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Title: The effect of electron scattering from disordered grain boundaries on the resistivity of metallic nanostructures

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Highlights

We calculate the electrical resistivity of a metallic specimen, under the combined effects of electron scattering by impurities, grain boundaries, and rough surfaces limiting the film, using a quantum theory based upon the Kubo formalism. Grain boundaries are represented by a one-dimensional periodic array of Dirac delta functions separated by a distance “d” giving rise to a Kronig-Penney (KP) potential. We use the Green’s function built from the wave functions that are solutions of this KP potential; disorder is included by incorporating into the theory the probability that an electron is transmitted through several successive grain boundaries. We apply this new theory to analyze the resistivity of samples S1, S2, S7 and S8 measured between 4 K and 300 K reported in *Appl. Surf. Science* **273**, 315 (2013). Although both the classical and the quantum theories predict a resistivity that agrees with experimental data to within a few percent or better, the phenomena giving rise to the increase of resistivity over the bulk are remarkably different. Classically, each grain boundary contributes to the electrical resistance by reflecting a certain fraction of the incoming electrons. In the quantum description, there are states (in the allowed KP bands) that transmit electrons unhindered, without reflections, while the electrons in the forbidden KP bands are localized. A distinctive feature of the quantum theory is that it provides a description of the temperature dependence of the resistivity where the contribution to the resistivity originating on electron-grain boundary scattering can be identified by a certain unique grain boundary reflectivity R , and the resistivity arising from electron-impurity scattering can be identified by a certain unique ℓ_{IMP} mean free path attributable to impurity scattering. This is in contrast to the classical theory of Mayadas and Shatzkes (MS), that does not discriminate properly between a resistivity arising from electron-grain boundary scattering and that arising from electron-impurity scattering, for MS theory does not allow parameters (ℓ_{IMP} , R) to be uniquely adjusted to describe the temperature dependence of the resistivity data. The same data can be described using different sets of (R , ℓ_{IMP}); the latter parameter can be varied by 2 orders of magnitude in the case of small grained samples $d < \ell$, and by a factor of 4 in the case of samples made out of large grains $d > \ell$ (where ℓ is the bulk mean free path). For samples $d > \ell$, *the increase of resistivity is attributed not to electrons being partially reflected by the grain boundaries, but to a decrease in the number of states at the Fermi sphere that are allowed bands of the KP potential; hence the reflectivity required by the quantum model turns out to be an order of magnitude smaller than that required by the classical MS theory.* For samples $d < \ell$, *the resistivity increase originates mainly from Anderson localization induced by electron grain*

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