Scaling Laws for the Resistivity Increase of sub-100 nm Interconnects

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***Abstract*— A physically based model is used to describe the resistivity increase of sub-100 nm copper interconnect structures. The main factors determining the increase are additional scattering of electrons at the surface as well as at the grain boundaries of the conductor. The model has been applied to several sets of experimental data. The parameters of the model, each of them with physical meaning, are appropriate to fit the model to the experimental data very well. A compact model for the surface contribution of the model has been derived capturing the essentials in a simple, analytical expression.**

Keywords- interconnects; resistivity; size-effect; scaling; grain boundary

I. INTRODUCTION

In the last years interconnects have been investigated experimentally and theoretically due to their impact on the RC delay that seriously limits signal propagation in integrated circuits. It has been shown recently that the specific resistance of interconnects increases significantly when the lateral dimensions of the lines (width and height) are scaled to the sub-100 nm regime [1-3]. For example the conductivity of electroplated copper rises from 1.8 μΩ cm for wide lines embedded in SiO_2 to 4.6 μΩ cm for 45 nm wide lines [4]. This finding is in contrast to the common expectation that the specific resistance of metals is constant independent of line width. The physical reasons for this size effect are well known in principle: The size effect manifests itself due to the scattering processes of the conduction electrons at the external interfaces (surface) and at the internal interfaces (grain boundaries) of the line. The first mechanism has been described by Sondheimer [5], the latter by Mayadas and Shatzkes [6]. Both mechanisms come into play, when the lateral dimension of the wire is scaled to the mean free path (about 50 nm for copper at room temperature). However, for practical application the surface scattering model has to be modified because the approximations made for the geometry of the wire (circular cross-section) are generally not precise enough. In this paper both scattering models will be combined and adapted to the specific geometry of sub-100 nm copper interconnects described elsewhere [7]. The parameters of the combined scattering model include besides the geometrical dimensions the mean free path and the resistivity of the bulk material, the reflectivity of the surface, the reflection coefficient of the grain boundaries and the average distance of the grain boundaries.

II. METHODOLOGY

A. Surface Scattering (Integral expression)

An integral expression for the resistivity increase due to surface scattering is derived and solved numerically. For wires with rectangular cross-section we utilize the Fuchs-Sondheimer-model (FS) and follow the approach of Chambers based on kinetic-theory arguments [8]. The main idea is that the mean free path of a conducting electron in a thin wire has to be modified because the electron has a finite probability to reach the surface and encounter scattering there. The fraction of diffusely scattered electrons is determined by the specularity parameter p which takes values between 0 and 1. As a result the effective mean free path of a specific electron is reduced depending on the position of the cross-section and on the direction. Therefore the surface scattering contribution of the resistivity is calculated (see Fig. 1) by integration over all directions and all positions of the cross-section. The

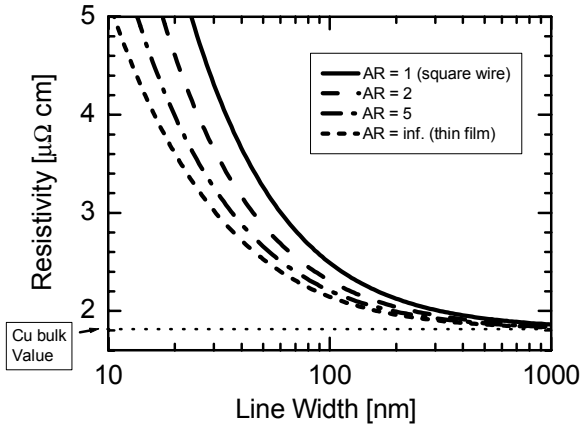

Figure 1. Surface scattering contribution to the resistivity of thin copper wires with different aspect ratio. 100% diffuse scattering and a temperature of 300 K is assumed.

following integral expression is obtained for pure diffuse scattering (p=0), where w is the width of the wire, h is the height, l is the mean free path of electrons in the bulk material, and ρ_0 the bulk resistivity:

$$\left(\frac{\rho_0}{\rho}(l)\right)_{p=0} = 1 - \frac{6}{4\pi h\, w}\int_0^w dx \int_0^h dy \int_{-\arctan(y/x)}^{\arctan((h-y)/x)} d\phi \int_0^\pi d\theta \sin\theta \cos^2\phi \left[1 - \exp\left(\frac{-x}{l \sin\theta \cos\phi}\right)\right] - \quad (1)$$
$$- \frac{6}{4\pi h\, w}\int_0^w dx \int_0^h dy \int_{-\arctan(x/(h-y))}^{\arctan((w-x)/(h-y))} d\phi \int_0^\pi d\theta \sin\theta \cos^2\phi \left[1 - \exp\left(\frac{-(h-y)}{l \sin\theta \cos\phi}\right)\right]$$

For $p>0$ the resistivity is determined by a series expansion:

$$\left(\frac{\rho_0}{\rho}(l)\right)_p = (1-p)^2 \sum_{k=1}^{\infty} \left\{ k\, p^{k-1} \left(\frac{\rho_0}{\rho}(l/k)\right)_{p=0} \right\} \quad (2)$$

The solution is exact in the framework of the FS model and does not rely on approximations for the limiting cases of very small or very large width compared to the mean free path. This approach is necessary because the width of the investigated wires is in the range of the mean free path.

