Investigation of the thermophysical properties of liquid iron by an ab initio molecular dynamics

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Iron is an important constructive material for nuclear power. In this regard, accurate knowledge of the parameters at which the phase transition occurs has a special meaning. However, the properties of liquid iron at low densities under static conditions were measured only in a limited range of temperatures and densities. On the other hand, the results of high-temperature measurements in dynamic experiments by different authors are in contradiction with each other. In addition, there is an uncertainty in the slope of the thermal expansion curve and the estimate of the critical temperature, which varies from 4.8 to 12 kK. Quantum molecular dynamics (QMD) is nowadays widely used for calculation of thermophysical properties of condensed matter. Since it relies only upon fundamental physical constants, therefore, it can be considered as a reference method for the analysis of available experimental data and obtaining new data for areas unavailable in the experiment.

The purpose of this work is to study the thermodynamic properties of iron in the vicinity of the boundary of the two-phase liquid–gas region using the QMD method. The selection of optimal parameters for subsequent modeling, QMD calculations of a detailed grid of isotherms and isochores for the liquid phase, an estimate of the near-zero isobar and critical parameters of iron are carried out. Available corresponding experimental data are also analyzed and discussed.

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