these parameters. Finally, by investigating the relationship of resistivity versus d and compare our *ab initio* data to the Fuchs-Sondheimer model, we deduce the surface roughness scattering parameter p as a function of roughness parameter x. Our results show good qualitative and reasonable quantitative agreement with available experimental data and show that the resistivity increases significantly due to surface roughness scattering where p can be as small as around 0.29, suggesting a strong diffusive scattering at the rough surfaces.

The rest of the paper is organized as follows. In Sec. II, we present the theoretical method and the model of the Cu films. Section III presents the results, and a short summary is included in Sec. IV.

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II. THEORETICAL METHOD

Before presenting a detailed description of our *ab initio* model for disordered systems, we first point out the major difficulties and challenges that have always been associated with the study of disordered systems within any atomistic first-principles framework. Because unintentional disorder or defects are located at random positions in a system, any physical quantity must be averaged over disordered atomic configurations. In atomic calculations, the disorder averaging can be carried out by generating many atomic structures with a given disorder concentration, performing calculations for each of them and finally averaging the results. Such a brute force calculation is extremely difficult to apply for our problem here due to two reasons. (i) In order to deduce resistivity, resistance of Cu films for many values of (l,d,x) must be calculated as discussed in Sec. I, and each calculation involves large number of atoms (up to ~1800 atoms for this work). Our experience indicates that for each concentration x, thousands or more disorder configurations must be averaged to obtain a converged result.[24,25] Together with the large system size, a brute force calculation becomes impractical since first-principles calculations are very time consuming even for just one system configuration. (ii) When the disorder concentration x is small (say a few percent), the system size can become prohibitively large in order to contain a reasonable number of disordered sites; as such a first-principles treatment can become almost impossible. Clearly, we need a more practical and efficient technique to address the above issues.

Our solution to the above-mentioned disorder averaging problem is to derive analytic expressions for the relevant physical quantities (i.e., electronic density matrix and conductance) as functions of the impurity positions and then to average over these random positions analytically to obtain a final formula which can be then computed numerically. In this way we need to perform only one calculation for a particular value of x. We have recently developed this idea by formulating the theory of nonequilibrium vertex correction (NVC).[23] NVC deals with multiple scattering caused by disorder that correlates the nonequilibrium Green's functions (NEGF) by analyzing a disorder vertex function. Its equilibrium counterpart is well known in calculations of Kubo formula by Feynman diagrammatic techniques.[26] The main qualitative difference between NVC and the equilibrium vertex correction (VC) is that NVC depends on the nonequilibrium quantum statistical information of the device scattering region while the equilibrium VC does not. We have implemented the NVC theory into a Keldysh NEGF-based density-functional theory (DFT) package.[23] The NEGF-DFT-NVC technique is capable of treating disorder averaging in a very practical and efficient manner for fairly large systems within atomistic first-principles and at nonequilibrium transport conditions. The technical details of this method are rather complicated, and we do not present it here for clarity of the paper. We refer interested readers to Ref. 23 and its associated online EPAPS document[27] for the technical details. In the following we apply the NEGF-DFT-NVC technique to investigate effects of surface roughness scattering on the resistivity of thin Cu films.

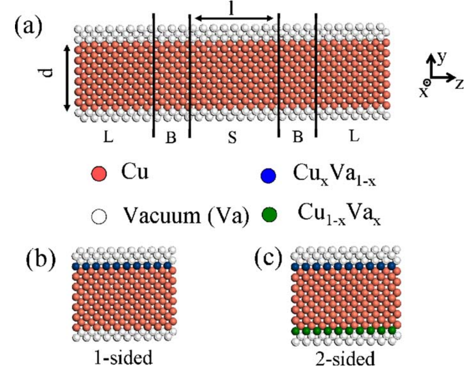

FIG. 1. (Color online) (a) Atomic structure of the Cu thin film. For the transport calculation, the film is treated as a two probe device where the scattering region (denoted by S) has specific length (l) and thickness (d) and it is assumed periodic in the width direction. The two leads (denoted by L) and the buffers (denoted by B) are perfect Cu films without any disorder. The buffer regions connect the leads to the scattering region. The atomic models used for surface roughness are shown in (b) for one-sided roughness and (c) for two-sided roughness. Roughness is modeled by randomly replacing Cu atoms with vacuum sites of specific concentrations (denoted by x and $1-x$) and is introduced at the outermost surface layer of the film.

