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## Abstract

We report the resistivity measured at temperatures between 5 K and 300 K of a Cu film 63 nm thick with grains that have a diameter d = 10.5 nm on the average. The resistivity of this film is described by the first quantum theory of resistivity of nano-scale metallic connectors [R C Munoz *et al*, App. Phys. Rev. **4** (2017) 011102]. We also report an improved version of this theory that includes a new analytical description of the effect of grain boundary disorder on electron transport. We employ the surface roughness and grain size distribution measured on this Cu film as input data to compute, using our heory, the room temperature resistivity of Cu wires of rectangular cross section, and compare with the resistivity of these wires reported in the literature [M H Van der Veen *et al*, 2018 IEEE International Interconnect Technology Conference (IITC) (2018)], that are used for designing Integrated Circuits (IC) for the 14 nm, 10 nm, 7 nm, 5 nm, 3 nm and 2 nm nodes, respectively. The quantum theory predicts an increase in resistivity with diminishing wire dimensions that accurately agrees with the room temperature resistivity measured on these Cu wires. The resistivity induced by electron-rough surface scattering accounts for about half of the increase over the bulk observed in the 3 nm and 2 nm tech node; scattering by non-uniform grain boundaries contributes the remaining increase in resistivity—the latter is responsible for the weak Anderson localization. According to the description of electron motion furnished by this improved quantum theory, the break down of Moore's law with shrinking wire dimensions is to be expected, since it *originates from size effects triggered by electron scattering with rough surfaces and scattering by non-equally spaced grain boundaries, which become dominant as the dimensions of the metallic wire shrinks.*

## 1. Introduction

Co-founder of Intel, Gordon Moore in 1965 proposed an empirical relation, which states that the number of transistors per unit area doubled approximately every 24 months; this became known as 'Moore's law'. For this relation to hold, the resistivity of the metallic connectors inside an IC— called interconnects—must remain unaltered as the linear dimensions diminish. However, in 2016 INTEL announced that 'Moore's law' is slowing down and is even coming to a halt, because the resistivity of the Cu connecting lines has been observed to grow as the dimensions of the connectors are reduced. Although the increase in resistivity with shrinking wire dimensions seems an accepted fact, the reasons why such an increase takes place remain unknown, and this has become a major obstacle in the continuing effort of circuit miniaturization. According to information provided by the International Road Map for Devices and Systems (IRDS), interconnects are expected to reach widths on the range of 10 to 20 nm within the next decade [1]. Therefore, elucidating why such an increase takes place has become a central problem within the electronic industry. At these short scales of length, the scattering of the electrons with the grain boundaries, and with the rough surfaces is expected to play a major role in the increase in resistivity of the connectors with shrinking wire dimensions.

In this manuscript we present the first application of this quantum theory to describe the resistivity of rectangular cross section Cu interconnects being considered for designing and building IC's, employing an improved version of this quantum theory that includes a new analytical description of the effect of grain boundary disorder on electron transport. The room temperature resistivity measured on these rectangular cross section Cu interconnects has been reported by M H Van der Veen and coworkers at 2018 IEEE International Interconnect Technology Conference (IITC) ([2]). The goal of this paper is, then, to compare the theoretical predictions based upon this improved version of the quantum theory, with published resistivity data on these wires that has become available.

This paper includes the following sections: In section 2 we review some theoretical and some experimental results published over the last few years, concerning charge transport in metallic wires and the break down of Moore's law with shrinking wire dimensions. In section 3 we describe the experimental work performed to measure the resistivity between 5 K and 300 K on a Cu film 63 nm thick deposited on cleaved mica. In section 4 we briefly review the quantum theory of resistivity. In section 5 we present an improved version of this quantum theory, a version that includes an analytical formulation of the effect of disorder on charge transport across a set of disordered grain boundaries. This improvement allows an estimation of the relative increase in resistivity induced by the exponential decay of the electron wave function caused by grain boundary positional disorder, which can be computed from the statistical parameters that describe such disorder on the wires (parameters that are directly measurable on the metallic specimen). In section 6 we assess how well this improved version of the quantum transport theory describes the growth in room temperature resistivity observed with shrinking wire dimensions in nanometric rectangular cross section Cu interconnects. We conclude in section 7 with a critical discussion of the content of this paper and in section 8 we present a summary of this work.

## 2. Recent theoretical and experimental results regarding electrical transport in metallic interconnects of nanometric size

Regarding theoretical work related to the break down of Moore's law and the attempts to generate a formalism that would allow an accurate calculation of the relative growth in resistivity of metallic connectors induced by shrinking scales of length, there is a central issue that must be addressed at the beginning. There are two distinct regimes regarding charge transport: (a) Diffusive transport, where electrons move uncoherently and experience energy dissipation as they undergo scattering events traveling from one electrode to another. This is the opposite of (b) Ballistic transport, where electron motion occurs without experiencing any scattering events (except when they arrive at the electrodes); *that is, the dissipation of energy occurs only at the electrodes.* As discussed in section VII.C of a recent review [3], the length-scale that determines whether electron transport is diffusive or ballistic is the length $L_{ph}$, the distance over which the phase of the electron wave function is modified because of electron scattering. If the typical length L of the specimen is such that $L < L_{ph}$, a ballistic mechanism dominates, while for $L \gg L_{ph}$, electron transport will be diffusive.

The resistance at 300 K of Cu cylindrical wires of nanometric dimensions computed using the formalism of ballistic transport proposed by Bütikker and Landauer was recently reported [4]. In a pure sample made out of crystalline Cu at 300 K, the electronic mean free path is set by the scattering of electrons with phonons and is characterized by a length $\ell_{Cu}(300) = 39$ nm. Hence it is expected that the electrical resistivity of a Cu interconnect of nanometric dimensions, at room temperature, computed using the Bütikker-Landauer formalism, is accurate when $L \approx \ell_{Cu}(300) = 39$ nm, but is underestimated for interconnects whose length L is bigger than about $2.5\ell_{Cu}(300) \approx 100$ nm, and the error will increase with growing L. Therefore, the applicability of Landauer´s formalism to estimate the resistivity of Cu interconnects with nanometric dimensions, for wires longer than 100 nm used in IC's today seems highly questionable.

A review regarding tools available for quantum atomic and electronic scale modeling was published this year containing over 190 references [5]. In this work, the conceptual differentiation between transport of ballistic type and diffusive type, as well as the empirical evidence pointing towards the break down of Moore's law—which has become one of the major obstacles that is demanding huge resources in the continuing effort of circuit miniaturization—are entirely ignored. In section 8.5 of this review, a method is presented to calculate the transport coefficients based on solutions of the Boltzmann Transport equation (BTE). As discussed in section VII.C of [3] and as depicted in figure 25 of that work, the description of the transport of charges based on the BTE is expected to fail for metallic interconnects of nanometric dimensions, because at these short length-scales, quantum effects will very likely dominate the transport of charges, *and such effects are not included in BTE*. This issue will be revisited at the end of this paper.

Following a different approach, a model for the resistivity of nanometric Cu connectors was published, based upon the assumption that the resistivity $\rho$ within the connector can be described as a function of the distance r between the observation point and the nearest metal or dielectric interface, $\rho(r) = \rho_b + \rho_q \exp(-r/\lambda_q)$, where $\rho_b$,

$\rho_q$ and $\lambda_q$ are adjustable parameters [6]. Since this model does not arise from a theoretical description of the scattering of electrons via different collision mechanisms acting at the microscopic scale that give rise to the resistivity within the connector, it has no predicting power whatsoever regarding how and why the resistivity growths as dimensions decrease. In fact, it becomes necessary to perform expensive and detailed experiments for different wire dimensions corresponding to different tech nodes in order to calibrate the unknown adjustable parameters ($\rho_b$, $\rho_q$ and $\lambda_q$); every change of wire dimensions or fabrication method, requires a new set of costly experiments.

