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Electrical Resisitivity in Metals and Metallic Alloys from First Principles ALEXANDER SLEPKO, The University of Texas at Austin; Intel Corporation, Santa Clara, California, USA, SADASIVAN SHANKAR, JUSTIN WEBER, Intel Corporation, Santa Clara, California, USA, ALEXANDER DEMKOV, The University of Texas at Austin — We have developed a method for estimation of resistivity of metals and their alloys based on ab initio methods. The formalism is based on quantifying electron phonon interactions using Boltzmann-based electronic transport and plane wave-based density functional theory for electronic structure and phonon frequencies. We explicitly take into account long wave length scattering, energy band dispersion and interaction between impurities, often omitted in previous approaches. Given the detailed nature of our formalism, we will explain deviations from the most-used Matthiessen's Rule. We have tested our technique on Al, Cu, and Al-doping in Copper. Our resisitivity values compare very well with experimental data at room temperature; Al 2.75 $\mu\Omega$ cm (experimental, 2.83 $\mu\Omega$ cm), Cu 1.81 $\mu\Omega$ cm (experimental, 1.66 $\mu\Omega$ cm). We were also able to estimate the drops in conductivity of Cu due to alloying with Al for a wide range of composition (from dilute to concentrated alloys) which are consistent with the experiments. Given the general nature of our formalism, we believe that it is extendable to nanostructures.

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