Ab initio calculations of conductivity and optical properties of metals in the vicinity of the critical point: Zr and Pb as examples

Fokin V B[1,2,@]**, Minakov D V**[1,2]**, Paramonov M A**[1,2] **and Levashov P R**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] Vladimir.Fokin@phystech.edu

Zirconium and Lead are the metals which has a lot of application in the nuclear industry.

We calculated transport and optical properties of these metals in the vicinity of the critical point for the first time. The behavior of the metals in the region of the phase diagram corresponding to the expanded heated matter was simulated by the first-principles method of the quantum molecular dynamics (using the VASP package). To calculate the dynamical electrical conductivity the Kubo–Greenwood formula [1] was used. After the calculation of electrical conductivity, the optical properties (normal spectral emissivity, reflectivity, refractive index) were reconstructed using the Kramers–Kronig transform [2].

A comparison of the electrical resistivity and the normal spectral emissivity of Zr and Pb to the experimental data is presented [3].

[1] Knyazev D V and Levashov P R 2013 *Computational Materials Science* **79** 817–829
[2] Fokin V B, Minakov D V and Levashov P R 2023 *Symmetry* **15** 48
[3] Paramonov M A, Minakov D V, Fokin V B, Knyazev D V, Demyanov G S and Levashov P R 2022 *Journal of Applied Physics* **132** 065102