A model for the resistivity of metallic films where the metal displays an irregular Fermi surface has been published [7]; the model was applied to films made out of Cu and Ru. This model is based upon an extension of the theory of Mayadas and Shatzkes (MS) [8], to the case where the electron effective mass is not isotropic and, hence, it varies significantly along different crystallographic directions as a consequence of the anisotropy of the Fermi surface. It seems remarkable that *despite some severe conceptual difficulties of the classical MS the*ory already discussed in papers previously published [3, 9], the MS model is still taken as the staring point—without any criticism whatsoever—as a model of wide applicability that offers a reasonable description of electron motion in the case where the conduction band of the metal is nearly isotropic. The evidence contained in figures 22 and 23 of [3] point to the contrary, in the case of electron motion taking place in gold films deposited on mica.

An entirely different and innovative approach was published recently, employing an atomistic model of grain boundaries combined with neural network, it was used to compute the grain boundary resistance of Cu interconnects [10].

Attempts have been published using Ru connectors of ever decreasing dimensions [11–15]. An investigation has also ben published using Co connectors [16]. An overview of the efforts regarding Cu connectors of increasingly smaller dimensions (developed over the last 20 years) has been published [17].

The room temperature resistance of lines of (approximately) rectangular cross section made out of Ru, Co and Cu has been recently reported [2]. In the present manuscript, we used the line resistance displayed in figure 3(a) of [2], to evaluate the typical resistivity expected of the 2 nm, 3 nm, 5 nm, 7 nm, 10 nm and 14 nm nodes, following the width and thickness recommendations reported by P. P. Shah in her MS Thesis regarding interconnect node dimensions for future technology or tech nodes [18]. For the definition of technology nodes or simply nodes, see [19]. Because of the apreciable scatter in the line resistance data reported on [2], we employed an estimation of the line resistance based upon a linear regression applied to a logarithmic representation of the data. The data and the corresponding linear regression are displayed in figure 1. The width and height of the Cu interconnect of rectangular shape corresponding to the different tech nodes according to the report by Shah [18], and the corresponding typical resistivity ($\rho_{Exp}$) estimated for each tech node on the basis of the linear regression representing the line resistance reported in [2], are displayed in table 1.

Experiments performed on gold thin films made up of grains where the average diameter ranges from some 12 nm to about 110 nm [20], suggest that the growth in resistivity with diminishing dimensions may originate from size effects (from scattering of electrons by non-equally spaced grain boundaries and perhaps, also, from scattering by rough surfaces), that may become dominant at smaller length-scales. However, the predictictions made by the quantum transport theory applied to nanometric Cu wires depends on the surface roughness of the wires as well as on the distribution of the grain size present on these wires. Unfortunately, this information is not available from [2]. The predictions of the quantum theory also depend on the reflectivity R associated to electron scattering *by a single grain boundary*; such information is not available either.

In order to be able to account for the resistivity of the Cu wires of rectangular shape, originating from the scattering of the electrons with rough surfaces and with grain boundaries employing the quantum theory, we need information regarding the grain boundary reflectivity R of a single grain boundary, the surface roughness modeling parameters and the grain size Gaussian distribution parameters measured in thin Cu films where the average grain diameter is approximately 10 nm, which is close to the average size of the grains expected in the 2 nm and 3 nm tech node. For this reason we prepared and measured Cu films varying the grain size in a UHV evaporation station, this experimental work is described below.

## 3. Experimental

We evaporated Cu films onto cleaved mica substrates employing Cu 99.9999% pure as a starting material, using a UHV evaporation station schematically shown in figure 2. Changing the substrate temperature from −190 °C to some 30 °C, we were able to change the average grain diameter d making up the samples from some 10 nm to

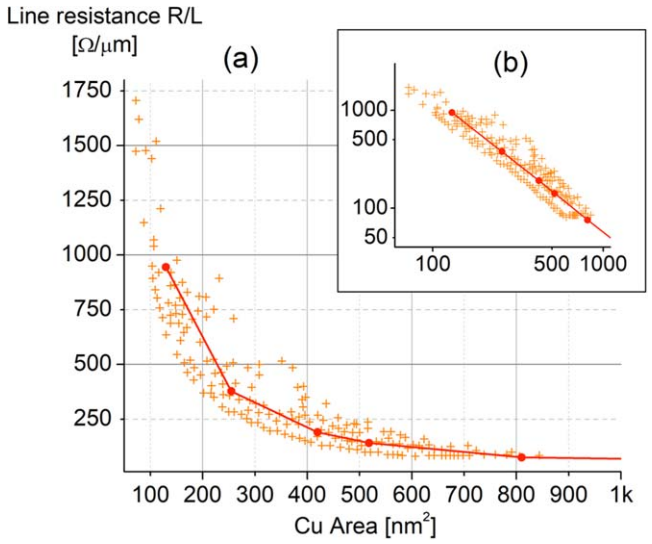


**Figure 1.** Line resistance of Cu interconnects of rectangular shape measured at room temperature, data from [2]; the red line displays the linear regression used to represent the data. The inset shows the data and the linear regression (in a logarithmic scale) used to estimate the resistivity of the 2 nm, 3 nm, 5 nm, 7 nm 10 nm and 14 nm nodes, respectively, following the width and height recommendations contained in [18].

**Table 1.** Resistivity of Copper interconnects of rectangular shape being considered for IC manufacturing. $\rho_{Exp}$: resistivity of Cu lines of rectangular shape at 300 K corresponding to each node, based on the line resistivity data reported in [2]. $\rho_{Dis.\ Flat\ Wire}$: Resistivity of a Copper rectangular shape interconnect, limited by atomically flat (perfectly reflecting) surfaces, made out of disordered grains. $\rho_{Dis.\ Rough\ Wire}$: Resistivity of a Copper rectangular shape interconnect limited by Rough surfaces, made out of disordered grains. $L_{Eff}$: Anderson Localization length.

| Node | Width [nm] | Height [nm] | $\rho_{Exp}$ [nΩ-m] | $\rho_{Dis\ Flat\ Wire}$ [nΩ-m] | $\rho_{Dis\ Rough\ Wire}$ [nΩ-m] | $L_{eff}$ [nm] |
|---|---|---|---|---|---|---|
| 14 | 37.8 | 69.9 | 40 | 38.6 | 48.2 | 155 |
| 10 | 22.5 | 36 | 61.3 | 42.3 | 61.9 | 92.9 |
| 7 | 18 | 28.8 | 73.5 | 44.6 | 70.7 | 75.5 |
| 5 | 16.2 | 25.9 | 80.1 | 46.2 | 76.9 | 67.5 |
| 3 | 12.6 | 20.2 | 96.1 | 50.2 | 92.2 | 52.9 |
| 2 | 9 | 14.4 | 122 | 58.9 | 128 | 38.7 |

about 32 nm. Following results published by Zarate *et al* [21], the Cu films were covered with a 3 nm thick TiO film evaporated with the Cu films held at room temperature to passivate the samples when transferred to a cryostat, in order to perform transport measurements. The resistivity plotted as a function of temperature, of a sample 63 nm thick with an average grain diameter d = 10.5 nm (computed over images recorded with an AFM on more than 500 grains), is displayed in figure 3, along with the theoretical description of the resistivity based upon the improved version of the quantum theory of resistivity outlined below [3, 9]. The measurement of the resistivity was performed using the 4 point method (2 contacts used for feeding current to the sample, and the other 2 contacts used for measuring the voltage drop across the film employing a digital voltmeter). A current of 1 mA was fed to the sample employing a computer controlled current source that performed periodic current reversal, in order to eliminate systematic voltage errors that might arise from undesired contact potentials.

