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Size-dependent resistivity of metallic wires in the mesoscopic range

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As the lateral dimension of conductors approaches the mesoscopic regime, deviations of electric resistivity from that of bulk material are observed. Size effects come into play as the lateral dimension of the wire is in the range of the mean free path of the conduction electrons and below. In order to probe the size effects in systems confined in both lateral dimensions copper wires with widths ranging from 40 to 800 nm were prepared in a SiO_2 matrix. The resistance of the wires was measured in the temperature range from 77 to 573 K. A size-dependent increase of the resistivity was found for decreasing wire widths. For the narrowest wires the resistivity is a factor of 2.6 higher than the copper bulk value (1.75 $\mu\Omega$ cm). The experimental data was compared to theoretical predictions over the whole investigated range of size and temperature using a semiclassical model. The model includes diffusive scattering of the conduction electrons at the surface and the grain boundaries of the wire. Very good agreement of theory with experimental data was found. In this way a coherent picture of the size dependent resistivity has been obtained.

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I. INTRODUCTION

The electrical resistivity of metallic conductors is increased compared to the bulk resistivity if the diameter of the wire is in the range of or smaller than the mean free path of the electrons (about 40 nm for copper at room temperature). Investigations of this size effect date back to 1938, when Fuchs derived an expression for the resistivity of thin films.[1] Later the theory was extended to include thin wires [Fuchs-Sondheimer[2] (FS) model]. Both authors based their work on the semiclassical concept of the relaxation time τ, where dt/τ is the probability that an electron experiences a collision during the infinitesimal time interval dt. They accounted for the size effects by including scattering at the external surfaces of the film or wire. It was assumed that the electrons will be specularly reflected at the surface or scattered diffusively depending on an empirical specularity parameter p. Later, Mayadas and Shatzkes (MS) observed that electron scattering at grain boundaries also increases the electrical resistivity of a thin film (MS model[3]). For the scattering probability at the grain boundary they introduced a further parameter that can also be understood as an empirical specularity parameter. Both models have been extensively tested against experimental data for thin films.[4,5] Furthermore efforts have been made to develop quantum mechanical descriptions of the empirical parameters of the MS model[6] and to include quantum effects from the surface scattering going beyond the FS model.[7] However for thin wires ($\leqslant$100 nm) little experimental data exist for Cu and Au.[8,9] These investigations were limited to room temperature and to a small range of lateral dimensions (20 to 50 nm). In order to assess the validity of the FS and MS models for conductors confined in two dimensions a much more extensive data base is necessary.

Copper has been chosen as a model system due to its technological applications. In this work extensive resistivity data for 40 to 800 nm wide copper wires will be presented covering the temperature range from 77 to 573 K. The method used to prepare the copper wires has been described elsewhere.[10] The electrical data will be analyzed within the framework of the FS and MS models. Information on the microstructure of the copper lines is extracted using transmission electron microscopy (TEM) and correlated with the parameters used in the MS model.

II. EXPERIMENTAL

The copper wires were prepared in a SiO_2 layer deposited on a (100)-oriented silicon substrate. 230 nm deep trenches were etched in a SiO_2 layer using 248 nm ultraviolet lithography in combination with a silicon hard mask narrowed by a spacer (for full details see Ref. 10). Using this approach a reduction of the line width below the limits of the lithography has been achieved. The resulting trenches were lined with a tantalum adhesion layer and a copper seed layer used for subsequently electrochemically filling with copper. The excess copper was polished back and the resulting wires were finally covered with an insulating passivation layer. In this way 40 to 800 nm wide, 230 nm high, and 200 μm long copper line structures have been obtained.