B. Surface Scattering (Compact Model)

It is argued that models of this kind should be incorporated in future EDA tools that extract parasitic elements from the layout of ULSI circuits in order to determine the resistance more precisely. Analytical expressions for the size effect model are desired because the numerical calculation of the surface contribution is cumbersome. Therefore, a compact model is given for the surface dependent contribution and compared to the size effect model. It has the form

$$\rho = \rho_0 \left(1 + C\,(1-p)\,\frac{U}{S}\,l\right), \quad (3)$$

where ρ_0 is the resistivity of the bulk material, C a constant, U the perimeter and S the area of the cross-section of the line, l the mean free path. In Fig. 2 the compact model is compared to the surface model for a copper wire with rectangular cross-section. 100% diffuse scattering is assumed. The deviations are small for line widths ranging from 10 nm to 1000 nm.

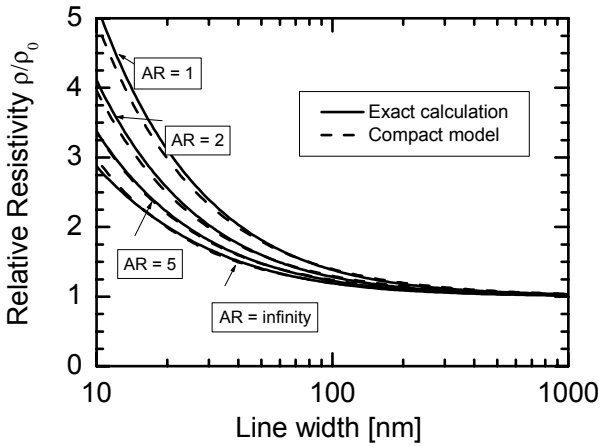

Figure 2. Comparison of the exact calculation of the surface contribution to the compact model (p=0). The constant C of the compact model is 1.2 in this case.

C. Grain Boundary Scattering

The microstructure of metallic interconnects is generally not monocrystalline. The wires consist of microcrystallites (so-called grains) separated from each other by grain boundaries. These grain boundaries act as scattering centers for the conducting electrons. In order to model this phenomenon the theory of Mayades and Shatzkes has been applied [6]. They extended the FS model by including internal surfaces (i.e. grain boundaries) of the conductor. Similar to the surface scattering model the mean free path of an electron is decreased by the existence of additional scattering centers assumed to be statistically distributed in the conductor. When an electron passes a grain boundary it has to overcome a potential barrier. The probability for the electron to be reflected at the barrier depending on the height and thickness of the barrier is denoted by the reflection coefficient R. These electrons do not contribute to the electrical current. From this theory the grain boundary component of the resistivity is

$$\frac{\rho_0}{\rho} = 3\left[\frac{1}{3} - \frac{\alpha}{2} + \alpha^2 - \alpha^3 \ln\left(1 + \frac{1}{\alpha}\right)\right] \text{ with } \quad \alpha = \frac{l}{d}\frac{R}{1-R} \quad (4).$$

The average distance of the grain boundaries is denoted by d. Obviously the resistivity increase is very sensitive to the reflection coefficient (see Fig. 3).

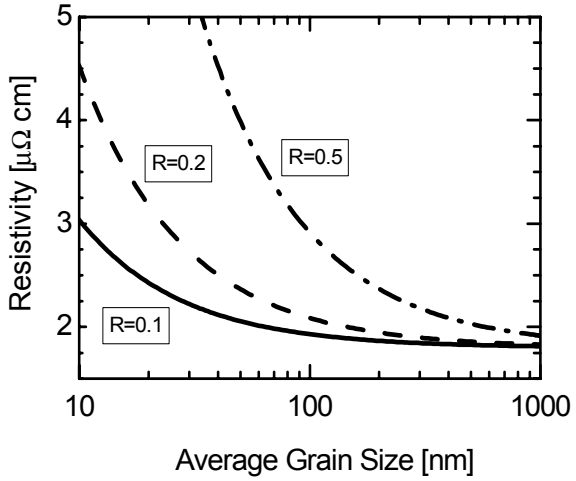

Figure 3. Resistivity increase for thin copper wires due to scattering at grain boundaries. R is the reflection coefficient: It denotes the fraction of diffuse scattering at the grain boundaries.

