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Electron Transport in Graphene-Versus Al/Pd-Coated Thin Cu Films With Low-Surface Roughness: A First Principles Study

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ABSTRACT Surface scattering is a major issue in thin Cu films at reduced scales. The rise in the diffusive scattering due to the surface roughness causes the electrical resistance to increase remarkably. In this paper, graphene, as opposed to Al and Pd, is considered as a liner layer for thin Cu film with low-surface roughness using first principles calculation. The surface roughness is simulated using the nonequilibrium coherent potential approximation combined with the linear muffin-tin orbital formulation. The coherent potential approximation band structure shows that the graphene π-bands is not significantly affected by the surface disorder at the Cu surface and that graphene acts as a parallel path to the electrons. On the other hand, the bands of Cu–Al/Pd around the Fermi level are substantially broadened due to the surface disorder. Moreover, the graphene-coated Cu shows less electrical resistance than Al/Pd-coated Cu for surface disorder $x \lessapprox 5\%$ for thin films with 0.245 nm in width, and 1.23 nm in thickness. The enhancement in the transport properties in Cu–Gr is attributed to the weak electronic interaction at the interface. The obtained results suggest that graphene is better than Al and Pd as a liner material for thin Cu films.

INDEX TERMS Thin films, surface scattering, copper, graphene, electron transport.

I. INTRODUCTION

At reduced scales, electron transport faces many challenges including electron surface scattering, electron grain boundary scattering, surface roughness scattering, impurity scattering and electron phonon scattering [1], [2].These scattering mechanisms cause an increase in the electrical resistivity and give rise to reliability issues [3]–[5]. The rise in the resistivity due to the scattering mechanisms are referred to as ''size effect'' [1], which becomes very critical for dimensions less than 50 nm, resulting in $\sim$ 100% decrease in the conductivity [2], [6], [7].

In electron surface scattering, the electrons are subjected to three types of scattering events, depending on the nature of the surface. The first event is the specular scattering in which the forward momentum is conserved and the surface does not contribute to the total resistivity. The second event is the partially specular scattering, where some of the electrons may be redirected to a random direction with a stoppage period at the surface. The third type is the diffusive scattering where all the electrons are diffused at the surface and the contribution of the electron surface scattering to the resistivity is substantial. The surface roughness scattering is due to the roughness at the film surface. If the surface is perfect, then the electrons hitting the surface still pointing to the transport direction. For a rough surface, the electrons may get redirected to a direction opposite to the initial direction depending on the part of the surface that the electrons collide with. There are many models which have been proposed to describe the surface scattering mechanisms. Starting from the early

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models by Fuchs and Sondheimer [8], [9] for the electron surface scattering and its modified versions [1], [10], [11] to account for the surface roughness scattering.

Cu is the backbone material for the micro- and nanoelectronics in the last two decades. With its advantages over its precedent Al, Cu will dominate in the area of integrated circuits for another period. The electron mean free path is ≈40 nm in Cu, which makes the size effect a severe issue in the nanostructure devices. Specially, the electron scattering due to the surface roughness. In fact the contribution of the surface roughness scattering to the total scattering mechanisms can reach ∼ 50%. [2]

A thin Cu film with a perfect surface is not possible to fabricate. At least for the time being. Even when using annealing processes after the deposition of Cu films as still some roughness in the surface is observed [12]. Therefore, the study of the geometric and the electronic behavior of the electrons at the surface is very crucial since it has a direct impact on the transport properties in the nanoscale devices.

Many liner materials have been proposed before to smooth out both the geometric and electronic structure of the Cu surface. The capping material may fill the gaps in the rough surface leading to less diffusive scattering [1]. However, not only the geometry structure, but the electronic structure at the surface needs to be smoothed. Common liner materials like Ti, Ta, Ru, Al, Au and Pd have been examined experimentally [1], [13]–[15]. Among these materials, Al [16], [17] and Pd [17] were found to decrease the resistivity of the Cu thin film. Other materials including Pt [1], Zr and Hf [18] were found to increase the resistivity and cause the scattering at the surface to be completely diffusive. Controversially, researchers have different views on Ta, which is the diffusion barrier currently used in integrated circuits. While authors in [19] and [17] showed that Cu-Ta has completely diffusive scattering and leads to an increase in the electrical resistivity. Others reported that deposition of Ta on Cu leads to a partial specular scattering [20], [21].

Two-dimensional materials (2D-materials) such as graphene and hexagonal boron nitride have been considered before as a capping material for Cu surfaces. These 2-D materials possess unusual properties that can enhance the electrical conductivity and prevent oxidation. Graphene is the name given to the one-atom-thick planar sheet of sp^2 bonded carbon atoms, arranged in honeycomb crystal lattice. Since its discovery in 2004 [22], graphene fascinated the world with its extraordinary properties such as electrical conductivity [22], thermal conductivity [23] and impermeability [24]. In [25], a Cu nanowire was capped with graphene and both the electrical and the thermal conductivity were substantially enhanced. While in [5], the resistance of the Cu interconnect was reduced by capping Cu with a multilayer graphene (MLG). Graphene was also used as a diffusion barrier between Cu and Si. Taking advantage of its near-zero-thickness [26]. Graphene may also play an importance role to enhance oxidation resistance, which is a major problem for Cu surfaces. A sheet of graphene helped to protect Cu from electrochemical degradation [27], [28]. Recently, graphene was used to preserve Shockley surface states of Cu surfaces because of the weak interaction between the Cu surface and graphene [29]. In addition, graphene coating decreased the resistance of a rough Cu surface by reducing the surface roughness scattering effect [30], [31].

