Investigation of the high-temperature properties of uranium in liquid and near-critical states from the first principles

Paramonov M A[1,2,@], Minakov D V[1,2] and Levashov P R[1,2]

[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

[@] mikhail-paramon@mail.ru

Reliable data on the thermophysical properties of uranium in the vicinity of the boundary of the two-phase liquid-gas region are necessary for the analysis of the nuclear safety of nuclear reactors. There are three areas of critical point estimation, corresponding to different estimation methods: by heat of vaporization, by plasma properties, and by extrapolation of thermal expansion data. However, these regions of the uranium phase diagram are inaccessible for precise experimental study due to high temperatures and high pressures.
Thus, it seems that at present the only available theoretical approach that can provide information of the thermophysical properties of a substance in the region of a hot expanded liquid is the first-principle method of quantum molecular dynamics (QMD) based on the electron density functional theory.
The purpose of this work is to study the thermodynamic properties of uranium in the vicinity of the boundary of the two-phase liquid-gas region using the QMD method. The study of influence of relativistic effects on the thermodynamic properties, QMD calculations of a detailed grid of isotherms and isochores for the liquid phase, an estimate of the critical parameters, critical isobar and specific enthalpy of uranium are carried out. Available corresponding experimental data are also analyzed and discussed.
Calculations were carried out in the Joint Institute for High Temperatures RAS under financial support of the Russian Science Foundation (Grant No. 20-79-10398).