Ab initio calculations for the transport properties of metals within Boltzmann transport theory: From a one- to two-temperature representation

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The paper presents a new approach for ab initio calculations of the electron transport properties of solid metals in the two-temperature approximation with account for electron-phonon interaction. Using the method to solve the Boltzmann transport equation proposed by Allen [*Phys. Rev. B* **17**, 3725 (1978)], formulas were obtained for calculating the electrical resistivity (dc conductivity) and thermal conductivity of metals at different electron and lattice temperatures. The presented approach also works well in the one-temperature case. It performs most effectively if it is necessary to allow for the smearing of the electron distribution function and the energy dependence of the electron–phonon spectral function. Four metals—Cu, Ag, Au and Pd—are considered as an example. The obtained results are in good agreement with the available experimental data. Thus, in the one-temperature case, it was possible to reproduce with good accuracy the increase in the thermal conductivity of palladium at temperatures above 300 K. The results obtained for the two-temperature regime of heating, reproduce quite well the temporal evolution of the dc electrical conductivity of gold, observed in experiments [*Nat. Commun.* **12**, 1638 (2021)] for the interaction of thin gold foils with ultrashort laser pulses.