In this paper, a qualitative comparison between graphene and Al/Pd is carried out using first principles calculation to investigate the effect of its coating on thin Cu films. Al and Pd are known to enhance the conductivity of Cu. However, graphene is found to show more specular scattering and lower electric resistance for low surface roughness. To the best of our knowledge, there is no direct comparison between graphene and Al/Pd as a liner layers for thin Cu films. This study aids to fill this gap.

The reminder of this paper is organized as follows: Section II presents the atomic structure and the simulation details. The coherent potential approximation band structure, the calculation of the specular and the diffusive transmission coefficients, and the electrical resistance of the Cu-Al/Pd/Gr are presented and discussed in Section III. Finally, the conclusions are presented in Section IV.

II. THEORETICAL MODEL

In this paper, the NanoDsim [32] package is used for simulation. NanoDsim adopts the nonequilibrium coherent potential approximation-density functional theory (NECPA-DFT) formalism. The NECPA [33] treats the quantum transport in disordered systems, in which the disorder average is carried out analytically within the coherent potential approximation, instead of brute-force calculation. The obtained quantities such as the band structure, density of states and the transmission coefficient are disordered and averaged. The linear muffin-tin orbitals (LMTO) is adopted as a basis set [34]. Since it is compatible with the NECPA theory and has less computation cost. Atomic sphere approximation (ASA) is adopted with the LMTO theory [35], in which the unit cell is filled with spheres to maintain the close-packed structure. Local density approximation (LDA) is chosen as the exchange correlation functional [36]. The calculations take place in two steps: First the Hamiltonian and the charge density are solved self-consistency. Then the LMTO Hamiltonian is used to calculate the electronic and the transport properties. The threshold of the electronic self-consistency is taken to be 10^{-6}. The quantum transport is simulated using a two probe system [37]. Where two leads are connected to the central region. The central region contains the device under consideration, and it may also contains disorder sites as shown in Fig. 1. Two buffer layers are included between the leads and the center to smooth the connection. The band structure is calculated for a bulk system using the coherent potential approximation-linear muffin-tin orbital (CPA-LMTO) method as will be shown later. The surface disorder is considered in the top layer of the central region, i.e., blue spheres in Fig. 1. Above the disordered layer, Al and Pd (green spheres), graphene (black spheres) are positioned as a liner

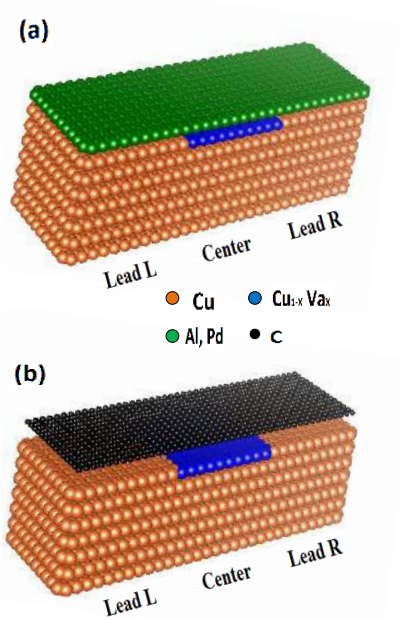


FIGURE 1. Two-probe system of (a) Al/Pd-coated Cu. (b) Gr-coated Cu. The left and the right leads are connected to the central area through buffer layer. The top layer of the central area of Cu (blue spheres) contains x% disorder as vacuum and $1 - x$% Cu.

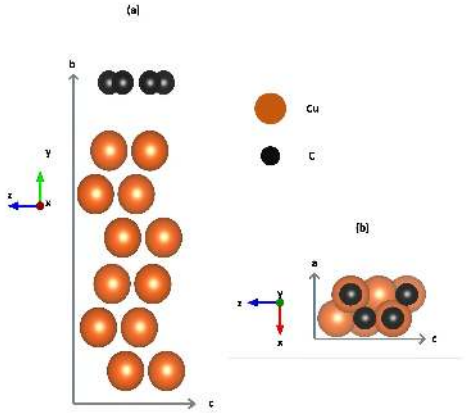


FIGURE 2. The unit cell of Cu-Gr. It contains twelve atoms of Cu arranged in six layer, four atoms of C positioned in a top-fcc configuration. (a) Side view. (b) Top view.

materials as shown in Fig. 1(a) and (b), respectively. It is worth mentioning that the obtained results are of a more qualitative character, since Al and Pd liner layers are assumed to replace an additional Cu layer on top of the disordered surface. This approximation is adequate and has been used before [16], [17]. Every atom in the disordered layer contains disorder concentration x% as vacuum. In other words, if $x = 5$%, that means for every 100 atoms there are 5 missing atoms represented as vacuum.