Since the quantum theory describing charge transport in these wires of rectangular cross section is available but, unfortunately, the grain size data and surface roughness data is not available for these Cu wires whose line resistance is reported in [2], the question remains open concerning how well the quantum theory performs regarding the resistivity data on the wires considered for these 2 nm to 14 nm tech nodes. To answer this question, in this paper we chose to use as input data, the grain size distribution and the surface roughness measured with an AFM on the 63 nm thick Cu film (whose resistivity is displayed in figure 3). The reason for this choice is that the average grain size measured on this Cu film is close to the grain size of 9.0 nm expected on the 2 nm tech node and 12.6 nm expected on the 3 nm tech node, if the grain diameter is constrained not to exceed the smallest wire dimension, the wire width.

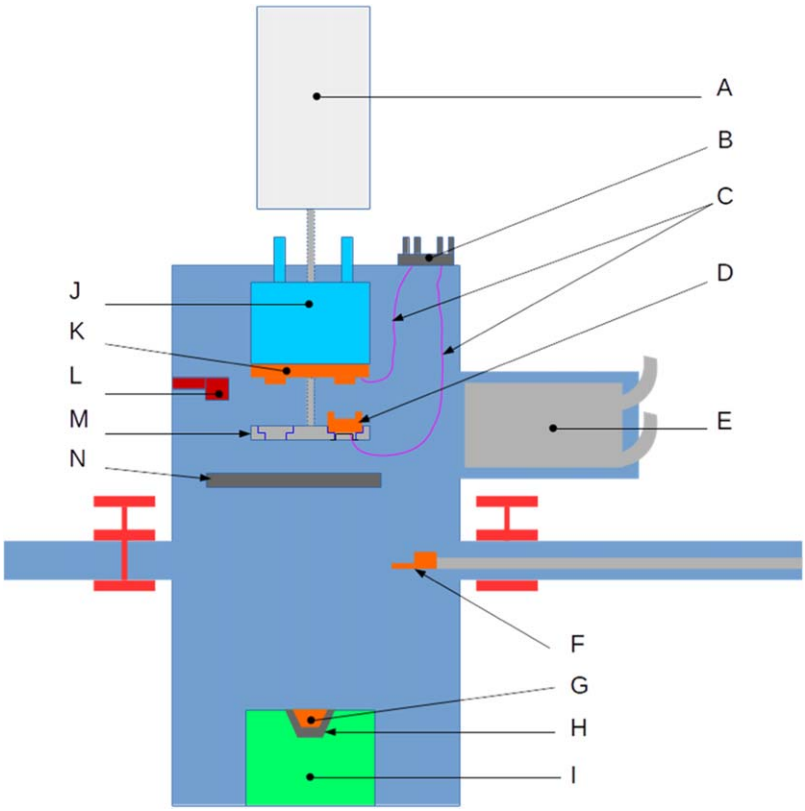


**Figure 2.** Vacuum station used to evaporate copper samples in UHV. (A): Sample manipulator, (allows for vertical and horizontal sample positioning). (B): Feedthrough connecting to thermocouples. (C): Thermocouple cables. (D): Sample holder. (E): Ti sublimator cooled to liquid nitrogen. (F): Insertion (movable) arm. (G): Material to be evaporated using the electron gun. (H): Electron gun crucible. (I): Electron gun. (J): Liquid nitrogen cold trap. (K): Copper oven. (L): Quartz crystal microbalance. (M): Metal disc carrying 4 samples. (N): Shutter plate.

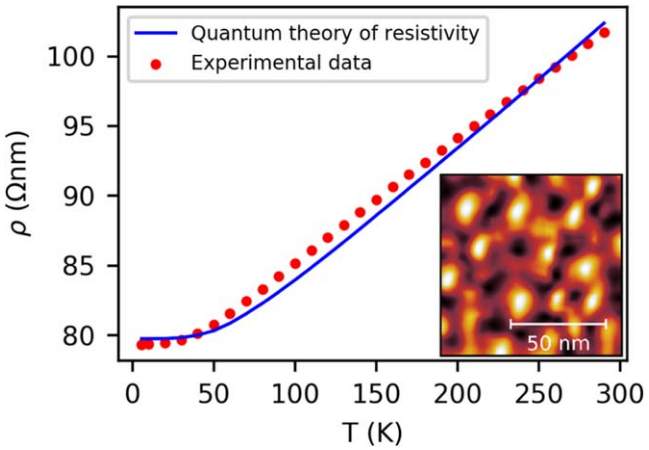


**Figure 3.** Temperature dependence of the resistivity of a copper film 63 nm thick evaporated onto a freshly cleaved mica substrate, covered with a 3 nm thick TiO film. The average grain diameter (measured on over 500 grains) is d = 10.5 nm. Inset: AFM image of the surface of the sample. The mean free path describing the scattering of electrons with impurities/point defects is $\ell_{IMP} = 16.7$ nm; the grain boundary reflectivity is R = 0.12. The inset displays an image of the grains recorded with an AFM.

## 4. Theory

In our model [3, 9] we assume, as in MS [8], that the external electric field **E** is parallel to the x directions, with grain boundaries modeled by (y, z) planes perpendicular to x. The effect of grain boundaries is captured by a set of delta function barriers placed at the sequence of positions $\{x_n\}$, all having the same strength S:

$$V(x) = \sum_{n=-N/2}^{N/2} \left(\frac{\hbar^2}{2m}\right)\delta(x - x_n) \tag{1}$$

In contrast with the classical MS theory, our quantum theory is based on the analytical solution of the Green´s function for the potential of equation (1) corresponding to equally spaced grains. In case all the grain boundaries are uniformily distributed, then

$$\cos(\xi) = \cos(k_x d) + (S/2k_x)\sin(k_x d) \tag{2}$$

where $\xi$ is the Kronig-Penney (KP) parameter and d is the mean grain diameter.

After calculating the analytical expression for the Green´s function corresponding to the periodic array of grain boundaries, the conductivity is computed employing the linear response theory by Kubo. Thus, the electrical conductivity of a wire of rectangular shape is computed using the following [equation (42) in [3]:

$$\sigma = \frac{q^2}{4\pi\hbar D_y D_z}\sum_{m,n}\frac{I(k_{m,n})}{|D(k_{m,n})^2|}T_N(k_{m,n})$$

Here q is the electron charge, $D_y$ and $D_z$ are the width and height of the rectangular wire, $T_N$ stands for the probability that an electron is transmitted through N successive grain boundaries, D(k) = ksin(kd)sin($\xi$), and I(k) is the expression given by equations (37), (38), (39) and (40) in [3]. The double sum is such that m, n and $k_x$ satisfy equation (2) (and therefore $k_x$ lies inside one of the allowed Kronig-Penney bands), and that also satisfy

$$k_x{}^2 + \left(\frac{n\pi}{D_y}\right)^2 + \left(\frac{m\pi}{D_z}\right)^2 = k_F{}^2$$

which is equation (43) in [3]. Further details regarding the Green's function built out of the solution of the Schrodinger equation describing an electron immersed in a periodic array of grain boundaries, as well as details leading to the calculation of the conductivity of a metallic wire of rectangulat shape, can be found in section II.E of [3].

