

# Thermodynamic, transport and optical properties of nickel in the vicinity of melting from *ab initio* calculations and pulse heating experiment

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Nickel is a heat-resistant metal and an important component of various alloys. It determines the use of nickel as a structural material in products exposed to intensive thermal and mechanical loads. So, it is of great importance to obtain reliable data both on equation of state of nickel and its transport and optical properties.

In this work, the properties of nickel in the vicinity of melting are found independently from quantum molecular dynamics calculations and from pulse heating experiment. We pay special attention to accounting for spin polarization in the part devoted to *ab initio* calculations. Comparison with several experiments is presented, including new data obtained in the experimental group of our team. We discovered that spin-polarized calculations for liquid nickel provide better agreement between calculated and measured thermodynamic properties.

The electrical resistivity of solid and liquid nickel near melting and its normal spectral emissivity are also considered. These calculations are based on Kubo-Greenwood formula combined with Kramers-Kronig transform.

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