The microstructure of the copper wires has been analyzed with TEM (see Fig. 1). To a good approximation the cross

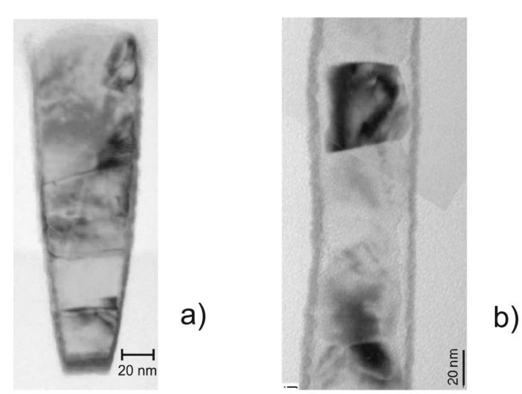

FIG. 1. TEM micrograph of a sub 50 nm trench filled with copper: (a) cross section, (b) top view.

section of the wire is trapezoidal. The size of the copper grains is evidently limited by the width of the trench. In the direction along the trench the typical distance of two grain boundaries is also about the same as the line width. This observation has important consequences for the resistivity. From the TEM micrographs the thickness of the Ta layer has been extracted and the fraction of Ta content has been estimated. It ranges from 5% for the 40 nm trenches to 10% for the 800 nm trenches. The resistivity of Ta is at least an order of magnitude higher than that of copper.

The resistance of the wires has been measured with a commercial probe system using a probe current of 10 μA to avoid heating of the wire. This is at least a factor of 1000 larger than the probe current required for burn out. Typical resistances were 1 kΩ for the narrowest wires with lengths of 200 μm. The resistivity of the conductor was calculated from the resistance and the known geometry of the wires.

III. MODEL

A. Fuchs-Sondheimer model

In order to compare the FS model with experimental data typically an approximate formula for wires with circular or quadratic cross sections is used:[2]

$$\frac{\rho}{\rho_0}=1+\frac{3}{4}(1-p)\frac{l}{d}, \tag{1}$$

where ρ_0 is the resistivity of the bulk material, p the fraction of electrons scattered specularly at the surface, d the width of the wire, and l the mean free path of the bulk material. For our data the requirements of this approximation are not fulfilled. First, it is not valid for the range $d/l\approx 1$, as is the case for our data. Secondly the aspect ratio (ratio of height to width) of the cross sections varies from 5 to 1 and is generally not square. Chambers derived an integral expression for the resistivity of wires with rectangular cross sections based on kinetic-theory arguments:[11]

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

Here h,w denote the height and the width of the wire, respectively. Completely diffusive scattering is assumed at the surface. This expression has been used to evaluate the resistivity of rectangular wires with different aspect ratios (see Fig. 2). The deviations from the results of Eq. (1) are significant. In real systems there exists a nonvanishing fraction of specular scattering events at the surface, denoted p. The resistivity is determined by a series expansion:[11]

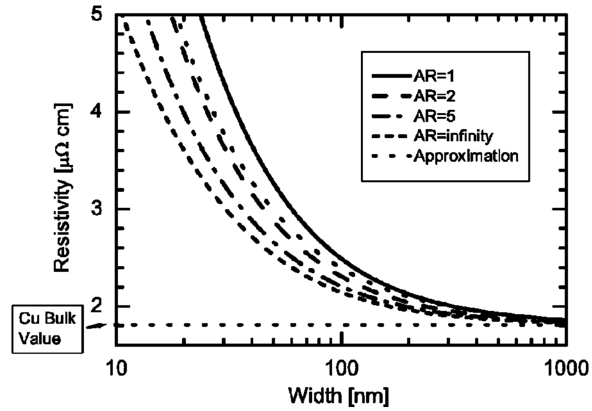

FIG. 2. Calculated resistivity of rectangular copper wires with different aspect ratios of the cross-section (AR) using Eq. (2). 100% diffuse scattering at the surface of the wire and a temperature of 300 K is assumed. For illustration the approximation for square wires is also included [Eq. (1)].

$$\left(\frac{\rho_0}{\rho}\right)_{p,l}=(1-p)^2\sum_{k=1}^{\infty}\left\{kp^{k-1}\left(\frac{\rho_0}{\rho}\right)_{p=0,l/k}\right\}. \tag{3}$$

This solution is exact in the framework of the FS theory and does not rely on approximate equations for the limiting cases of very small or very large widths compared to the mean free path.

