The Changes of Thermophysical Properties of Iron under Isothermal Compression

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Coming from the pair potential of interatomic interaction in the Mie–Lennard-Jones form, and the Einstein's model of crystal, without of the fitting parameters the state equation and the baric dependencies of thermophysical properties are received for BCC iron. The calculations were executed along two isotherms: 300 and 1500 K, for pressure from zero till 8000 kbar, i.e. for the relative volume from 1 up to 0.5. The good coincidences with experimental data are received. The graphs of baric dependencies for the next thermophysical properties are calculated: for the Debye temperature, for the first, second and third Gruneisen parameters, for the isothermal compression modulus and for its derivative with respect to pressure, for the isochoric heat capacity and for its derivative with respect to pressure, for the coefficient of thermal expansion and for its derivative with respect to pressure, for the isobaric heat capacity, for the specific (per unit area) surface energy and for its derivative with respect to pressure. It was shown that for ultrastrong compression the next regularities are carried out: the dependencies from pressure for the Debye temperature and for the second Gruneisen parameter tend to maximum, the dependencies from pressure for the first and for the third Gruneisen parameters go to zero, the dependencies from pressure for the isothermal compression modulus and for the specific surface energy are changing by a linear manner, the dependency of the coefficient of thermal expansion from pressure tend to constant value.