Wide-range calculation of equations of state for Mo, Ti, Nb, and Re using quantum-statistical approach

Kadatskiy M A[1,2,@] **and Khishchenko K V**[1,3,4]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny 141701, Russia
[3] South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia
[4] Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka 142432, Russia

[@] makkad@yandex.ru

The quantum-statistical approach is commonly used for constructing the equation of state for matter in a wide range of temperatures and densities. In this approach, lattice models of an average atom are of particular interest for describing substances in states with high energy densities. These models are using the self-consistent field approximation and are relatively simple to implement. One previously developed model of the average atom is the Hartree–Fock–Slater (HFS) model, which is widely used for simple substances at densities close to normal ones and relatively high temperatures. Previous implementations of this model led to discontinuities in thermodynamic functions associated with the transition of electron states between the discrete and continuous spectrum, or required the introduction of an additional free parameter to define the values of the energy boundary of electron states belonging to the continuous spectrum in a specific region of input thermodynamic parameters. In this work, a variant of the HFS model, for which no additional free parameters are required in the thermodynamics calculation over a wide range of temperatures and densities, and the resulting thermodynamic functions remain continuous, is presented. The study includes calculations of Hugoniots of Mo, Ti, Nb and Re using the HFS model for pressure ranges from 1 to 10^7 GPa, and a comparison of the results with available experimental data.