## 5. Effect of grain bondary positional disorder

The positional disorder in the array of grain boundaries plays a central role in the theory. To account for it, we started from $\varphi_n(x)$, the wave functions which describe the electron states of the system with grain boundaries that are located at $x = x_n$ and *are unequally spaced*. For this, we write

$$\varphi_{n-1}(x = x_n) = \varphi_n(x = x_n);\left\{\left(\frac{d\varphi_n(x)}{dx}\right)_{x=x_n} - \left(\frac{d\varphi_{n-1}(x)}{dx}\right)_{x=x_n}\right\} + S\varphi_n(x = x_n) = 0$$

leads to the $2 \times 2$ $P_n$ transfer matrix defined by $\begin{pmatrix} A_n \\ B_n \end{pmatrix} = P_n \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix}$ The $2 \times 2$ transfer matrix describing the effect of N consecutive grain boundaries is $M = P_N \times P_{N-1} \ldots \times P_1$. The statistical average of $P_n$ over a Gaussian distribution with zero mean and s standard deviation, is

$$\langle P_n \rangle = \begin{pmatrix} 1 + i\frac{S}{2k_x} & i\frac{S}{2k_x}(\exp(-2ik_x nd)\exp(-2k_x{}^2 s^2) \\ -i\frac{S}{2k_x}(\exp(2ik_x nd)\exp(-2k_x{}^2 s^2) & 1 - i\frac{S}{2k_x} \end{pmatrix} \tag{3}$$

It is useful to write the matrix $\langle P_n \rangle$ in terms of the Pauli $2 \times 2$ matrices, that can be employed to derive an analytical expression for the transmission coefficient $T_N(k_x) \approx \frac{1}{\langle |M_{22}(N,k_x)|^2 \rangle}$ (Section II.E.5 of [3]). While in our 2017 work we performed the statistical average numerically, in the present paper we present an upgraded version of the theory, with analytical expressions for the statistical average over disorder. These expressions are summarized in the set of equations:

$$T(N, k_x) = C(N, k_x)\exp^{-N/\Lambda(k_x)} \text{ with } C(N, k_x) = \frac{1 + \frac{\gamma^2}{N^2}\frac{\sin^2(N\vartheta/2)}{\sin^2(\vartheta/2)}}{1 + \frac{\gamma^2}{N^2}\frac{\sin^2(N\vartheta/2)}{\sin^2(\vartheta/2)}\cos^2(u)}$$

where $S = 2k_F\sqrt{\frac{R}{1-R}}$ represents the strength of a delta function potential appearing in equation (1), and is related to the *reflectivity R of a single grain boundary*, and

$$\nu = \frac{S}{2k_x};\ \gamma = \exp(-2s^2k_x{}^2);\ \vartheta = 2dk_x;\ \alpha = \tan^{-1}(\nu\sqrt{1+\gamma^2})$$

with $u = N\alpha\frac{1}{\sqrt{1+\gamma^2}}\left[1+\frac{\gamma^2}{N^2}\frac{\sin^2(N\vartheta/2)}{\sin^2(\vartheta/2)}\right]^{1/2}$; and $\Lambda^{-1}(k_x) = \ln(1+\nu^2(1+\gamma^2))$

The variables $\alpha, \nu, \gamma, \theta$, are all auxiliary variables that depend on the momentum $k_x$, that have been introduced to simplify the notation as well as the numerical calculations. Replacing N by $\ell/d$ leads to

$$T\left(\frac{\ell}{d}, k_x\right) = C\left(\frac{\ell}{d}, k_x\right)\exp\left(-\frac{\ell}{L(k_x)}\right) \tag{4}$$

$$\text{where } L(k_x) = d\Lambda(k_x) = \frac{d}{\ln(1+\nu^2(1+\gamma^2))} = \frac{d}{\ln\left(1+\frac{S^2}{4k_x{}^2}(1+\exp^{-4k_x{}^2s^2})\right)} \tag{5}$$

is the Anderson localization length arising from the positional disorder of the grain boundaries. To include the effect of disorder we were guided by the following considerations:

1. N = 1 if $\ell$ < d, and

2. N = Int($\ell$/d) if $\ell$ > d, where Int(z) is the integer part of z, and $\ell$(T) is the electronic mean free path in the massive bulk sample at temperature T.

This approach leads to *the well known Anderson localization* mechanism, but in this case only *weak localization* is achieved, since after traversing the grains contained in a mean free path $\ell$(T), the wave function of the electron will be modified and will lose coherence because of the scattering events of the electron in the bulk. Equations (4) and (5) reproduce the 'clean' limit in the absence of disorder, which corresponds to s → 0. This corresponds to $\gamma \to 1$, which implies $\alpha \to 0$ and hence u → 0. Thus, $C(N, k_x) \xrightarrow[s\to 0, u\to 0]{} 1$, and similarly $L(k_x) \xrightarrow[s\to 0, \gamma\to 1]{} \infty$, which implies $T(N, k_x) \xrightarrow[s\to 0]{} 1$, i.e. full transmission is achieved in the absence of disorder.

Quite often, the standard deviation s of the *Gaussian distribution* which models grain boundary disorder is of order 20%–30% of d. This means that for Cu, Al, Ag and Au for which $k_F$ is of order 10 $nm^{-1}$, $\gamma^2 \ll 1$. Consequently, in this case C is a quantity of order 1 and

$$T \sim C\exp(-N/\Lambda) \sim C\exp[\ln(1+\nu^2(1+\gamma^2)^{-N}] \sim (1+\nu^2)^{-N} \sim \left(1+\frac{S^2}{4k_F{}^2}\right)^{-N}$$

$$\sim \left(1+\frac{R}{1-R}\right)^{-N} \sim (1-R)^N$$

This is an essential difference with the classical MS theory where T = 1: *The transmission coefficient T (and therefore the conductivity of a sample involving electrons propagating through N consecutive grain boundaries found along an electronic mean free path $\ell$) decreases as (1-R)* $^N$. This turns out to be one of the reasons underlying the increase of resistivity induced by shrinking wire dimensions to a scale smaller than the mean free path of the electrons in the massive bulk sample.

## 6. Resistivity of copper interconnects with rectangular section

The typical resistivity of the Cu wires of rectangular shape at room temperature contained in table 1 ($\rho_{Exp}$) is displayed in figure 4, along with the resistivity predicted by our improved quantum theory. This is the main content of this paper.

The assumptions used to compute the predictions based on the quantum theory are the following: (a) The mean free path of the electrons in the bulk (determined by scattering of electrons by impurities and point defects as well as phonon scattering at 300 K), is the same for all wires, $\ell$ = 29 nm. (b) The grains exhibit an average diameter d in the wire that is equal to the smallest dimension (the wire width) in all wires; the positional disorder of the grain boundaries is s/d = 0.30 = 30%. (c) The average rms surface roughness is $\delta$ = 0.60 nm and the lateral correlation length is $\xi$ = 2.2 nm in the four surfaces of all wires. The values of ($\delta$, $\xi$) and of s/d correspond to what we measured with an AFM on the 63 nm thick Cu film whose resistivity is displayed in figure 2. (d) The grain boundary reflectivity R = 0.12 is the same for all wires, and is close to R = 0.11 used to describe the resistivity of sample S1 on table I of our work [3], that refers to a Au film 49 nm thick deposited on mica having a grain diameter d = 11 nm.