The atomic structure of the system used in our calculations is shown in Fig. 1. It is a thin Cu film of fcc structure with lattice constant (denoted by a) of 3.61 Å which is the standard experimental value. The atomic structure is formed as such that the $\langle 010\rangle$ direction is along the thickness (denoted by d) of the film while the $\langle 101\rangle$ and $\langle 10\bar{1}\rangle$ directions are along the length (denoted by l) and the width of the film, respectively. The layer-to-layer distance along the thickness direction is 1.81 Å ($\frac{a}{2}$), while it is 2.55 Å ($\frac{a}{\sqrt{2}}$) along the length and the width directions. The Cu film is assumed to be periodic in the width direction, whereas the length and the thickness of the film are varied in our calculations. We employ two different models for the surface roughness: one-sided roughness [Fig. 1(b)] and two-sided roughness [Fig. 1(c)]. In both cases the roughness at the surface is modeled by randomly removing Cu atoms (i.e., replacing them by vacuum) of specific concentrations $(1-x)$. In this work, disorder has been added only to the *outermost* surface layer of the film in both the one-sided and two-sided roughness models. In order to solely focus on the surface roughness scattering, we consider single-crystal Cu film without any impurity atom but with random surface roughness. This way, the only contribution to the resistivity in our calculation is the surface roughness.

In our calculation method,[23] the electronic structure is determined by DFT within the tight-binding linear muffin-tin orbital (TB-LMTO) implementation.[28] The disorder averaging of the DFT Hamiltonian and single particle Green's function is treated by coherent potential approximation (CPA).[29] After the NEGF-DFT self-consistent iteration of the density matrix is converged, we evaluate the disorder averaged conductance within the NEGF-DFT-NVC formalism.[23] This is a fully self-consistent atomistic formalism of quantum trans-

port for two probe systems. In a general NEGF-DFT-NVC analysis, the configurational averaged electronic density matrix $\bar{\rho}$ is calculated using the NEGF formalism[30,31] as follows:

$$\bar{\rho} = (1/2\pi)\int_{-\infty}^{\infty} \bar{G}^{<}(E)dE,$$

$$\bar{G}^{<} = \overline{G^R\Sigma^{<}G^A} = \bar{G}^R(\Sigma^{<} + \Omega_{\rm NVC})\bar{G}^A,$$

$$\Sigma^{<} = i(f_L\Gamma_L + f_R\Gamma_R), \quad (2)$$

where $\overline{(\ldots)}$ indicates the configurational average; ρ is the density matrix; $G^{R,A}$ are the retarded and the advanced Green's functions; $\Gamma_{L,R}$ are the self-energies of the left and right leads which describe the interactions between the leads and the scattering region of the device; $f_{L,R}$ are the Fermi-Dirac functions of the two leads; and $\Omega_{\rm NVC}$ is the nonequilibrium vertex correction term.[23] All quantities are calculated for each (k_x,k_y) point and summed over the two-dimensional (2D) Brillouin zone (BZ). After convergence of the self-consistent iteration of the density matrix, the impurity averaged conductance is calculated from the following expression:

$$\bar{G} = \frac{e^2}{h}({\rm Tr}[\Gamma_L\bar{g}^R\Gamma_R\bar{g}^A] + {\rm Tr}[\Gamma_L\bar{g}^R\Gamma_{\rm VC}\bar{g}^A]), \quad (3)$$

where $\bar{g}^{R,A}$ are the retarded and the advanced auxiliary Green's functions that have been averaged over the impurities: they are calculated by the CPA iterations; and $\Gamma_{\rm VC}$ is a second vertex correction term, i.e., a self-energy, due to multiple impurity scattering which describes interactions between the impurities and electrons.[23,29] The conductance expression in Eq. (3) is written in two parts, a coherent term and a vertex correction term.

More specific to the Cu films of this work, the NEGF-DFT-NVC formalism becomes simpler to apply because we are only interested in equilibrium conductance obtained at zero-bias voltage. In this situation, NEGF $G^{<}$ is reduced to the retarded Green's function G^R whose impurity average can be done by CPA,[23,29] so that the only vertex correction necessary is associated with the quantity $\Gamma_{\rm VC}$. Details of its calculation can be found in Ref. 23 and references therein. All the self-consistent NEGF-DFT-NVC calculations are performed at zero temperature. Since we consider Cu films which have infinite extent in one transverse direction and a finite width d in the other transverse direction, the 2D BZ is sampled by $(k_x,k_y)=(60,1)$ k mesh for each energy point. The energy integration (see Eq. (2)) has been performed with 28 energy points along a complex energy contour in the upper half plane.[23] Since at zero bias voltage (equilibrium) $G^{<}$ is reduced to R^R which is analytic on the upper half energy plane, Eq. (2) can be very efficiently calculated by a contour integration.[23] We have checked that these computational parameters produced converged numerical values. In the transport calculations, both the coherent and the vertex parts in Eq. (3) are evaluated with (100,1) k mesh in the k sampling. One of the main advantages of our NEGF-DFT-NVC formalism is that it can handle quite large systems: we have performed calculations of Cu film with up to around 1800 atoms without any difficulty.

