ELECTRON SCATTERING AT COPPER SURFACES

by

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ABSTRACT

As interconnects are scaled to smaller dimensions, the resistivity of the copper lines increases above the bulk resistivity due to a phenomena known as the size effect. Three components are known to contribute to the size effect: surface roughness, grain boundary scattering, and surface scattering. Of these, surface roughness and grain boundary scattering have been researched previously, and methods to minimize the resistivity increase due to these mechanisms have been proposed. The focus of this thesis research was to address the issue of surface scattering, which is the least understood component of the size effect. In particular, little is known about the materials and surface structure which lead to completely specular scattering (i.e. no increase in resistivity for thin layers).

This research has built on the reported observation of partial specular scattering in both gold and silver films. The most promising layers have been shown to be single crystals. These single crystal films have the added advantage of simplifying the resistivity characterization, as there is no grain boundary component to the resistivity. Thus, particular focus was spent on determining the growth conditions required to produce high quality single crystal copper layers. Epitaxial copper layers were grown on single crystal magnesium oxide substrates with $(001)_{Cu}||(001)_{MgO}$ with $[001]_{Cu}||[001]_{MgO}$ for samples grown at a substrate temperature T_s of 100 °C or less. The lattice mismatch between copper and MgO is 14.29%, which is resolved by 7×7 copper unit cells occupying 6×6 MgO cells. The highest crystalline quality was found for those layers grown at T_s = 100 °C, while the layers grown at T_s = 40 °C demonstrated the smoothest surface and lowest buried interface roughness.

Surface morphology was studied through the use of *in-situ* scanning tunneling microscopy (STM). From these characterizations, the epitaxial copper surfaces have a self-affine surface structure, with a scaling exponent α of 0.82±0.03, independent of annealing. The mound width increased from 31±8 to 39±6 nm for increasing layer thickness, *d*, of 24 and 120 nm, respectively. The heights of the as-deposited mounds were nearly constant, independent of film thickness. *In-situ* annealing at T_a = 200 and 300 °C results in thermodynamically driven mass transport that minimized the surface step density. This resulted in mounds with a larger mound radius and smaller root mean

square roughness σ. The effect was most pronounced on the thinnest layer, d = 24 nm, with the mound radius increasing from 31±8 to 70±20 nm, and σ decreasing from 1.3±0.1 to 0.74±0.08 nm, for the as-deposited and 300 °C annealed layers, respectively. Thus annealing resulted in a reduction in the mound aspect ratio when compared to the as-deposited layers. In the best case, terrace widths were increased from 1.5 to 6.3 nm, for the 24-nm-thick as-deposited and 300 °C annealed layer, respectively. These terrace widths correspond to terraces which consist of 6 to 25 atoms per step. Further annealing at higher temperatures resulted in rough, partially discontinuous layers, attributed to oxidation of the copper-substrate interface as well as thermodynamically driven copper islanding in order to reduce the interfacial area between the copper and magnesium oxide.

Electron transport experiments have shown that resistivity is highly dependent on the crystalline quality of the copper layers. Single crystal copper layers have resistivities that are a minimum of four times smaller than the polycrystalline layers, which is due to the absence of grain boundaries, which act as additional scattering centers. As-deposited copper layers resulted in completely diffuse scattering, which was attributed to the short length scales of atomically smooth terraces. Annealing resulted in layers which were smoother, but all layers exhibited completely diffuse surface scattering with a specularity parameter of p = 0. Low temperature and *in-situ* electron transport measurements were used in order to determine whether oxidation or surface smoothness is the key constraint to specular scattering. Both experiments show that specular scattering is highly dependent on the atomic level surface perfection, as sheet resistance measurements increased by 10% for copper layers after they were exposed to air or to deposition of a partial monolayer of tantalum, corresponding to R_s values of 0.197-0.216 to 0.214-0.234 Ω/□, respectively. This increase is unexpected, as conduction should still occur through the copper layer, which has not changed. Thus, the presence of tantalum and/or oxygen causes in an atomic level disturbance in the surface perfection. This disruption results in a switch from partial specular scattering at the top surface to diffuse surface scattering.