D. Combined Model

For comparison with experimental data the surface scattering model (FS model) has been combined with the grain boundary model (MS model) by adding the resistivities. This is in accordance with Matthiessen's rule stating that the total resistivity is described by a combined relaxation time

$$\frac{1}{\tau} = \frac{1}{\tau_{FS}} + \frac{1}{\tau_{MS}} + \frac{1}{\tau_{bg}}, \qquad (5)$$

where τ_{bg} corresponds to the background scattering of the electrons.

Combining the surface scattering part with the grain boundary part of the resistivity an easy-to-use model for the size-dependent resistivity increase of interconnects is at hand:

$$\rho = \rho_0 \left(\frac{1}{3} \Big/ \left[\frac{1}{3} - \frac{\alpha}{2} + \alpha^2 - \alpha^3 \ln\left(1 + \frac{1}{\alpha}\right) \right] + C\,(1-p)\,\frac{U}{S}\,l \right), \qquad (6)$$

where C is 1.2 and α defined in (4). It may be applied to copper interconnects with rectangular cross-sections and also to other metals besides copper after calibration with experimental data.

III. Results and Discussion

A. Data Set 1

The model has been applied to different sets of resistivity data of copper interconnects in the sub-50 nm range. Electrical measurements of copper wires embedded in a SiO_2 damascene structure have been performed in our group [4]. The resistivity has been extracted from the resistance data set 1 using SEM and TEM measurements for the heights and widths. The widths of the wires ranged from 40 nm to 800 nm whereas the height was constant at 230 nm. The resistivity was observed to rise from 2.45 μΩ cm for the widest wires to 4.6 μΩ cm for the narrowest wires. This increase could not be modelled by surface scattering. Even for an extreme choice of parameters assuming 100% diffusive scattering at the boundary and a bulk resistance for copper of 2.45 μΩ cm the predictions of the FS model have been more than 50% too low. In consequence the combined model was employed to describe the data.

From SEM and TEM images information of the grain structure has been collected [9]. The copper grains extend usually over the whole width of the wire and are limited in size by the height of the wire. The assumption was made that the grain boundary distance is equal to either the width or the height depending on what was the smaller one. With this input the combined model has been evaluated and fitted to the experimental data (see Fig. 4). The agreement with the experimental data is excellent. The parameter set for the best fit was: reflectivity coefficient at grain boundary R=0.50, bulk resistivity ρ_0=1.9 μΩ cm (corresponds to mean free path 40 nm), specularity parameter at external surface p=0.6.

The value of the bulk resistivity is close to that of electroplated copper for larger wires (1.8 μΩ cm [10]). That means that the background scattering due to defects is just merely increased for the investigated copper wires. For the wider wires the significant resistivity increase related to the bulk resistivity ρ_0 of 30% is mainly due to grain boundary scattering.

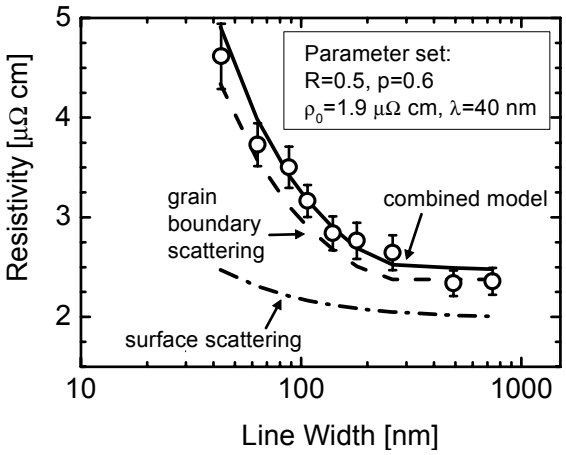

Figure 4. Contributions of the surface scattering effect and grain boundary scattering to the total resistivity. A sum of both terms yields an excellent fit to the experimental data.

The value for the reflectivity at grain boundaries lies in the range of values found in the literature. Mayadas et al. [6] reported for bulk copper R=0.24, Kuan et al. [1] for 50 nm PVD deposited copper films R=0.3, and Ramaswamy et al. [11] for 100 nm CVD deposited copper films R=0.65-0.8. A very large reflectivity of R=0.9 has been published by Durkan et al. [3] for gold wires ranging in thickness between 20 and 60 nm. The enlarged R value in this work compared to the bulk value is interpreted as an enhanced potential barrier between grain boundaries due to eventually existing defects at the grain boundaries.