The rectangular unit cell is adopted throughout this paper [38]. The cuboid structure helps to build a thin film with dimensions parallel to the x, y and z direction. Fig. 2 shows the primitive unit cell of graphene-coated Cu. One layer of graphene is positioned on six layers of Cu (111) forming a top-fcc structure [39]. The inter-layer distances between Cu–Cu and Cu–C are 2.08 and 3.26 Å, respectively [39]–[41]. The primitive unit cell of the Cu-Al/Pd structure is the same as in Fig. 2, except that the graphene layer is replaced by the Al/Pd layer. In order to build a thin film, the unit cell is repeated in the x, y and z directions as needed.

III. RESULTS AND DISCUSSIONS

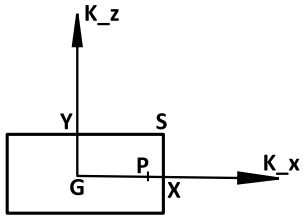
A. BAND STRUCTURE

The band structure is usually plotted by calculating the eigenvalues as a function of the wave vector k, which links the high symmetry points in the first Brillouin zone. However, in disordered systems the periodicity is lost and the calculation of the eigenvalues is no longer valid. Fortunately, the band structure can still be obtained through coherent potential approximation (CPA) band structure. For a clean system, the delta functions constitute the k-resolved DOS (Bloch spectral function) over the Bloch states. In the presence of the surface disorder, the delta functions are broadened due to the disorder effect. The trace of these broadened delta functions form the band structure of disordered bulk system. The CPA band structure (sometimes referred to as the k-resolved DOS) is calculated using the formula [35]

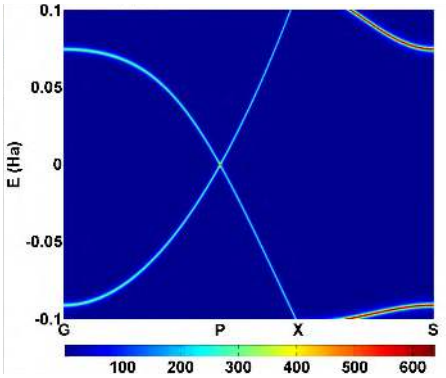
$$D(E, k) = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr} \overline{G^r}(E, k) \tag{1}$$

where $\overline{G^r}$ is the disorder-averaged retarded Green's function and is calculated from the CPA-LMTO equations. First, the band structure of bare Gr is calculated, then the band structure of the hybrid Cu–Gr is plotted to investigate the interaction between Cu and Gr. The first Brillouin zone of the rectangular unit cell is shown in Fig.3a with its high symmetry points. Fig.3b shows the band structure of a pristine graphene. The well-known linear dispersion relationship of Gr is shown around the crossing point P (Dirac point) at which the conduction and the valence bands meet. The P point in a rectangular unit cell is equivalent to the K point in the rhombus unit cell. When Gr is deposited on Cu, the band structure of both materials get affected. However, the linear dispersion at the point P is maintained as shown in Fig.3c. Indicating that the electronic interaction between Cu and Gr is weak and the Cu band structure is not substantially disturbed. This weak interaction can be attributed to the physisorption interface between Cu and Gr. Moreover, there is an upward shift of 0.0428 Ha for the Fermi level with respect to the conical point of Gr, as a result of an electron transfer from Cu to Gr, which is described as n-doping effect [41].

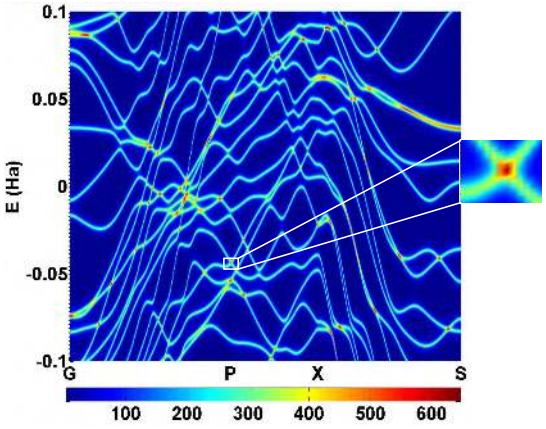
In the presence of the surface roughness, the bands get broadened due to the disordered atoms at the Cu surface. Such "broadening effect" is similar to the impurity broadening [42]. In Fig. 4, the band structure of Cu–Al, Cu–Pd and Cu–Gr are plotted for different disorder concentrations. For Al and Pd, all the bands are broadened, specially, the bands that are crossing the Fermi level as shown in Fig. 4(a-c) and (d-f), respectively. The broadened bands indicate that both Al and Pd are affected by the surface disorder at



(a)



(b)



(c)

FIGURE 3. Band structure of a rectangular unit cell. (a) The high-symmetry points in the first Brillouin zone of the rectangular unit cell. (b) Band structure of pristine graphene. (c) Band structure of Cu-Gr. Inset: The linear dispersion relation of Gr around the point P.

the Cu surface beneath them. On the other hand, Cu–Gr bands are also affected with the increase in the disorder. However, the π-bands of Gr still visible and distinguishable even at high disorder ($x = 25\%$) as shown in Fig. 4(g-i). The lower sensitivity of the Gr band to surface disorder may be justified by the weak binding at the interface between Cu and Gr. which ultimately helps to enhance the transport properties by offering more conduction channels.

