Ab initio calculations of Ni and Fe resistivity and optical properties

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Iron and nickel are the widely used construction materials both in everyday life and in industry. Since these metals are ferromagnetic, their behavior and properties are differ from other common metals. The resistivity and optical properties of Fe and Ni in the temperature range up to 10 kK have been 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]. The effect of the spin polarization and various exchange-correlation functionals influence to the calculated properties of ferromagnetic metals is tested.

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[1] Knyazev D V and Levashov P R 2013 *Comput. Mater. Sci.* **79** 817–829
[2] Fokin V B, Minakov D V and Levashov P R 2023 *Symmetry* **15** 48