B. Mayadas-Shatzkes model

In order to model the scattering at grain boundaries the theory of Mayadas and Shatzkes has been applied.[3] They extended the FS model by including *internal* surfaces of the conductor as scattering sources. In a way similar to the FS model the mean free path of an electron is decreased by the existence of additional scattering sites assumed to be statistically distributed in the conductor. The fraction of electrons that are not scattered by the potential barrier at a grain boundary is described by a reflectivity coefficient R. From this theory the grain boundary component of the resistivity is given by

$$\frac{\rho_0}{\rho}=3\left[\frac{1}{3}-\frac{\alpha}{2}+\alpha^2-\alpha^3\ln\left(1+\frac{1}{\alpha}\right)\right],$$

$$\alpha=\frac{l}{d}\frac{R}{1-R}, \tag{4}$$

where l denotes the mean free path of the bulk material and d the average distance of grain boundaries.

C. Combination of the FS and MS models

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

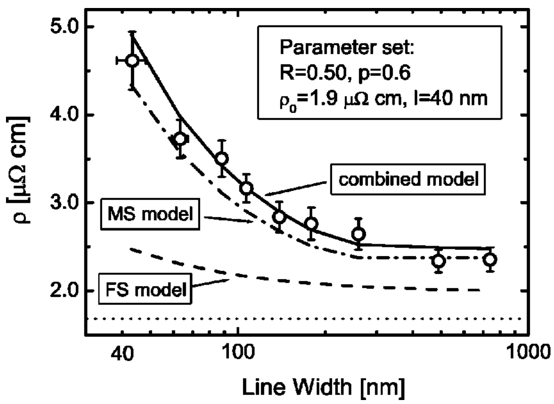

FIG. 3. The experimental resistivity of thin copper wires at room temperature (circular symbols) compared with the Cu bulk value (Ref. 12) (dotted line), the combined model (solid line), MS model (dash-dot line), and FS model (dashed line).

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

where τ_{bg} corresponds to the background scattering of the electrons by phonons, electrons and defects. Although deviations from Matthiessen's rule are expected in the presence of grain boundary scattering this assumption will be used to estimate the relative importance of surface scattering versus grain boundary scattering.

IV. RESULTS AND DISCUSSION

In Fig. 3 the experimental data for the resistivity of thin copper wires (not corrected for Ta content) are shown for room temperature. Typically ten measurements from different structures have been collected for each point. The resistivity was observed to rise from 2.45 $\mu\Omega$ cm for the widest wires to 4.6 $\mu\Omega$ cm for the narrowest wires whereas the resistivity of bulk copper is 1.75 $\mu\Omega$ cm. This increase could not be modeled by surface scattering alone (FS-model). Even for an extreme choice of specularity parameter $p=0$ (100% diffusive scattering at the surface) and bulk resistivity $\rho_0=2.45$ $\mu\Omega$ cm the prediction of the FS model is more than 50% too low. As a consequence scattering at grain boundaries has to be included. The width of the copper grains usually extends over the whole lateral dimension of the wire whereas the height of the grains is limited in size by the vertical dimension (see Fig. 1). As a result the average distance between grain boundaries was taken to be the smallest dimension of the wire. The best fit of the combined model to the experimental data is shown in Fig. 3 with the parameters $\rho_0=1.90$ $\mu\Omega$ cm (corresponds to a mean free path of 40 nm), $p=0.6$, and $R=0.50$. The agreement with the experimental data is excellent.

The value of the bulk resistivity, corrected for the 10% Ta content in the wire of 1.80 $\mu\Omega$ cm (see Sec. II) is remarkably close to the bulk value of copper (1.75 $\mu\Omega$ cm). That means that background scattering due to defects within the grains in the wires is not significant. For the wider wires the comparatively large value of 2.45 $\mu\Omega$ cm (30% increase over the bulk resistivity ρ_0) is mainly due to grain boundary scattering.

The fraction of specular reflection at the wire surface $p=0.6$ is quite large. This indicates that the surface scattering contribution to the resistivity increase is considerably smaller than the grain boundary contribution. However, the surface roughness would also affect the specularity parameter. In the presented model this scattering source cannot be separated from diffuse scattering.