B. TRANSMISSION COEFFICIENT

A good quantification of the diffusive scattering at the surface can be made through the decomposition of the disorder-averaged transmission coefficient $\overline{T}(E)$ into a specular and diffusive transmission coefficient. In NECPA theory [33], $T(E)$ can be generelized to the calculation of the disorder-averaged transmission coefficient $\overline{T(E)}$ as

$$\overline{T}(E) = \mathrm{Tr}[\overline{G^R(E)\Gamma_l(E)G^A(E)\Gamma_r(E)}] \tag{2}$$

where Γ_β is the line width function of the left and the right leads, and $G^{R,A}$ are the retarded and the advanced Green's functions, respectively. To calculate $\overline{T}(E)$, Eq. 2 needs to be simplified to the calculation of disorder-averaged Green's function as follows (hereafter the argument E is omitted from equations for simplicity)

$$\Sigma^< = i\Gamma_l f_l + i\Gamma_r f_r \tag{3}$$

where $\Sigma^<$ is the lesser self-energy and f_β is the Fermi function of the left and the right leads. By setting $f_l = 1$ and $f_r = 0$,

$$\Sigma^< = i\Gamma_l, \quad \Gamma_l = -(i)\Sigma^< \tag{4}$$

Substituting Eq. 4 into Eq. 2, we get

$$\overline{T} = \mathrm{Tr}[\overline{G^R(-i\Sigma^<)G^A}\Gamma_r] \tag{5}$$

and

$$\overline{T} = \mathrm{Tr}[-i\overline{G^<}\Gamma_r] \tag{6}$$

$\overline{G^<}(E)$ can be decomposed into two components [33]

$$\overline{G^<} = \overline{G^R}\Sigma^<\overline{G^A} + \overline{G^R}\tilde{\epsilon}^<\overline{G^A} \tag{7}$$

where $\tilde{\epsilon}^<$ is the lesser coherent potential. The first term is a simple average and the second term is the contribution from the lesser coherent potential. Similar to the nonequilibrium vertex correction in (NVC) in coherent potential approximation-nonequilibrium vertex correction (CPA-NVC) theory [43]. Consequently, the transmission coefficient can be written from Eqs. 6 and 7 as

$$\overline{T} = \overline{T}_S + \overline{T}_D \tag{8}$$

where $\overline{T}_S$ and $\overline{T}_D$ are the specular and the diffusive transmission coefficients, respectively. Conceptually, the leads are clean and in good quantum number. If the central region is disorder free and the surface is perfect, the incoming wave with a transverse momentum k would be scattered to an outgoing wave with the same transverse momentum k. Resulting in a complete specular transmission coefficient $\overline{T}_T = \overline{T}_S$. On the other hand, any disorder in the central area would make the incoming wave with a transverse momentum k scatters to an outgoing wave function with $k' \neq k$, giving rise to a diffusive transmission coefficient $\overline{T}_D$.

The calculated diffusive, specular and total transmission coefficient are shown in Fig. 5 for lengths 1.27 and 2.55 nm. As the disorder concentration x increases, the specular (diffusive) transmission coefficient decreases (increases). The increased $\overline{T}_D$ is due to the increased disorder in the Cu surface, which means more scattering incidents in the central area, resulting in a decreased $\overline{T}_S$ as well. Cu–Gr shows more

