The Resistivity Bottleneck: The Search for New Interconnect Metals

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ABSTRACT

The resistivity increase of Cu interconnects with decreasing line width is a major challenge for the continued downscaling of integrated circuits. Various approaches can be employed to mitigate this resistivity bottleneck including (a) facilitating specular interface scattering by using an insulating lattice-matched liner, (b) increasing the grain size or the grain boundary transmission through Fermi surface matching, and (c) choosing a metal with a low product of the bulk resistivity times the bulk electron mean free path. Electron transport measurements on epitaxial metal layers in combination with first-principles simulations are used to quantify the resistivity scaling for a series of metals including Cu, W, Ru, Mo, Co, Rh, and Ir, and to provide insight into the interface structure and chemistry requirements that lead to specular electron scattering and therefore a low resistivity for narrow interconnects.

INTRODUCTION

Electron scattering at surfaces and grain boundaries causes the resistivity of 10-nm-wide Cu interconnect lines to be approximately an order of magnitude larger than that of bulk Cu [1]. This motivates diverse research efforts to reduce diffuse scattering at the Cu-liner interface [2-4] and electron reflection at Cu grain boundaries [5-8], but also the search for conductors which may replace Cu as interconnect material at small dimensions [9]. The evaluation of Cu replacement options is challenging because (i) the resistivity size effect is due to both surface and grain boundary scattering which depend on a myriad of parameters including interface roughness [10-13], orientation [14], and chemistry [2,15,16], and grain boundary density [17,18], structure [5] and orientation distribution [6,8,19], and (ii) the widely used classical models fail in predicting the resistivity increase for narrow metal lines [19,20]. A more detailed summary of the work presented here can be found in the recent perspectives article in [21].

ELECTRON SURFACE SCATTERING

Electron scattering at the interface between the conducting metal and the liner layer is one of the primary reasons for the interconnect resistivity increase with decreasing line width. Classical models use a phenomenological specular parameter to distinguish between diffuse and specular surface scattering [22]. Specular scattering is desired, because it causes no increase in the line resistance.

Specular scattering requires that the metal-liner interface is atomically smooth because electrons have a typical Fermi-wavelength on the order of 1 Å such that even atomic scale roughness results in diffuse surface scattering and a corresponding resistivity increase [23]. This requirement is only important over short lateral length scales over which the electron wave is coherent, yielding mostly specular electron scattering at atomically smooth terraces even in the presence of some roughness [3,24]. On the contrary, regular atomic-level roughness disturbs the flat potential step at the conductor-liner interface and leads to diffuse electron scattering [12]. This effect is similar to the reported deposition of Ta or Ti adatoms or the adsorption of oxygen on an atomically smooth Cu surface, which disturbs the flat surface potential to cause effectively a roughening of the conducting Cu and a transition from specular to diffuse surface scattering [2-4,15].

The second requirement for specular scattering at the metal-liner interface is a negligible localized density of states at the Fermi level such that electrons cannot scatter into states where their momentum is randomized, which effectively corresponds to diffuse scattering. This requires insulating liners with a negligible interface density of states, as has been demonstrated experimentally using in situ transport measurements during oxidation of epitaxial Cu(001) layers which show a considerably larger conductivity if coated with monolayers of Al2O3 or TiO than if coated with metallic Al or Ti [4,25].

GRAIN BOUNDARY SCATTERING

Electron scattering at grain boundaries contributes to the resistivity size effect. This is because the grain size in microscopic conductors typically scales with the conductor size, such that narrow wires have small grains and correspondingly a large grain boundary density that leads to considerable electron scattering. There are two general approaches to suppress the resistivity contribution from grain boundary scattering: Scattering becomes negligible if grains are large in comparison to the bulk electron mean free path or the line width. More specifically, if the average grain size is > 200 nm or larger than 10× the line width (for lines with d < 20 nm) then the resistivity contribution from grain boundary scattering is expected to be < 10% [21]. Alternatively, grain boundary scattering becomes negligible if the boundaries exhibit small electron reflection coefficients. This requires low-energy boundaries which may be facilitated by annealing sequences or boundary doping [5] and electronic state matching which is facilitated by spherical Fermi surfaces and/or grain alignment (texturing) or high-symmetry boundaries [21].

RESISTIVITY SCALING: METALS COMPARISON

The classical expression for the resistivity size effect predicts that the resistivity contributions from electron scattering at external surfaces and grain boundaries are proportional to the product of the bulk resistivity times the bulk electron mean free path $\rho_o \times \lambda$. Therefore, in the limiting case of thin wires and/or small grain sizes, the wire resistivity becomes proportional to $\rho_o \times \lambda$ for any given fixed wire dimension and grain size distribution. Thus, the metal with the lowest product $\rho_o \times \lambda$ is expected to exhibit the highest conductivity in the limit of a small wire width [26].

The product $\rho_o \times \lambda$ is independent of temperature and electron scattering at impurities and crystalline defects and can be directly calculated with numerical methods from the Fermi surface without the need to account for any electron-phonon interactions. Therefore, such calculations provide a direct ranking of metals which are promising for narrow high-conductivity lines, as shown in Table I [26]. Experimental verification is done by measuring the resistivity $\rho$ as a function of film thickness and fitting the data with the classical
transport models. This is done most effectively using epitaxial layers, because in that case grain boundary scattering can be neglected, which reduces the number of free fitting parameters [14,24,27-35]. This is illustrated in Fig. 1. The experimentally determined $\rho_o \times \lambda$ products are also included in Table I. Comparison of the two columns indicates considerable deviations between predictions and experiments, which can be attributed to the breakdown of the classical models at small length scales [23] as well as experimental variations in crystalline quality and surface scattering specularity. Based on the presented data, Ir is the most promising elemental metal for narrow interconnect lines. For a more detailed discussion see [21].

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<table>
<thead>
<tr>
<th>$\rho_o \times \lambda$ ($10^{16}$ $\Omega$ m$^2$)</th>
<th>Theory</th>
<th>Experiment</th>
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<tbody>
<tr>
<td>Rh</td>
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</tr>
<tr>
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<tr>
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<tr>
<td>Cu</td>
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<td>6.6</td>
</tr>
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</table>

Table I: Product of bulk resistivity $\rho_o$ times mean free path $\lambda$ determined from theory and experiment.

Figure 1: Measured resistivity $\rho$ vs thickness $d$ of epitaxial metal layers [21].

REFERENCES