The value of $R=0.50$ for reflectivity at grain boundaries lies within the range of values found in the literature. Mayadas *et al.*[3] reported $R=0.24$ for bulk copper, Kuan *et al.*[8] $R=0.3$ for 50 nm PVD (physical vapor deposition) deposited copper films, and Ramaswamy *et al.*[13] $R=0.65-0.80$ for 100 nm CVD (chemical vapor deposition) copper films. A very large reflectivity of $R=0.9$ has been published by Durkan *et al.*[9] for gold wires ranging in thickness between 20 and 60 nm. The larger R value in our work compared to the bulk value is interpreted as an enhanced potential barrier between grain boundaries possibly due to defects at the grain boundaries.

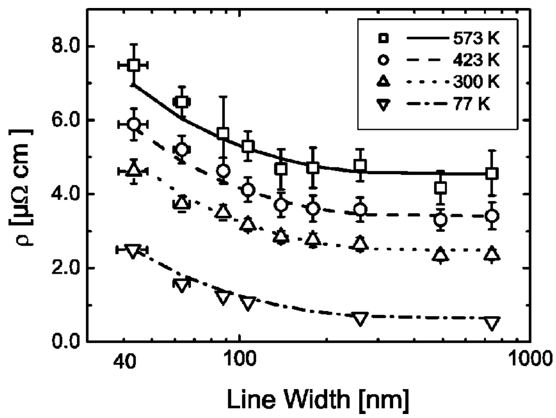

FIG. 4. Temperature dependence of the electrical resistivity for thin copper wires. (Symbols: experimental data, lines: calculations with the combined FS and MS models).

The temperature dependent resistivity results are shown in Fig. 4 for the range from 77 to 573 K. As expected the resistivity increases for increasing temperature. The temperature-dependent parameters have to be modified for comparison with the model. For the investigated range of temperature it is a plausible assumption that the scattering parameters related to the surface and to the grain boundary do not change whereas the resistivity due to background scattering shows the behavior known from bulk data. Temperature-dependent modifications of the diffuse surface scattering induced by electron-electron interaction have been neglected.[14] We used tabulated values for the resistivity of bulk copper (see Table I) and assumed that the product of resistivity and mean free path does not depend on temperature and again obtained very good agreement between the calculated resistivity and the experimental data. There is no indication of a further temperature-dependent scattering mechanism. The temperature dependence of the resistivity was included in the combined model without introducing a further parameter.

TABLE I. Temperature dependent resistivity of bulk copper.

Temperature [K]	77	300	423	573
Resistivity [$\mu\Omega$ cm]	0.2[a]	1.9	2.83[b]	3.97[b]
Mean free path [nm]	330[a]	40	26.5[b]	19[b]

[a]From Ref. 12.

[b]Determined from the linear relation $\rho/\rho_0 = 1 + \alpha(T - T_0)$ with $\alpha = 4.0\times 10^{-3}$ and ρ_0 room-temperature value.

V. CONCLUSIONS

The resistivity increase for copper wires in the 50 nm range is determined by geometrical and structural properties. As the lateral dimension of the wire approaches the mesoscopic range a size-dependent electrical resistivity has been observed. In addition to nonspecular scattering at the surface of the wire, scattering of conduction electrons at grain boundaries is the dominant source of the resistivity increase. The surface scattering is intimately connected with the geometrical dimensions of the wire. It becomes important when the width of the wire is comparable or smaller than the mean free path of the conduction electrons. On the other hand, the critical scale for grain boundary scattering is the average grain size along the direction of the electrical current. The existence of grain boundaries is not limited to copper. These considerations apply generally for the charge transport in metallic conductors. It is left to the object of further investigations to change the density of grain boundaries in mesoscopic wires by modifying the deposition and patterning process. As a result the effect of grain boundary scattering could be reduced even for wires narrower than the mean free path of the conduction electrons. The question arises whether thin wires of metals other than Cu show a different microstructure and how the microstructure influences their resistivity.

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