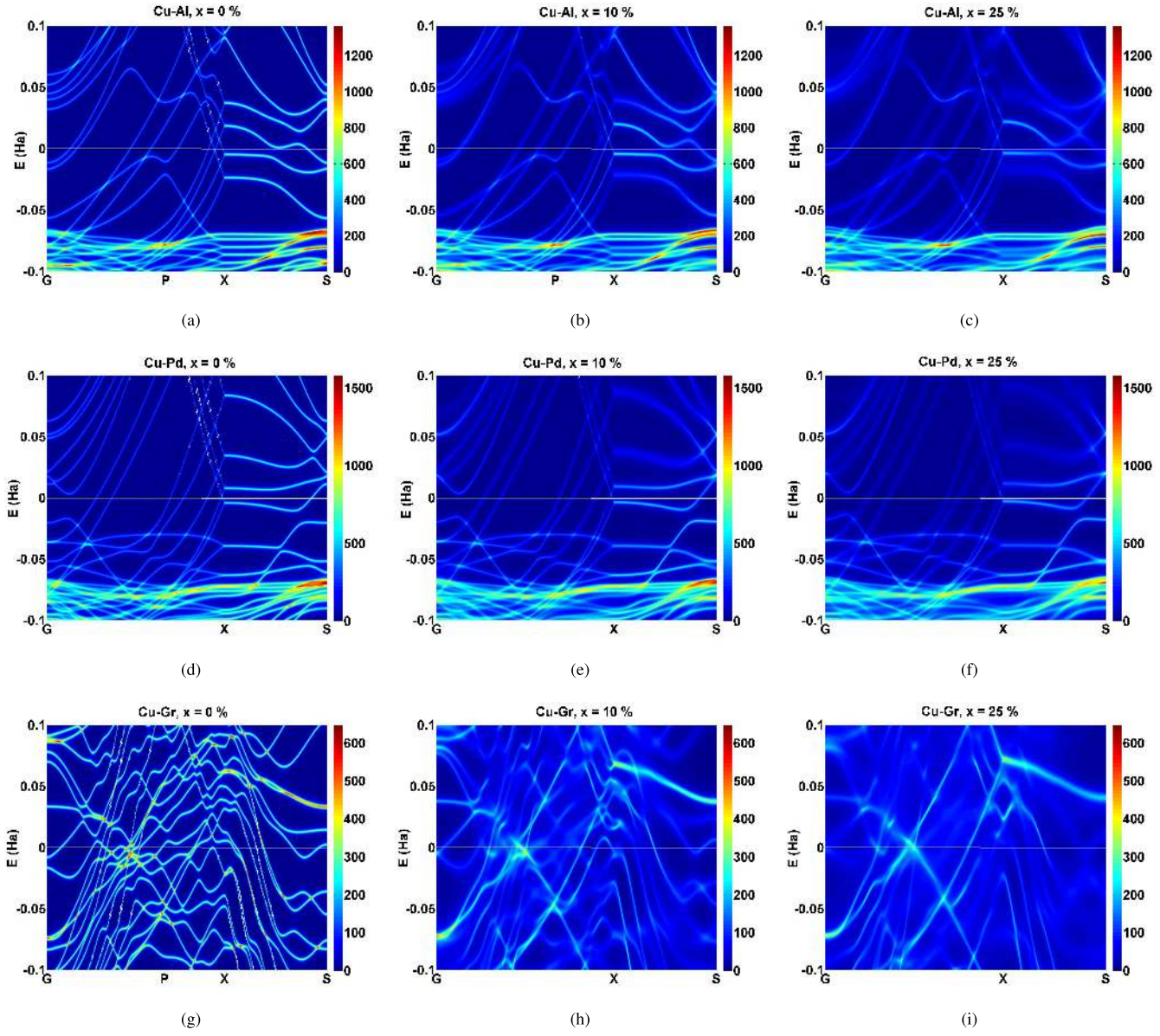


FIGURE 4. CPA band structure of Cu–Al (a-c), Cu–Pd (d-f) and Cu-Gr(g-i) for 0, 10 and 25%, respectively. As the disorder x increases, the bands get broadened. For Cu–Gr, the π-bands are visible and distinguishable from Cu bands. Indicating a weak interaction with the Cu surface.

$\overline{T}_T$ when compared with Cu–Al and Cu–Pd. This can be attributed to the higher $\overline{T}_S$ as shown in Fig. 5a and Fig. 5b. $\overline{T}_T$ is calculated from (8) and shown in Fig. 5c and Fig. 5d. Cu–Gr has higher $\overline{T}_T$ than Cu–Al/Pd, except for $x \approx 3.81\%$ and $x \approx 5\%$ for Pd and Al, respectively. Although the increased $\overline{T}_T$, Cu–Gr seems very sensitive to the disorder increase at relatively longer films. As shown in Fig. 5b, Cu–Gr starts with a higher $\overline{T}_S$ at $x = 0\%$ but drops very fast afterwards. The sensitivity of Cu–Gr to surface disorder is due to the increased $\overline{T}_D$, which makes the total transmission of the film very sensitive to any increase in the surface disorder or the length. Moreover, Cu–Pd shows better $\overline{T}_S$ when compared to Cu–Al, in consistent with previous report [17]. Fig. 5a and Fig. 5b also show that for a perfect Cu surface, i. e., $x = 0\%$, the transmission is completely specular and independent of the length. And the transverse momentum is conserved. The enhancement in the specular transmission of Cu film when coated with Gr can be linked with CPA band structure shown in Fig. 4. The weak interaction, lack of hybridization between Cu and Gr prevent the disorder at the Cu surface from disturbing the π-bands of Gr. In other words, the contrast between the Gr π-bands and Cu bands shows that Gr works as an additional path, parallel to the Cu channels. And most importantly, not significantly affected by the surface disorder.

To calculate the electrical resistance, the disorder-averaged electric conductance is obtained using the formula