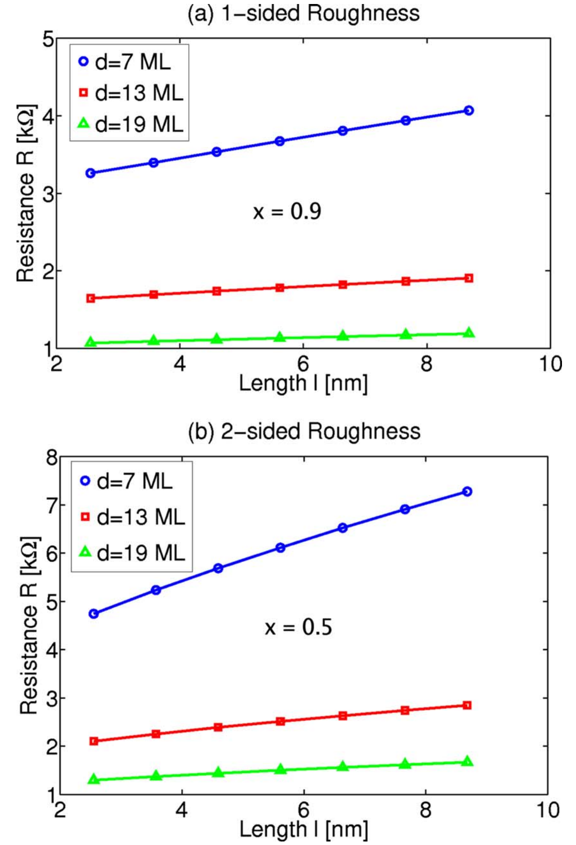

FIG. 2. (Color online) Surface roughness induced resistance R (i.e., purely due to surface roughness scattering) as a function of length l of the film for two cases. (a) x=0.9, i.e., 10% disorder and one-sided roughness. The conductance is high for this case. (b) x=0.5, 50% disorder and two-sided roughness, and the conductance is low. It shows largely linear behavior for all situations, and the slopes give the resistivity.

III. RESULTS AND DISCUSSION

We begin by calculating the resistance R of the Cu film for different thicknesses and lengths. The results are presented in Fig. 2 for one-sided roughness with 10% disorder (x=0.9) and for two-sided roughness with 50% disorder (x=0.5). The former is very conductive with little surface roughness whereas the latter is low conducting with high roughness concentration. In both cases, resistance increases rather linearly with the length for all thickness of the film, showing an expected Ohmic behavior. A resistance of several kΩ suggests significant contributions from the surface roughness.

From the slope of resistance versus length curves in Fig. 2, we obtain resistivity ρ of the Cu films; the results are presented in Fig. 3 as a function of roughness concentration $(1-x)$ for different thicknesses of the film. The resistivity values shown here are solely due to the surface roughness scattering. The surface is perfect if $x=1$ (no disorder, i.e.,