Under such assumptions, *the quantum theory predicts accurately the observed trend of increasing resistivity (by almost one order of magnitude) with shrinking wire width.* However, we need to elucidate how much of the growth in resistivity with decreasing dimensions, comes from the scattering of the electrons by the rough surfaces

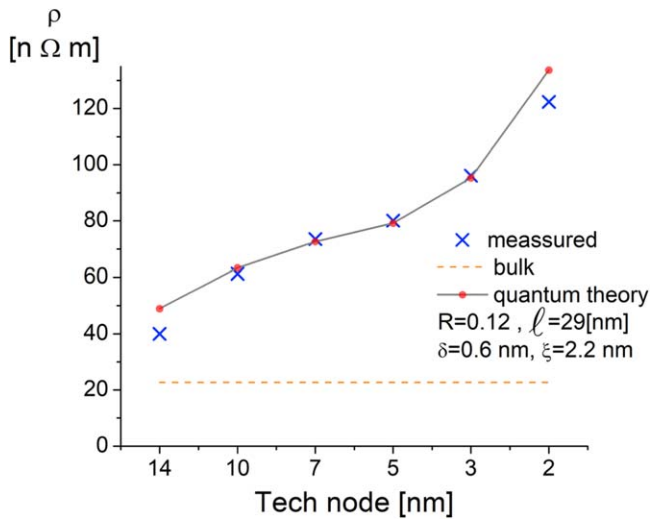


**Figure 4.** Room temperature resistivity of Cu interconnects with rectangular shape being considered for chip manufacturing. The blue crosses represent the room temperature resistivity of the wires being considered for the different tech nodes, estimated from the typical line resistance of Cu wires of rectangular shape reported in [2]. The red dots represent theoretical predictions, under the following assumptions: $k_F = 13.6\ nm^{-1}$. (a) The electronic mean free path $\ell$ describing the scattering of electrons with phonons and with impurities/point defects in the bulk is the same for all wires, $\ell = 29$ nm. (b) The average grain diameter d is equal to the smallest dimension (the wire width) in all wires. (c) The degree of disorder is $s/d = 0.3$ in all wires. (d) The grain boundary reflectivity $R = 0.12$ is the same for all wires. (e) The average rms surface roughness is $\delta = 0.60$ nm and the lateral correlation length is $\xi = 2.2$ nm in the four surfaces of all wires.

limiting the wire, and what is the contribution that arises from grain boundary disorder. To explore the role that disorder plays on this increase in resistivity, in figure 5 we plot the dependence of the transmission coefficient T computed according to equation (4), on the wave vector $k_x$ and on the degree of disorder s. There are interesting new features displayed on this figure that are in sharp contradiction with the predictions of the classical MS theory for which $T = 1$.

The first, is that *for certain regions of $k_x$ the transmission coefficient is close to zero;* these regions correspond to the forbidden states of the Krönig-Penney (KP) potential arising from periodic grain boundaries, regions which are already excluded by the KP band selection [equation (2)]. The second interesting result, is that *for a degree of disorder s/d that exceeds a rather small fraction of approximately 2%, the effect of weak Anderson localization sets in,* and turns the transmission coefficient T (plotted as a function of s/d for a given $k_x$) into almost a constant, *whose value is appreciably smaller than that obtained when s/d* $< 0.02$. This is one of the driving mechanisms underlying the increase in resistivity observed in nanometric Cu wires of rectangular cross section with shrinking wire width.

Since the localization length defined by equation (5) depends on the wave vector $k_x$, for convenience we write the conductivity of an interconnect with rectangular shape in the form:

$$\frac{\sigma}{\sigma_0} = \sum_{states} T(\ell,\ k_x\ ) f_{KP}(\ell,\ k_x) \tag{6}$$

where $\sigma_0$ is the conductivity of the bulk (that is, the conductivity of a fictitious reference wire of the same dimensions that carries the same concentration of both impurities and point defects, but without any grain boundaries and that is bounded by atomically flat, perfectly reflecting surfaces), $\sigma$ is the conductivity of the interconnect with rectangular shape, and the sum implied by equation (6) includes the function $f_{KP}(\ell,\ k_x)$ that is evaluated only over all states allowed by the KP periodic potential.

We define an 'effective localization length $L_{eff}$' that is independent of the wave vector $k_x$,

$$\sum_{states} T(\ell,\ k_x\ ) f_{KP}(\ell,\ k_x) = \sum_{states} C\left(\frac{\ell}{d},\ k_x\right) \exp\left(-\frac{\ell}{L(k_x)}\right) f_{KP}(\ell,\ k_x) = \exp\left(-\frac{\ell}{L_{eff}}\right) \sum_{states} C\left(\frac{\ell}{d},\ k_x\right) f_{KP}(\ell,\ k_x) \tag{7}$$

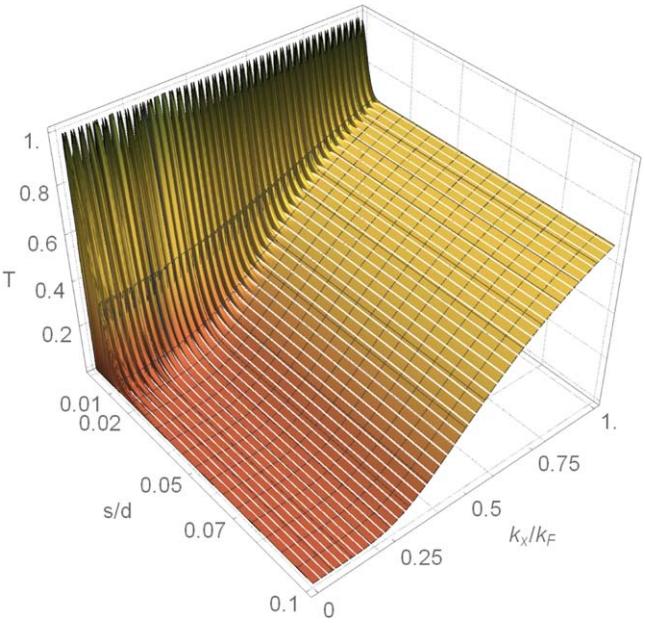


**Figure 5.** Dependence of the transmission coefficient T computed from equation (4), on the degree of disorder and on the wave vector $k_x$. The wave vector $k_x$ is plotted as a fraction $k_x/k_F$ relative to the Fermi wave vector for Cu. The degree of disorder is plotted as a function of s/d (where s corresponds to the Gaussian standard deviation of the distribution $f(\Delta_n) = \frac{1}{\sqrt{2\pi s^2}} \exp\left(-\frac{\Delta_n{}^2}{2s^2}\right)$ describing the fluctuations $\Delta_n$ of the location of the grain boundaries placed at $x_n = nd + \Delta_n$, with respect to their average position $x_n = nd$ when $\Delta_n = 0$ (d is the average diameter of the grains). The electronic mean free path used is $\ell = 36$ nm, the average grain diameter $d = 10$ nm, the grain boundary reflectivity is $R = 0.1$.

$$\text{hence } L_{eff} = -\frac{\ell}{\ln\left(\frac{\sigma/\sigma_0}{\sum_{states} C\left(\frac{\ell}{d}, k_x\right) f_{KP}(\ell, k_x)}\right)} \tag{8}$$

In order to elucidate the effect that shrinking the wire width has on the resistivity arising from size effects, that is, on the contribution to the resistivity growth originated in the scattering of the electrons by the rough surfaces as well as by grain boundaries, we display in table 1 the effective localization length for each of the tech nodes, as well as the resistivity of the wire made out of disordered grains limited by atomically flat (perfectly reflecting) surfaces, as well as the resistivity of the wire made out of disordered grains limited by rough surfaces. Table 1 displays some interesting new information.