$$\overline{C} = \frac{e^2}{h}\overline{T}(E) \tag{9}$$

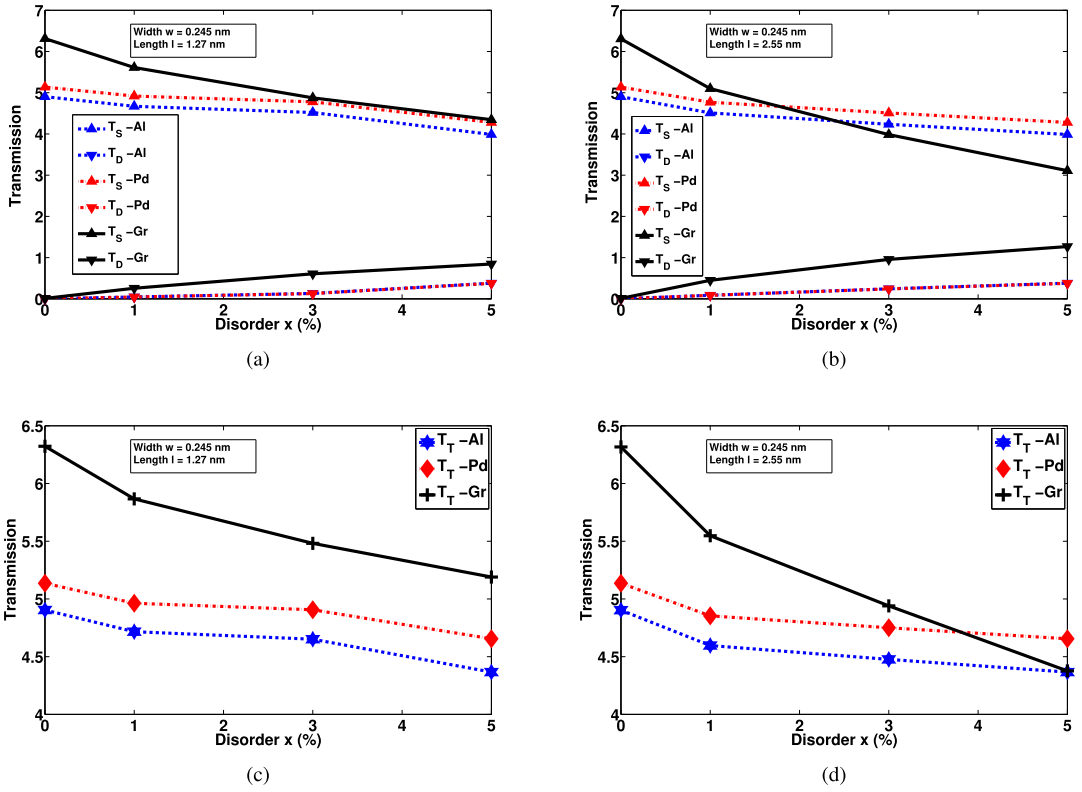


FIGURE 5. The calculated transmission coefficient for Cu–Al, Cu–Pd and Cu–Gr. (a-b) $\overline{T}_S$ and $\overline{T}_D$ for lengths 1.27 and 2.55 nm respectively. (c-d) $\overline{T}_T$ for lengths 1.27 and 2.55 nm respectively.

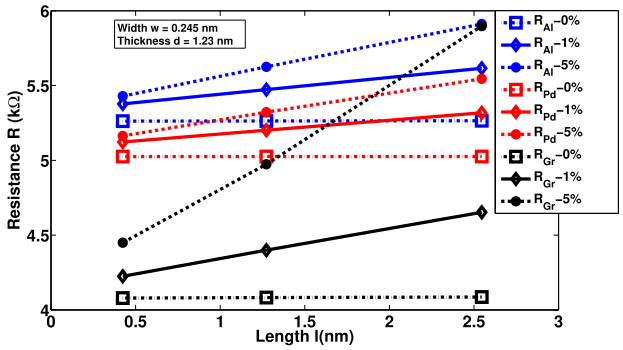


FIGURE 6. The calculated resistance of Cu–Al, Cu–Pd and Cu–Gr for disorder $x = 0$, 1 and 5%.

where e is the electron charge, and h is Planck's constant, and $\overline{T}(E)$ is the disorder-averaged transmission coefficient. Fig. 6 plots the electrical resistance for Cu–Al, Cu–Pd and Cu–Gr for $x = 0\%$, $x = 1\%$ and $x = 5\%$. As noted before, the resistance is independent of the length when the surface is clean. In this case, the transmission is completely specular and the transverse momentum k is conserved. For the chosen dimensions, i. e., 0.245 nm in width, 1.23 in depth, Cu–Gr exhibits less resistance than Cu–Al/Pd. Except for $x = 5\%$, when $l > 1.9$ and $l > 2.5$ nm for Pd and Al, respectively. The latter finding limits the application of Gr coating to thin Cu films with short lengths and low surface roughness.

IV. CONCLUSION

In this paper, graphene is compared to Al and Pd as a liner material for thin Cu films using first principles calculation. When the surface of Cu film is clean, graphene is found to reduce the resistance of Cu significantly. In the presence of low disorder in the Cu surface, graphene-coated Cu shows better transport properties than Al/Pd-coated Cu for surface disorder $\lessapprox 5\%$. The physisorption interface helps grapehene to work as a parallel path to the disordered Cu surface. Moreover, the relatively greater distance between Cu and graphene avoids the disorder at the Cu surface to affect the π-bands of graphene. The obtained results demonstrate graphene as rival liner material for Al, Pd in thin Cu films.

REFERENCES

[1] S. M. Rossnagel and T. S. Kuan, "Alteration of Cu conductivity in the size effect regime," *J. Vac. Sci. Technol. B, Microelectron.*, vol. 22, no. 1, pp. 240–247, 2004.

[2] J. J. Plombon, E. Andideh, V. M. Dubin, and J. Maiz, "Influence of phonon, geometry, impurity, and grain size on copper line resistivity," *Appl. Phys. Lett.*, vol. 89, no. 11, Sep. 2006, Art. no. 113124.

[3] Y. Shacham-Diamand, A. Dedhia, D. Hoffstetter, and W. Oldham, "Copper transport in thermal SiO_2," *J. Electrochem. Soc.*, vol. 140, no. 8, pp. 2427–2432, Aug. 1993.

[4] M. T. Bohr, "Interconnect scaling-the real limiter to high performance ULSI," in *IEDM Tech. Dig.*, Dec. 1995, pp. 241–244.

[5] C. G. Kang, S. K. Lim, S. Lee, S. K. Lee, C. Cho, Y. G. Lee, H. J. Hwang, Y. Kim, H. J. Choi, S. H. Choe, M.-H. Ham, and B. H. Lee, "Effects of multi-layer graphene capping on Cu interconnects," *Nanotechnology*, vol. 24, no. 11, Mar. 2013, Art. no. 115707.