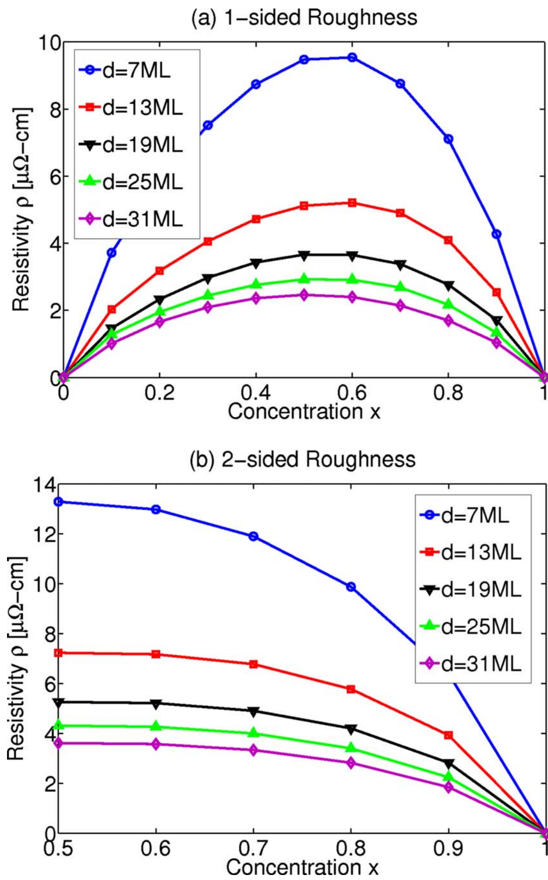

FIG. 3. (Color online) Surface roughness induced resistivity ρ as a function of roughness concentration parameter x for different thickness d of the Cu films. The thickness d is expressed as the number of monolayers (ML) of Cu planes. Since the system is symmetric around $x=0.5$ for the two-sided roughness ρ values for only x up to 0.5 are presented in (b). Note that for (a) one-sided roughness, the maximum ρ value is obtained at $x=0.6$, i.e., at 40% disorder of the system. Note that when $x=0,1$ corresponding to perfect Cu surfaces, the surface roughness induced ρ vanishes because there is no roughness scattering.

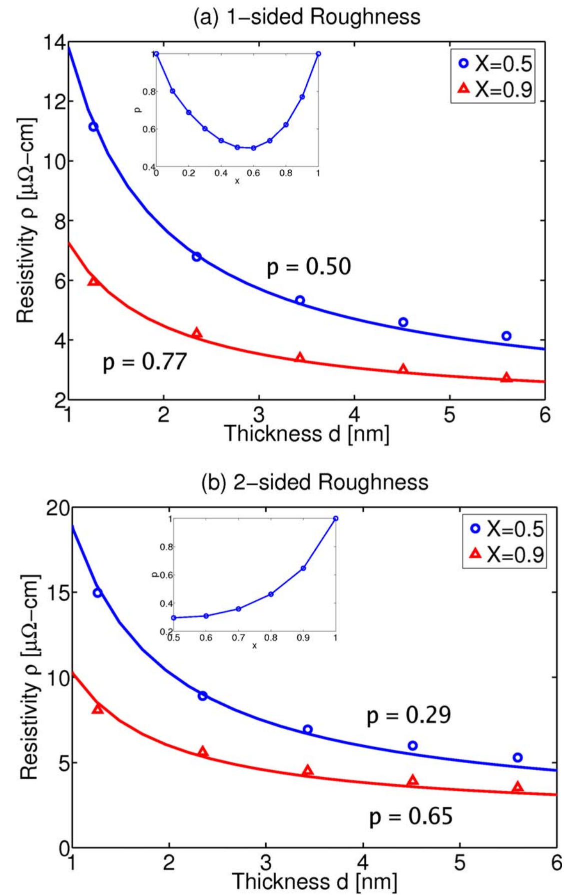

FIG. 4. (Color online) Resistivity ρ as a function of thickness (d) of the Cu film for different roughness concentrations $(1-x)$. The ρ values (which equal our calculated resistivity due to surface roughness scattering plus the bulk resistivity value of 1.67 $\mu\Omega$-cm) are shown by the circles and the triangles. Solid lines are the corresponding fit of our data with the Fuchs-Sondheimer analytic model where p is the specularity parameter. The p values obtained from the fitting are shown as a function of x in the inset.

roughness is zero); it is also perfect if $x=0$, i.e., when the topmost layer atoms are all replaced by vacuum sites so that the next perfect layer of Cu becomes the top surface. Since the scattering is completely specular at a perfect surface, the resistivity caused by roughness scattering is zero at both $x=0$ and $x=1$, as shown in Fig. 2. We observe that the resistivity is not quite symmetric around $x=0.5$ for the one-sided roughness model: this is expected since the atomic potentials of a Cu atom and a vacuum site are different. Interestingly, resistivity is maximum when the disorder is 40% (i.e., $x=0.6$). On the other hand, for two-sided roughness resistivity is completely symmetric around $x=0.5$ [the ρ values for $x<0.5$ are not shown in Fig. 3(b)]. We also notice that the resistivity is much higher at around $x=0.5$ for $d=7$ ML compared to the resistivity for the other thickness values, showing a substantial size effect when the film thickness is smaller.

