The thermodynamically consistent model of ionic and electronic subsystems within the average-atom framework

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In the routine approach to constructing a complete thermodynamic model of an electron–ion system within the average-atom framework, the electronic subsystem is described using thermodynamically consistent quantum-statistical models, while the ionic subsystem is typically treated within simpler approximations [1]. It is commonly assumed that the ionic contribution to the total thermodynamic functions is small compared to the electronic one, and therefore possible thermodynamic inconsistency in the ionic part does not significantly affect the final equation of state.
However, investigations of these models in parameter regimes characteristic of shock-compression experiments demonstrate that the ionic contribution can become comparable to the electronic one [2]. In the present work, an approach to constructing a thermodynamically consistent model of the ionic subsystem within the average-atom framework based upon the one-component plasma approximation [3] is investigated. An explicit expression is used for the ionic free energy as a function of the effective ion charge obtained from the Thomas–Fermi model, or the Thomas–Fermi model with corrections, or the Hartree–Fock–Slater model [1] for electronic subsystem.
This work is financially supported by the Russian Science Foundation (grant No. 25-19-00944, https://rscf.ru/project/25-19-00944/).

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