Research of high-temperature thermophysical properties of iron by first-principle calculations

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Iron, crucial in various industries, demands a comprehensive understanding of its thermodynamic properties for an accurate equation of state. Current analysis reveals insufficient, inconsistent data on the thermal expansion curve, especially in the liquid phase. The pulsed heating method, important for obtaining liquid metal thermophysical properties, faces challenges due to inaccurate sample expansion determination, resulting in significant resistivity data scatter in the liquid state.

To obtain the physical properties of materials in the temperature range where experimental data are difficult to reproduce, or the experiment is completely impossible, today a different approach is actively used—carrying out first-principles (ab initio) calculations based on the method of quantum molecular dynamics (QMD), which does not require any additional empirical information.

The purpose of this work is to obtain data on the thermal expansion curve of iron, its resistivity and normal spectral emissivity in the vicinity of melting from ab initio calculations. In addition, the temperature dependence of enthalpy was restored from calculations and experiments on pulsed heating. The critical parameters of iron were also assessed using QMD data.

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