Calculation of the transport properties of metals under non-equilibrium heating

Smirnov N A[@] and Ovechkin A A

Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk 456770, Russia

[@] deldavis@mail.ru

The work studies the transport properties of three noble metals–Ir, Pt and Au–under non-equilibrium heating when the electron temperature T_e is higher than the ionic temperature T_i, and their density corresponds to that of their solid state. The static conductivity σ and the thermal conductivity κ were calculated by two methods. At relatively low electron temperatures (form room temperature to a few eV), we used an approach based on solving the Boltzmann equation [1] and the FP-LMTO method of band structure calculation from first principles [2]. At higher temperatures, we used an average atom model implemented in the RESEOS code [3]. Here we calculated σ and κ from Ziman formula and the Wiedemann-Franz law and the relaxation time approximation too [4]. Results of calculation with the two approaches are compared and shown to agree quite satisfactory at T_e above 1 eV.

[1] Smirnov N A 2022 *Phys. Rev. B* **106** 024109
[2] Savrasov S Y 1996 *Phys. Rev. B* **54** 16470
[3] Ovechkin A A, Loboda P A, Novikov V G, Grushin A S and Solomyannaya A D 2014 *High Energy Density Phys.* **13** 20
[4] Ovechkin A A, Loboda P A and Falkov A L 2016 *High Energy Density Phys.* **20** 38