EQUATION OF STATE FOR LIQUID AND GASEOUS IRON AT HIGH PRESSURES AND TEMPERATURES

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The functional relationship of thermodynamic parameters that determines the properties of a substance is called the equation of state [1, 2]. This equation closes the system of equations expressing the laws of conservation of mass, momentum and energy, which makes it possible to carry out hydrodynamic modeling of processes in a wide region of the phase diagram. This work is devoted to the description of the thermodynamic properties of iron within the framework of the equation of state for its liquid and gas phases. The model is considered in the form of dependence of specific free energy on specific volume and temperature. The contributions of the elastic part, which describes the behavior of the substance at zero absolute temperature, and the thermal components of the electron and ionic subsystems are taken into account. The cold (elastic) part is given by a three-term dependence, which provides the possibility of a combined description of the speed of sound under normal conditions and the specific heat of evaporation. The thermal contribution of heavy particles is given on the basis of the quasi-harmonic approximation; the chosen form of the dependence of this contribution allows one to describe the shock-wave data and the specific entropy of evaporation. The thermal contribution of electrons is given in the simplest form of a degenerate electron gas.

Based on the developed equation of state, the boundary of the iron evaporation region, the temperature dependence of the density in the process of isobaric expansion of the liquid phase, and the thermodynamic characteristics of the metal in shock-wave processes were calculated. The calculation results are compared with the available data from the corresponding experiments, on the basis of which the applicability range of the obtained thermodynamic function is established. The resulting equation of state can be used for numerical modeling of high-intensity processes in liquid and gaseous iron.

References

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