[6] T. S. Kuan, C. K. Inoki, G. S. Oehrlein, K. Rose, Y.-P. Zhao, G.-C. Wang, S. M. Rossnagel, and C. Cabral, "Fabrication and performance limits of sub-0.1 μm Cu interconnects," in *MRS Online Proceeding Library Archive*, vol. 612, 2000.

[7] S. Aouadi, P. Shreeman, and M. Williams, "Real-time spectroscopic ellipsometry study of ultrathin diffusion barriers for integrated circuits," *J. Appl. Phys.*, vol. 96, no. 7, pp. 3949–3955, Oct. 2004.

[8] K. Fuchs, "The conductivity of thin metallic films according to the electron theory of metals," *Math. Proc. Cambridge Philos. Soc.*, vol. 34, no. 1, pp. 100–108, Jan. 1938.

[9] E. H. Sondheimer, "The mean free path of electrons in metals," *Adv. Phys.*, vol. 1, pp. 1–42, Jan. 1952.

[10] M. Lucas, "Electrical conductivity of thin metallic films with unlike surfaces," *J. Appl. Phys.*, vol. 36, no. 5, pp. 1632–1635, May 1965.

[11] W. Steinhögl, G. Schindler, G. Steinlesberger, M. Traving, and M. Engelhardt, "Comprehensive study of the resistivity of copper wires with lateral dimensions of 100 nm and smaller," *J. Appl. Phys.*, vol. 97, no. 2, Jan. 2005, Art. no. 023706.

[12] J. Purswani and D. Gall, "Surface morphological evolution during annealing of epitaxial Cu(001) layers," *J. Appl. Phys.*, vol. 104, no. 4, 2008, Art. no. 044305.

[13] D.-Y. Shih, C.-A. Chang, J. Paraszczak, S. Nunes, and J. Cataldo, "Thin-film interdiffusions in Cu/Pd, Cu/Pt, Cu/Ni, Cu/NiB, Cu/Co, Cu/Cr, Cu/Ti, and Cu/TiN bilayer films: Correlations of sheet resistance with Rutherford backscattering spectrometries," *J. Appl. Phys.*, vol. 70, no. 6, pp. 3052–3060, Sep. 1991.

[14] J. Chawla and D. Gall, "Specular electron scattering at single-crystal Cu(001) surfaces," *Appl. Phys. Lett.*, vol. 94, no. 25, Jun. 2009, Art. no. 252101.

[15] K.-L. Ou, M.-S. Yu, R.-Q. Hsu, and M.-H. Lin, "Comparative study of polycrystalline Ti, amorphous Ti, and multiamorphous Ti as a barrier film for Cu interconnect," *J. Vacuum Sci. Technol. B, Microelectron. Nanometer Struct. Process., Meas., Phenomena*, vol. 23, no. 1, pp. 229–235, Jan. 2005.

[16] V. Timoshevskii, Y. Ke, H. Guo, and D. Gall, "The influence of surface roughness on electrical conductance of thin Cu films: An *ab initio* study," *J. Appl. Phys.*, vol. 103, no. 11, Jun. 2008, Art. no. 113705.

[17] F. Zahid, Y. Ke, D. Gall, and H. Guo, "Resistivity of thin Cu films coated with Ta, Ti, Ru, Al, and Pd barrier layers from first principles," *Phys. Rev. B, Condens. Matter*, vol. 81, no. 4, Jan. 2010, Art. no. 045406.

[18] S. Yokogawa and Y. Kakuhara, "Role of impurity segregation into Cu/cap interface and grain boundary in resistivity and electromigration of Cu/low-k interconnects," *Jpn. J. Appl. Phys.*, vol. 50, no. 5S1, May 2011, Art. no. 05EA02.

[19] H. Kitada, T. Suzuki, S. Akiyama, and T. Nakamura, "Influence of titanium liner on resistivity of copper interconnects," *Jpn. J. Appl. Phys.*, vol. 48, no. 4S, Apr. 2009, Art. no. 04C026.

[20] G. Steinlesberger, M. Engelhardt, G. Schindler, and W. Steinhögl, A. Von Glasow, K. Mosig, and E. Bertagnolli, "Electrical assessment of copper damascene interconnects down to sub-50 nm feature sizes," *Microelectron. Eng.*, vol. 64, nos. 1–4, pp. 409–416, Oct. 2002.

[21] T. Sun, B. Yao, A. P. Warren, K. Barmak, M. F. Toney, R. E. Peale, and K. R. Coffey, "Surface and grain-boundary scattering in nanometric Cu films," *Phys. Rev. B*, vol. 81, Apr. 2010, Art. no. 155454.

[22] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, "Electric field effect in atomically thin carbon films," *Science*, vol. 306, no. 5696, pp. 666–669, Oct. 2004.

[23] A. A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, and C. N. Lau, "Superior thermal conductivity of single-layer graphene," *Nano Lett.*, vol. 8, no. 3, pp. 902–907, 2008.

[24] J. S. Bunch, S. S. Verbridge, J. S. Alden, A. M. van der Zande, J. M. Parpia, H. G. Craighead, and P. L. McEuen, "Impermeable atomic membranes from graphene sheets," *Nano Lett.*, vol. 8, no. 8, pp. 2458–2462, Jun. 2008.