The forth column, $\rho_{\text{Exp}}$, displays the resistivity of the Cu lines of rectangular cross section being considered for each node. The fifth column displays $\rho_{\text{Dis. Flat Wire}}$, the resistivity of a wire bounded by perfectly flat, reflecting surfaces. It indicates that the very fact of decreasing the wire width already induces a significant increase in the resistivity, even if the four surfaces of the wire are atomically flat, reflecting planes and the bulk resistivity is the same for all nodes. The reason is that, since the diameter of the grains making up the samples is assumed to be the same as the wire width, if the grain diameter is constrained not to exceed the wire width, then shrinking the wire width leads to smaller grains so there is more than one grain boundary found along a sinlge mean free path of the electrons in the massive bulk sample, and therefore the influence of the scattering of the electrons by the disordered grain boundaries is increased.

The sixth column, $\rho_{\text{Dis. Rough Wire}}$, displays the effect of including the surface roughness in all four surfaces. *Such an increase grows larger for smaller wire dimensions even when the wire is limited by surfaces that are characterized by the same surface roughness (for the roughness rms amplitude $\delta = 0.6$ nm and the lateral length of correlation $\xi = 2.2$ nm used in the calculation are the same for all nodes)*. We expected this to be the case, since for smaller wire dimensions the ratio between the surface and the volume is larger. It seems reassuring that the quantum theory and, in particular, the energy dissipation induced by the scattering of the electrons by the rough surfaces computed employing the Kubo linear response theory discussed in section II.E.7 of our work [3], quantitatively predicts that shrinking the dimensions of the wire will induce an increase in the resistivity due to electron-rough surface scattering. For the smaller nodes this effect turns out to be similar to or larger than the growth of electrical resistivity arising from the scattering of the electrons by the disordered grain boundaries.

New materials (such as Ru and Co) have been suggested to compensate the effects related to the break down of Moore's law. However, the change in material will hardly eliminate the effect of electrons being scattered by the rough surfaces limiting the wire that will become dominant as the wire dimension shrinks, and will hardly compensate the inherent loss of order of the grain boundaries along the metallic wire that leads to electron scattering by disordered potential barriers resulting in weak Anderson localization. Such localization is induced by the exponential decay of the wave function of electrons, describing a carrier that traverses several disordered potential barriers—that ultimately leads to a wire resistance that increases exponentially (instead of linearly) with increasing wire length [22].

## 7. Discussion

In this work we apply an improved version of our quantum transport theory of resistivity for metallic interconnects of nanometric dimensions, to model the room temperature resistivity of Cu interconnects of rectangular shape being considered for IC manufacturing. The theory describes in detail the resistivity of metallic structures with nanometric dimensions—based on quantum Kubo's linear response theory—which includes the scattering of the electrons with grain boundaries and with rough surfaces, that allows the calculation of the increase in resistivity of nanometric metallic interconnects of rectangular cross section and roughly explains the observed trend of increasing resistivity by almost one order of magnitude with shrinking wire dimensions. The input parameters of the model are the statistical parameters that describe the roughness of the surfaces limiting the wire (roughness modelled assuming a Gaussian distribution characterized by its rms amplitude and its length of lateral correlation), together with the statistical parameters that describe the grain size distribution in the wire (a Gauusian distribution described by an average grain diameter and its standard Gaussian deviation), as well as the reflectivity R of a *single grain boundary* and the mean free path $\ell_{\mathrm{IMP}}$ determined by the scattering of electrons by impurities and point defects in the bulk (which would be measured in the absence of the scattering of the electrons by surfaces and in the absence of electron scattering by grain boundaries).

The model presented here exhibits two distinct features: First, it is the only model available that allows the computation of the electrical resistivity of metallic interconnects of nanometric lateral dimensions arising from a quantum description of the different electron scattering mechanisms acting together, that includes: (i) electron scattering by point defects/impurities, (ii) scattering by phonons, (iii) scattering by rough surfaces, (iv) scattering by disordered grain boundaries. Second, it is the only theory that naturally predicts an exponential (rather than linear) increase in resistivity with wire length that takes place when electrons propagate through a disordered 1-D potential arising from several consecutive grain boundaries found within an electron mean free path $\ell$(T) in a massive bulk sample, an increase that is characterized by an Anderson localization length whose analytical expression is given by equation (8).

This model leads to some interesting conclusions: (a) *The break down of Moore's law with shrinking wire dimensions is to be expected, since it originates from size effects that become dominant at smaller scales of length.* (b) The model captures the entire range of morphological and structural features on the resistivity, ranging from perfectly periodic and monodisperse grain boundaries towards disordered ones. (c) The model allows for an assessment of how much of the increase in resistivity with shrinking dimensions (with respect to the resistivity of the bulk) arises from grain boundary disorder, employing the statistical parameters that describe the grain size population; these parameters can be measured on the metallic specimen. It also allows for an independent estimation of the extent to which the scattering of the electrons by the rough surfaces on the side walls of the wire also contribute to increasing the resistivity with shrinking wire dimensions, employing the statistical parameters that model its surface roughness, which can also be measured on the wire.

### 7.1. Resistivity arising from electron scattering by rough surfaces

To illustrate the relative growth in resistivity attributable to electron scattering by the rough surfaces that represent the side walls of the interconnects, induced by shrinking the wire dimensions, we plot in figure 6, the increase $\Delta\rho/\rho_0 = (\rho_{\mathrm{Dis\ Rough\ Wire}} - \rho_{\mathrm{Dis\ Flat\ Wire}})/\rho_0$, where $\rho_0$ is the resistivity of the bulk. It seems interesting that the very fact of decreasing the dimensions of the wire *for a surface roughness described by the same statistical parameters*, results in an appreciable raise of the resistivity arising from the scattering of the electrons by the rough surfaces. As pointed out above, we expected this to be the case, since for smaller wire dimensions the surface to volume ratio grows larger. The theoretical description contained in this manuscript leads to an increase of about 200% for the 3 nm node, and larger than 300% for the 2 nm node.

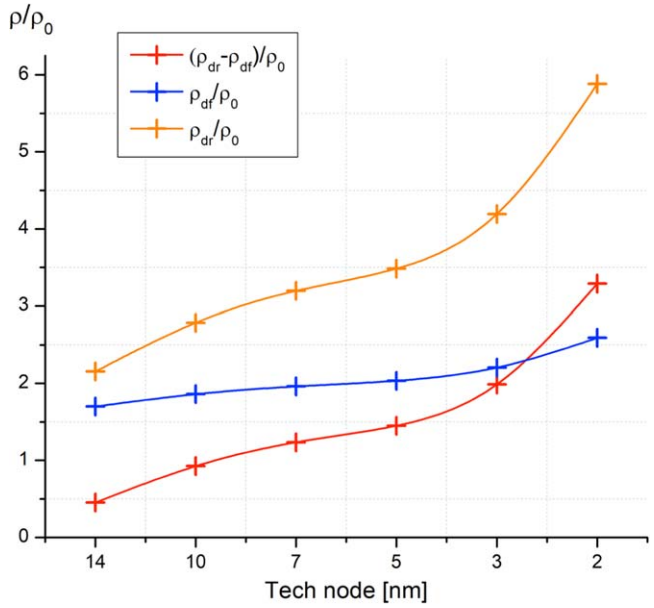


**Figure 6.** Increase in resistivity plotted as a fraction of the resistivity of the bulk $\rho_0$. Orange crosses: $\rho_{Dr} = \rho_{Dis\ Rough\ Wire}$, resistivity of a Disordered Rough Wire. Blue crosses: $\rho_{df} = \rho_{Dis\ Flat\ Wire}$, resistivity of a Disordered wire limited by flat, perfectly reflecting surfaces. $\Delta\rho = \rho_{Dr}$ - $\rho_{df}$, resistivity attributable solely to the electron scattering by the rough surfaces on the sides walls of the wire, plotted as a fraction of the resistivity of the bulk $\rho_0$.