Figure 4 plots the increase in resistivity with decreasing film thickness—this is the size effect as mentioned earlier. Our calculated values for resistivity ($\sim 2-14$ $\mu\Omega$-cm) are quite substantial compared to the room-temperature *bulk* Cu resistivity value of $\rho_b=1.67$ $\mu\Omega$-cm obtained experimentally. This shows that surface scattering can have a significant effect on the resistivity of very thin Cu films. When the surface roughness is small (i.e., $x\sim 1$), the resistivity becomes less dependent on the thickness of the film which is expected for specular scattering. On the other hand, for high level of surface roughness ($x\sim 0.5$) the resistivity shows strong dependence on thickness. For the two-sided roughness the resistivity becomes almost twice as large as for the one-sided roughness. It is not exactly twice as large because the roughness concentrations are not symmetric on both sides for the two-sided roughness model [see Fig. 1(c)], and the films are so thin that the top and the bottom surfaces can have some correlations. We wish to point out that quantum oscillation in resistivity versus thickness d is difficult to observe in Cu films even though the thickness values we have used are within the quantum regime. This is because a necessary condition to observe quantum oscillation is that the layer

TABLE I. Values for the specular parameter p obtained from the Fuchs-Sondheimer fitting where $\pm\Delta P$ is the error bound for the p value and RMSE is the root mean squared error for the fit. Low values for both $\pm\Delta P$ and RMSE indicate the goodness of our fit.

x	p	$\pm\Delta p$	RMSE
	(a) One-sided roughness		
0.1	0.80	0.016	0.14
0.5	0.50	0.024	0.21
0.9	0.77	0.015	0.13
0.99	0.97	0.002	0.01
	(b) Two-sided roughness		
0.5	0.29	0.049	0.43
0.7	0.36	0.056	0.49
0.9	0.65	0.043	0.37
0.99	0.94	0.004	0.03

spacing should be much smaller than $\frac{\lambda_F}{2}$ where λ_F is the Fermi wavelength.[16] For Cu film, the layer spacing is 1.81 Å while $\frac{\lambda_F}{2}$ is 2.33 Å as obtained from the calculated Fermi energy of −6.9 eV for Cu. These two length scales are too close for appreciable quantum oscillations to be observable.

It is somewhat difficult to compare our calculated results quantitatively with experimental data available in the literature for two reasons. (i) Almost all the available experimental data were obtained for Cu film of thickness greater than 10 nm which is too large a system for atomistic *ab initio* calculations; (ii) due to the presence of all scattering mechanisms (phonon, impurity, surface roughness, and grain boundary) in experimental systems, it is quite difficult to identify the contribution from each scattering process independently. Nevertheless, in a recent experiment,[7] great care was taken to minimize the bulk impurity and grain boundary scattering effects by growing thin Cu film of pure and single-crystalline nature, and the reported experimental value of resistivity is 8.35 $\mu\Omega$-cm at d=6.6 nm. In comparison, our calculated value at d=5.6 nm is 5.30 $\mu\Omega$-cm (which includes a bulk resistivity value of 1.67 $\mu\Omega$-cm to take into account the phonon scattering). The consistency is quite reasonable, and the remaining discrepancy can be attributed to the nature of the roughness model used in our calculations.

As mentioned before, surface scattering is conventionally described by a semiclassical model developed by Fuchs[10] and Sondheimer[11] and later modified by Rossnagel and Kuan[2] to take into account the surface roughness. This model proposes a relationship between the resistivity ρ and the thickness d of a thin film,

$$\frac{\rho}{\rho_b} = 1 + 0.375\frac{\lambda}{d}(1-p)S, \tag{4}$$

where ρ_b is the bulk resistivity, λ is the room-temperature electron mean free path, and p is called "specularity parameter" whose value ranges from 0 to 1 for completely diffusive to completely specular scattering, respectively. The surface roughness factor S is an empirical constant which quantifies the contribution due to *macroscopic* surface roughness. It can have a value greater than or equal to 1.0, with S=1 representing a perfect surface. It is obvious that the two phenomenological parameters p and S are interrelated since diffusive scattering is a direct consequence of the surface roughness. Therefore, it is almost impossible to independently determine p and S.