B. Data Sets 2 and 3

To assess the quality of the model the parameters have been fitted to two more datasets. They differ from the first set by processing conditions and by geometry: the height for dataset 2 is 125 nm, that for dataset 3 is 50 nm [12]. The resistivity was extracted from temperature dependent resistance measurements combined with SEM measurements of the height. With this method the line width can be calculated and must not be determined directly [13]. The result is shown in Fig. 5. The agreement for dataset 2 is very good, for dataset 3 the functional trend is captured qualitatively. All model parameters have been kept constant besides the specularity p. It has been decreased from p=0.6 to p=0.4 for both sets 2 and 3. That means that increased scattering at the surface of the wire is assumed. A plausible explanation is an enhanced surface roughness of the lines from set 2 and 3. It is about a factor of 3 larger compared to set 1 according to TEM measurements. In all datasets the grain boundary part dominates over the surface scattering part. This indicates that the surface scattering contribution to the resistivity increase is significantly smaller than the grain boundary contribution.

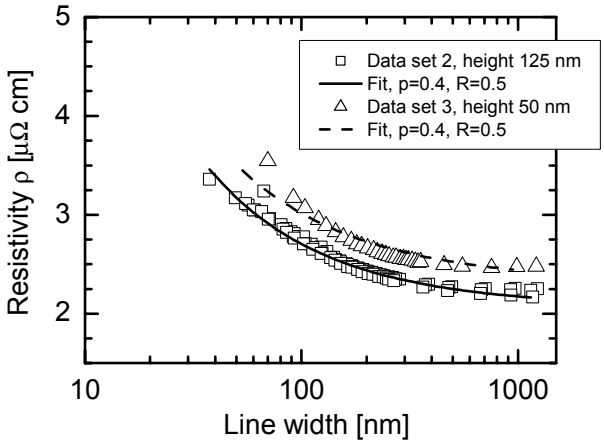

Figure 5. Comparison of the combined model to data set 2 and 3. The sets differ in the height of the wire: 125 nm for set 2 and 50 nm for set 3.

C. Temperature Dependent Data

For the dataset 1 the investigation was also extended to several temperatures covering the range from 4.2 K to 573 K without introducing new parameters, i.e. the scattering parameters of surface and grain boundaries were not changed. For the bulk parameters of copper including the mean free path and the resistivity the well-known temperature dependence according to the Bloch-Grüneisen theory was taken from the literature [14]. Again, good agreement with experimental data was achieved (see Fig. 6). This result shows that the resistance contribution due to the surfaces and the grain boundaries is not dependent on temperature. In other words the size-dependent contribution to the resistance is analogous to that of defects or impurities in a metal. Therefore it cannot be reduced by cooling the interconnect structure to cryogenic temperatures.

IV. SUMMARY AND CONCLUSION

It has been shown that the description of size-dependent resistivity data with the conventional Fuchs-Sondheimer model is not sufficient because it does not take into account the scattering contribution acting at the grain boundaries of a metallic wire. The Mayadas-Shatzkes model offers a natural extension to obtain a more complete description of the data. Both models have been joined using Matthiessen's rule to a physically based scattering model. Furthermore a plausible calibration of the model was feasible and excellent fits to several sets of experimental data have been obtained. The rather cumbersome integral expression for the surface contribution of the model was approximated by an analytical expression and a simple, easy-to-use equation has been derived. Especially for the demands of VLSI design a precise knowledge of the electrical properties of interconnects is undispensable. The phenomena discussed above are certain to be encountered in the manufacturing of integrated circuits in the near future for the technology node 50 nm and beyond.

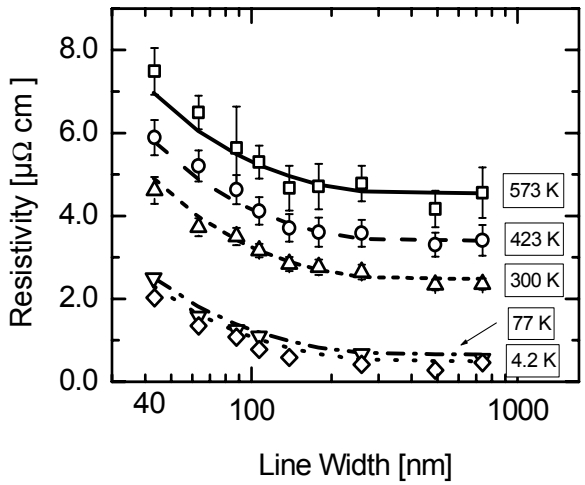

Figure 6. Temperature dependence of the electrical resistivity of copper interconnects. (Symbols: experimental data, lines: calculations with the combined model)

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