### 7.2. Growth of resistivity triggered by the scattering of electrons with rough surfaces and with non-equally spaced grain boundaries

In figure 6 we plot the relative growth of the resistivity triggered by the combined scattering of electrons with rough surfaces and with disordered grain boundaries. The increase in resistivity with decreasing wire dimensions exceeds 400% for the 3 nm node, and exceeds 550% for the 2 nm node. In the case of disordered grain boundaries, the relative growth in resistivity with smaller dimensions is due to the fact that the grain diameter was assumed to be constrained not to exceed the wire width, hence for smaller wire widths there are more grain boundaries found along the distance corresponding to a mean free path.

### 7.3. Effect of surface roughness and of the distribution of grain sizes on the increase in resistivity arising from size effects

It seems interesting to find out how the parameters used to characterize statistically the surface roughness and the grain size distribution describing the positional disorder of grain boundaries, affect both the resistivity $\rho$ of the specimen corresponding to different nodes, as well as the Anderson localization length $L_{eff}$. This is displayed in figure 7 and in figure 8.

Figure 7 reveals that the relative growth in resistivity due to electron scattering by rough surfaces does not exhibit a monotonic behavior with increasing the rms roughness amplitude $\delta$. The increase in resistivity with increasing $\delta$ exhibits a maximum roughly near $\delta/\lambda_F \sim 0.5$, where $\lambda_F$ is the Fermi wave length of electrons in Cu. The reason resides in the quantum theory used to compute the increase in resistivity arising from electron-surface scattering. As mentioned in section II.C.4 of [3], according to the quantum version of the Fuchs-Sondheimer theory [23], the quantum reflectivity $R(k_{\|})$ predicted by the theory of Sheng, Xing and Wang is given by

$$R(k_{\|}) = \left[\frac{1 - k_z Q(k_{\|})}{1 + k_z Q(k_{\|})}\right]^2$$

where $k_{\|}$ is the momentum of the electron parallel to the rough surface, $k_z$ is the momentum of the electron perpendicular to the surface, and $Q(k_{\|})$ is the self-energy of the electron gas induced by electron confinement within the film limited by rough surfaces. For a Gaussian distribution of surface roughness, $Q(k_{\|})$ is given by equation (14) in [3]. The effect of the surface roughness on the resistivity of the film is maximally enhanced when the parameters are in the vicinity of the condition of minimal reflectivity, i.e. $R = 0$. This condition is satisfied when $1 - k_F Q(k_F) = 0$. Using the asymptotic behavior of $Q(k_{\|})$, it can be shown that a null reflectivity is obtained, roughly when $\frac{\sqrt{\xi\delta}}{\lambda_F} \approx 1.57$, where $\xi$ is the surface roughness lateral correlation length. A more detailed numerical calculation yields that the surface roughness has a maximum effect roughly when $\delta/\lambda_F \sim 0.5$.

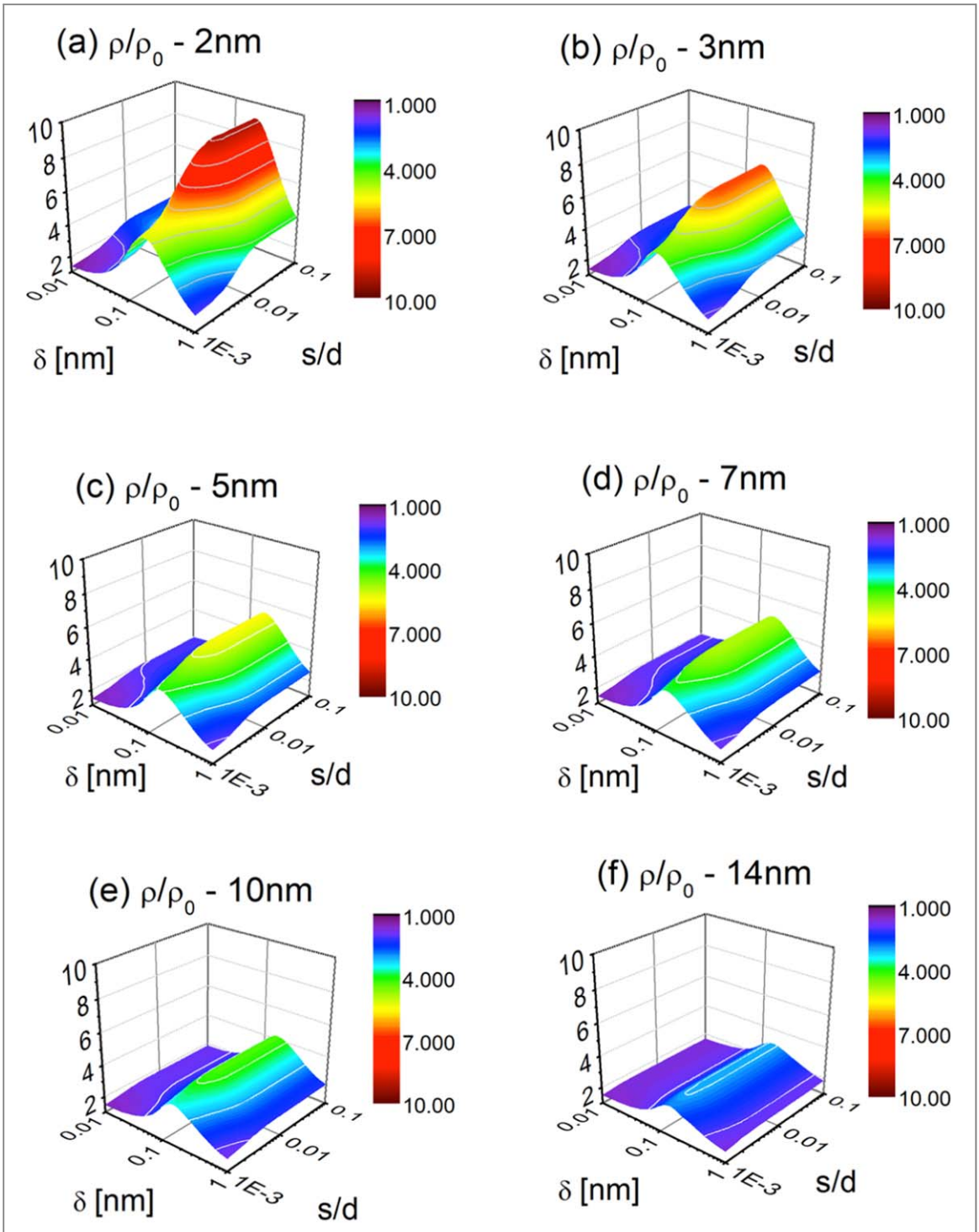


**Figure 7.** The effect of the statistical parameter $\delta$ describing rms roughness amplitude, and s/d (where s is the standard deviation describing the Gausian statistical distribution of the size of the grains around the mean grain diameter d), on the increase in resistivity$\rho/\rho_0$ associated to each node.