In order to estimate the value for p which is rather useful for experimental characterization of resistivity of rough films, we fit our calculated results with the FS equation [Eq. (4)] by tuning the specularity parameter p, and we employ the following values for the other parameters in Eq. (4): ρ_b =1.67 $\mu\Omega$-cm, λ=39 nm, $\rho=\rho_b+\rho_s$ (ρ_s is our calculated resistivity), and S=1 (in this study, we choose to focus solely on the parameter p). We observe a good fit (see the solid lines in Fig. 4) of our data to the FS model by adjusting p. The resulting p values are shown in Table I (also, see the insets of Fig. 4). The goodness of the fit is very satisfactory as suggested by the low values of $\pm\Delta p$ and root mean squared error (RMSE) in Table I. The minimum values of p for one-sided and two-sided roughness are 0.5 and 0.29 near x=0.5, respectively. We note here that these p values are obtained by directly fitting the data using Eq. (4), which assumes identical top and bottom surfaces. This assumption is likely reasonable for our two-sided roughness layers which have comparable morphologies on top and bottom surfaces. Thus, we expect that the p values in Table I correspond to the specularity of the simulated surfaces. In contrast, the p values shown in Table I represent an average of the perfectly flat bottom surface and the rough top surface of the one-sided layers. Assuming specular scattering (p=1) for the bottom surface, the p value for the rough top surface at x=0.5 drops exactly to p=0, corresponding to completely diffuse scattering. This is in agreement with various experimental studies which reported completely diffuse surface scattering.[2,7,8] Here, we would like to mention clearly that the good fit of our calculated *ab initio* data with the semiclassical FS model does not endorse or validate the FS formula for any quantum effects. In order to validate the FS model properly, one needs to perform a fitting with resistivity data for a much wider range of thickness values which includes both the quantum and semiclassical regimes. In addition we note that the *FS* relation in Eq. (4) is an approximation which becomes inaccurate for $d/\lambda<0.1$. Therefore, one could argue that Eq. (4) is not applicable to our computational approach since in the absence of true bulk scattering $\lambda=\infty$. However, a more sensible λ value for our simulated thin layers may be the system length l. In that case, Eq. (4) holds true since $\lambda \sim l$ <10 nm and thus $d/\lambda>0.1$ for all simulated thicknesses d >1 nm. Despite these uncertainties in how to interpret the *FS* model within our results, we believe that there is value in the presented fitting as it provides an estimate of the specularity parameter p.

Finally, we plot resistivity as a function of thickness in Fig. 5 for *diluted* concentrations of roughness, i.e., for nearly perfect Cu surfaces. We expect that for perfect surface the resistivity will be independent of thickness and it will not deviate much from the bulk value. However, we observe in Fig. 5 that the resistivity is still increasing with decreasing thickness even when x is as high as 0.99 (i.e., 1% disorder). In other words, our calculations show that a thin Cu film

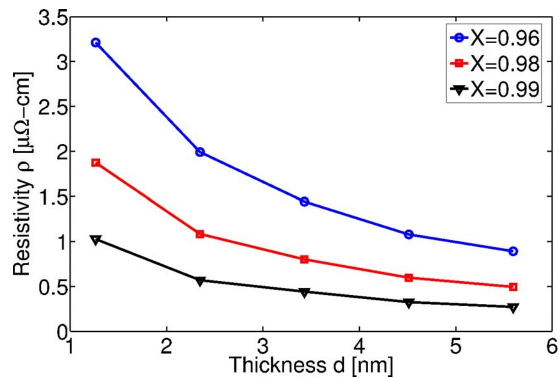

FIG. 5. (Color online) Resistivity (ρ) as a function of thickness (d) when the surface is almost perfect, i.e., the vacuum concentration $(1-x)$ is very low. The data presented here are for the two-sided roughness model. As expected, resistivity shows less dependence on the thickness at low roughness concentrations, even though there is still substantial contribution from the surface roughness scattering.

which misses 1 atom for 100 (i.e., $x=0.99$) is still rough enough to produce significant scattering at the surface. We also notice that at these diluted concentrations the resistivity is almost directly proportional to the disorder concentration.

IV. SUMMARY

In summary, we have calculated surface roughness induced resistivity of thin Cu films. The resistivity values are obtained using the NEGF-DFT-NVC *ab initio* formalism self-consistently. The inputs to our calculation are the atomic position and roughness concentration $(1-x)$. Our results show reasonable qualitative consistency with the available experimental data. They demonstrate that electron scattering due to surface roughness contributes significantly to the total resistivity of Cu thin films. Even in the low roughness regime, the resistivity of very thin Cu films remains substantial as compared with the bulk value. Our results can be fit to the Fuchs-Sondheimer semiclassical formula which allows us to estimate the degree of specular scattering, and we have obtained the $p=p(x)$ characteristics.

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