[25] R. Mehta, S. Chugh, and Z. Chen, "Enhanced electrical and thermal conduction in graphene-encapsulated copper nanowires," *Nano Lett.*, vol. 15, no. 3, pp. 2024–2030, Mar. 2015.

[26] J. Hong, S. Lee, S. Lee, H. Han, C. Mahata, H.-W. Yeon, B. Koo, S.-I. Kim, T. Nam, K. Byun, B.-W. Min, Y.-W. Kim, H. Kim, Y.-C. Joob, and T. Lee "Graphene as an atomically thin barrier to Cu diffusion into Si," *Nanoscale*, vol. 6, no. 13, pp. 7503–7511, 2014.

[27] S. Chen, L. Brown, M. Levendorf, W. Cai, S.-Y. Ju, J. Edgeworth, X. Li, C. W. Magnuson, A. Velamakanni, R. D. Piner, J. Kang, J. Park, and R. S. Ruoff, "Oxidation resistance of graphene-coated Cu and Cu/Ni alloy," *ACS Nano*, vol. 5, no. 2, pp. 1321–1327, Feb. 2011.

[28] R. K. S. Raman, P. C. Banerjee, D. E. Lobo, H. Gullapalli, M. Sumandasa, A. Kumar, L. Choudhary, R. Tkacz, P. M. Ajayan, and M. Majumder, "Protecting copper from electrochemical degradation by graphene coating," *Carbon*, vol. 50, no. 11, pp. 4040–4045, Sep. 2012.

[29] N. T. Cuong and S. Okada, "Suppression of conductivity deterioration of copper thin films by coating with atomic-layer materials," *Appl. Phys. Lett.*, vol. 110, no. 13, 2017, Art. no. 131601.

[30] D. M. Guzman and A. Strachan, "Enhanced electron transport in thin copper films via atomic-layer materials capping," 2018, *arXiv:1805.01517*. [Online]. Available: https://arxiv.org/abs/1805.01517

[31] M. Ahmed, E. Li, and Y. Li, "First principles calculation of effect of graphene coating on transmission coefficient of Cu thin film with low surface roughness," *J. Appl. Phys.*, vol. 125, no. 6, Feb. 2019, Art. no. 065305.

[32] Y. Zhu and L. Liu, *Atomistic Simulation Of Quantum Transport in Nanoelectronic Devices (With CD-ROM)*. Singapore: World Scientific, 2016.

[33] Y. Zhu, L. Liu, and H. Guo, "Quantum transport theory with nonequilibrium coherent potentials," *Phys. Rev. B, Condens. Matter*, vol. 88, Nov. 2013, Art. no. 205415. doi: 10.1103/PhysRevB.88.205415.

[34] H. L. Skriver, "The LMTO method," in *Springer Series in Solid State Sciences*, vol. 41. Berlin, Germany: Springer-Verlag, 1984.

[35] I. Turek, V. Drchal, J. Kudrnovsky, M. Sob, and P. Weinberger, *Electronic Structure of Disordered Alloys, Surfaces and Interfaces*. Berlin, Germany: Springer, 2013.

[36] J. P. Perdew and A. Zunger, "Self-interaction correction to density-functional approximations for many-electron systems," *Phys. Rev. B, Condens. Matter*, vol. 23, pp. 5048–5079, May 1981. doi: 10.1103/PhysRevB.23.5048.

[37] J. Taylor, H. Guo, and J. Wang, "Ab initio modeling of quantum transport properties of molecular electronic devices," *Phys. Rev. B, Condens. Matter*, vol. 63, no. 24, 2001, Art. no. 245407.

[38] J. Ruseckas, G. Juzeliūnas, and I. V. Zozoulenko, "Spectrum of π electrons in bilayer graphene nanoribbons and nanotubes: An analytical approach," *Phys. Rev. B, Condens. Matter*, vol. 83, Jan. 2011, Art. no. 035403.

[39] Z. Xu and M. J. Buehler, "Interface structure and mechanics between graphene and metal substrates: A first-principles study," *J. Phys., Condens. Matter*, vol. 22, no. 48, Nov. 2010, Art. no. 485301.

[40] G. Giovannetti, P. A. Khomyakov, G. Brocks, V. M. Karpan, J. van den Brink, and P. J. Kelly, "Doping graphene with metal contacts," *Phys. Rev. Lett.*, vol. 101, Jul. 2008, Art. no. 026803.

[41] P. A. Khomyakov, G. Giovannetti, P. C. Rusu, G. Brocks, J. van den Brink, and P. J. Kelly, "First-principles study of the interaction and charge transfer between graphene and metals," *Phys. Rev. B, Condens. Matter*, vol. 79, May 2009, Art. no. 195425.

[42] Y. Wang, F. Zahid, Y. Zhu, L. Liu, J. Wang, and H. Guo, "Band offset of GaAs/Al_xGa_{1-x}As heterojunctions from atomistic first principles," *Appl. Phys. Lett.*, vol. 102, no. 13, 2013, Art. no. 132109.

[43] Y. Ke, K. Xia, and H. Guo, "Disorder scattering in magnetic tunnel junctions: Theory of nonequilibrium vertex correction," *Phys. Rev. Lett.*, vol. 100, no. 16, Apr. 2008, Art. no. 166805.

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