However, in spite of these conclusions, we caution that this work may be considered as exploratory in several ways. First, the theoretical predictions displayed in figure 4 *by no means represent a parameter fitting to existing resistivity data on Cu wires of rectangular cross section*. Figure 4 is simply intended to illustrate the argument that the phenomena underlying the observed relative growth in resistivity with decreasing dimensions is to be expected. Scattering of the electrons by disordered grain boundaries leads to Anderson's weak localization that takes place when electrons traverse several grain boundaries; this will occur and may become dominant when the average grain diameter becomes shorter than the electronic mean free path in the massive bulk, *regardless of the metal making up the wire.* The loss of coherence of the electron wave function induced by electron scattering in the bulk prevents the electron from actually becoming localized.

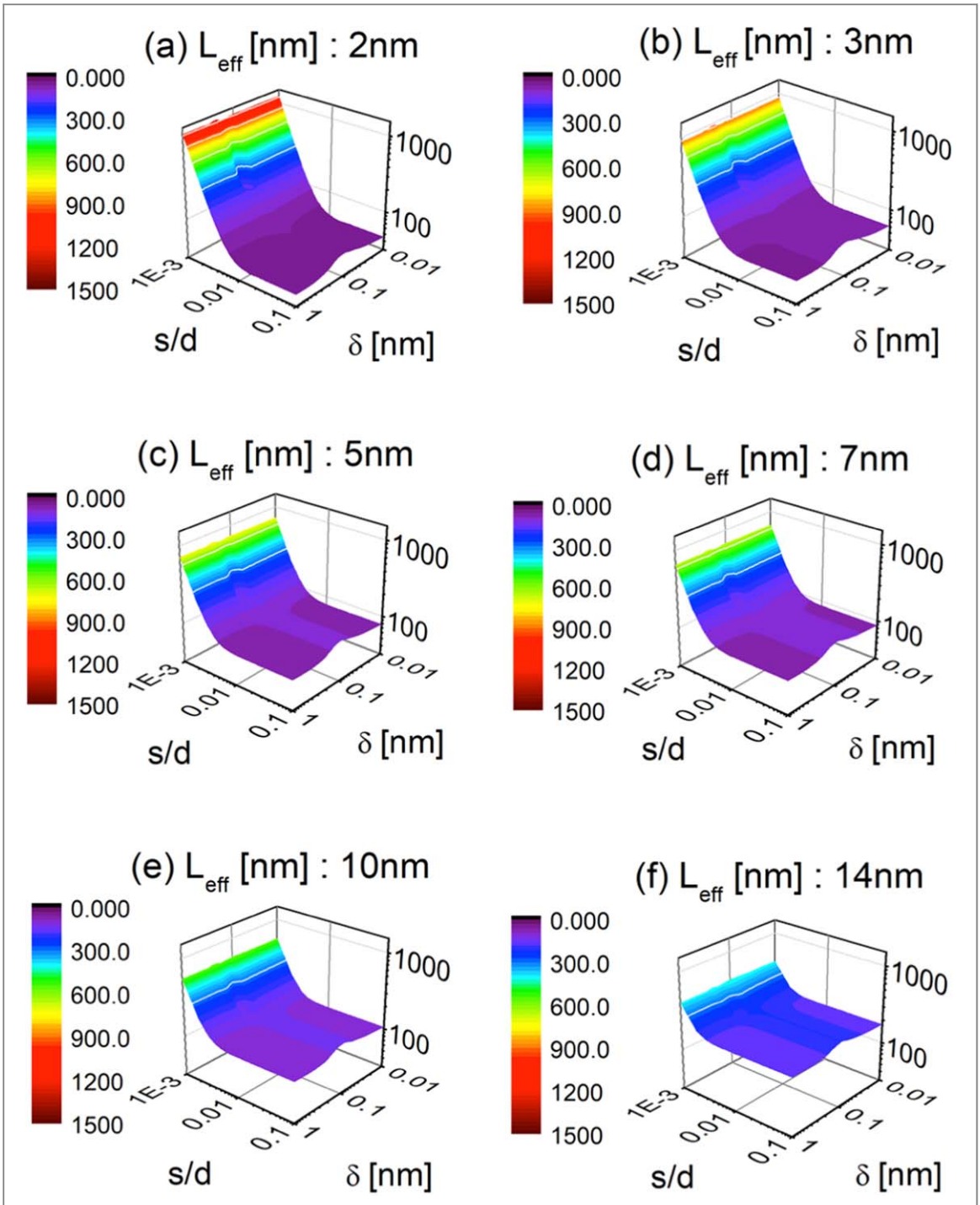


**Figure 8.** The effect of the statistical parameter $\delta$ describing rms roughness amplitude, and s/d (where s is the standard deviation describing the Gausian statistical distribution of the size of the grains around the mean grain diameter d), on the Anderson localization length $L_{Eff}$ associated to each node.

Another reason why this work may be considered as exploratory is because grains exhibit properties that have been entirely ignored in the theoretical model presented here. There is evidence indicating that shrinking dimensions influences significantly the texture and the distribution of grain boundaries, such significant influence has been entirely ignored in the present theory; this is discussed in section VII.D of our work [3]. To illustrate this point, we mention a report indicating that wires of 1.8 $\mu$m width show a strong $\langle 111 \rangle$ typical texture and is formed by micron size large grains; however moving to 180 nm leads to a $\{111\}\langle 110 \rangle$ texture which is bi-axial [24]. Additional evidence based upon computer simulations, predicts that grain boundaries with high angle are responsible for a large resistivity increase due to scattering of the electrons with these type of boundaries between grains [10, 25–28]. Such contributions are also ignored in the present model, for all grain boundaries are characterized by the same reflectivity R. Representing grain boundaries by a series of delta

function potentials having the same strength is a first step, a first idealization that can be refined and can certainly be improved.

## 8. Summary

In this work we use an improved version of a quantum transport theory—that is, a description of the resistivity based on the quantum description of the scattering of electrons with disordered grain boundaries and with rough lateral surfaces—and apply this theory to predict the resistivity of Cu interconnects of metallic rectangular shape with nanometric dimmensions, being considered for IC building. The theory predicts that the relative growth in resistivity measured in Cu wires reported in the recent literature, leading to the break down of Moore's law, is a natural phenomena. A distinct feature of the theory is that it contains only one adjustable parameter, *the reflectivity R describing the scattering of electrons by a single grain boundary* within the wire. The quantum theory with $R = 0.12$ provides a fair representation of the resistivity measured at temperatures between 5 K and 300 K on a 63 nm thick Cu film whose grains exhibit an average diameter of $d = 10.5$ nm. The other parameters controlling the increase in resistivity are: (i) The rms roughness amplitude and the length of lateral correlation which characterize the surface roughness limiting the wires, and (ii) The average grain size d and the standard deviation s which describe the positional disorder of grain boundaries within the wire.

A distinct feature of the quantum theory, is that it predicts the relative growth in resistivity arising from electron-grain boundary scattering that gives rise to weak Anderson localization, when the average grain diameter d is appreciably shorter than the mean free path in a massive bulk sample. In the process of measuring the resistivity of the Cu film reported in this work, we also measured the transverse magnetoresistance as well as the Hall voltage at 5 K on a family of Cu films some 65 nm thick made out of grains where d varies from some 10 nm to about 35 nm. *We found a negative magnetoresistance for films where* $d < 20$ nm *and a positive magnetioresistance in samples where* $d > 20$ nm. These results seem remarkable, fort *a negative magnetoresistance is considered the 'fingerprint' of weak electron localization* [29]. Details of these experiments will be published elsewhere [30].

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