Ab initio calculations of transport and optical properties of Zr in the vicinity of melting

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Zirconium and its alloys are widelly applied in nuclear reactors as a cladding for nuclear fuels because of its excellent resistance to corrosion, high melting temperature and a low neutron-capture cross-section.

In this work static and dynamic electrical conductivity for solid and liquid zirconium were calculated in the range of temperatures 300–3000 K. The calculation is based on the the first-principle method of quantum molecular dynamics (QMD) simulation, density functional theory and the Kubo–Greenwood formula [1]. The VASP package is used for QMD simulation. Then, using Kramers–Kronig transform, optical properties (normal emissivity, reflectivity and refraction index) are also calculated.

Calculations were perfomed with different technical parameters (total number of atoms in the QMD cell, **k**-points grid size, type of pseudopotentials) in order to show the convergence of the results.

Comparison with the experimental data is presented.

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[1] Knyazev D V and Levashov P R 2013 *Computational Materials Science* **79** 817–829