Investigation of the influence of ab initio simulation parameters on results of the transport and optical properties calculations using the Kubo–Greenwood formula and the Kramers–Kronig transform

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We calculate the electronic transport and optical properties of metals (Zr, Pb, Fe). Our calculations are based on the the first-principle method of quantum molecular dynamics (QMD) simulation, density functional theory and the Kubo–Greenwood (KG) formula [1]. The VASP package is used for QMD simulation. Then we find conductivity by the KG formula, it allows us to calculate other optical and transport properties (normal emissivity, reflectivity and refraction index). We investigate the simulation parameters (type of the pseudopotential, spin-orbital interaction, size of system, Kramers–Kronig transform parameters) influence on the results of our calculations.

This work has been supported by the Russian Science Foundation (grant No. 20-42-04421).

[1] Knyazev D V and Levashov P R 2013 *Comput. Mater. Sci.* **79** 817–829