Electron Scattering at Surfaces of Epitaxial Metal Layers

by

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Abstract

In the field of electron transport in metal films and wires, the ‘size effect’ refers to the increase in the resistivity of the films and wires as their critical dimensions (thickness of film, width and height of wires) approach or become less than the electron mean free path λ, which is, for example, 39 nm for bulk copper at room temperature. This size-effect is currently of great concern to the semiconductor industry because the continued downscaling of feature sizes has already lead to Cu interconnect wires in this size effect regime, with a reported 2.5 times higher resistivity for 40 nm wide Cu wires than for bulk Cu. Silver is a possible alternate material for interconnect wires and titanium nitride is proposed as a gate metal in novel field-effect-transistors. Therefore, it is important to develop an understanding of how the growth, the surface morphology, and the microstructure of ultrathin (few nanometers) Cu, Ag and TiN layers affect their electrical properties. This dissertation aims to advance the scientific knowledge of electron scattering at surfaces (external surfaces and grain boundaries), that are, the primary reasons for the size-effect in metal conductors.

The effect of surface and grain boundary scattering on the resistivity of Cu thin films and nanowires is separately quantified using (i) *in situ* transport measurements on single-crystal, atomically smooth Cu(001) layers, (ii) textured polycrystalline Cu(111) layers and patterned wires with independently varying grain size, thickness and line width, and (iii) *in situ* grown interfaces including Cu-Ta, Cu-MgO, Cu-vacuum and Cu-oxygen. In addition, the electron surface scattering is also measured *in situ* for single-crystal Ag(001), (111) twinned epitaxial Ag(001), and single-crystal TiN(001) layers.

Cu(001), Ag(001), and TiN(001) layers with a minimum continuous thickness of 4, 3.5 and 1.8 nm, respectively, are grown by ultra-high vacuum magnetron sputter deposition on MgO(001) substrates with and without thin epitaxial TiN(001) wetting layers and are studied for structure, crystalline quality, surface morphology, density and composition by a combination of x-ray diffraction θ-2θ scans, ω-rocking curves, pole figures, reciprocal space mapping, Rutherford backscattering, x-ray reflectometry and transmission electron microscopy. The TiN(001) surface suppresses Cu and Ag dewetting, yielding lower defect density, no twinning, and smaller surface roughness than if grown on MgO(001). Textured polycrystalline Cu(111) layers 25-50-nm-thick are deposited on a stack of 7.5-nm-Ta on SiO_2/Si(001), and subsequent *in situ* annealing at 350 ^{o}C followed by sputter etching in Ar plasma yields Cu layers with independently variable thickness and grain size. Cu nanowires, 75 to 350 nm wide, are fabricated from Cu layers with different average grain size using a subtractive patterning process.

In situ electron transport measurements at room temperature in vacuum and at 77 K in liquid nitrogen for single-crystal Cu and Ag layers is consistent with the Fuchs-Sondheimer (FS) model and indicates specular scattering at the metal-vacuum boundary with an average specularity parameter $p = 0.8$ and 0.6, respectively. In contrast, layers measured *ex situ* show diffuse surface scattering due to sub-monolayer oxidation. Also, addition of Ta atoms on Cu(001) surface perturbs the smooth interface potential and results in completely diffuse scattering at the Cu-Ta interface, and in turn, a higher resistivity of single-crystal Cu layers. *In situ* exposure of Cu(001) layers to O_2 between 10^{-3} and 10^{5} Pa-s results in a sequential increase, decrease and increase of the electrical resistance which is attributed to specular surface scattering for clean Cu(001) and for surfaces with a complete adsorbed monolayer, but diffuse scattering at partial coverage and after chemical oxidation. Electron transport measurements for polycrystalline Cu layers and wires show a 10-15% and 7-9% decrease in resistivity, respectively, when increasing the average lateral grain size by a factor of 1.8. The maximum resistivity decrease that can be achieved by increasing the grain size of polycrystalline Cu layers with an average grain size approximately ~2.5× the layer thickness is 20-26%.