

Resistivity of Pd: *s*- and *d*-contributions from *ab initio* calculations and Wannier formalism

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The scattering mechanism in transition metals, proposed by Mott, is known as *s-d* scattering [1]. Such scattering, primarily mediated by phonons, dominates electrical resistivity in transition metals. Understanding electronic transitions between *s*- and *d*- states is relevant for modeling ultrafast laser irradiation in thin metallic films [2]. Allen’s method [3] for first-principles transport properties calculations is applicable for a wide range of solid metals. Notably, it captures the anomalous nonlinear temperature dependence of resistivity in Pd at high temperatures by properly accounting for Fermi smearing. It was suggested [4] that the ρ_{ss} (initial and final states in scattering are both of *s*-type) contribution in Pd can be approximated by the resistivity of Ag—the nearest non-transition metal for Pd. In this work, we focus on evaluating of the aforementioned electronic contributions to the total resistivity in Pd using Allen’s method as implemented in our SKiES code [5] with support for *ab initio* calculations and Wannier interpolation. The results for electrical resistivity as well as for electron-phonon linewidth of Pd are demonstrated.

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