ESTIMATION OF CRITICAL PARAMETERS OF REFRACTORY METALS BASED UPON FIRST–PRINCIPLE SIMULATION

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Critical points of the majority of metals are currently unknown. An experimental measurement of critical parameters of metals is very difficult to carry out owing to extremely high temperatures (higher than 3000 K) and pressures (from kilobars to tens of kilobar). A theoretical calculation of near-critical metallic fluid causes significant difficulties because of the degeneration of the electronic subsystem and strong interaction. Only model estimations exist having a particularly big scatter for refractory metals [1]. Meanwhile, the position of the binodal and critical point on a phase diagram of metals is necessary to know for the creation of adequate equations of state at densities below normal. Moreover, in the near-critical region of metals interesting phenomena have been predicted, in particular, the metal–non-metal transition and the cluster formation.

Only pulsed experiments can give some information about the position of critical points, in particular, on isentropic [2] and isobaric [3] expansion. In experiments on isentropic expansion with porous samples it is possible to observe the evaporation of a metal under its expansion into different anvils. Isobaric expansion under the action of powerful current pulses allows one to investigate properties of matter near the liquid–vapor equilibrium curve. However, until recently there were no models able to consistently describe both these types of experiment, in particular, for tungsten and molybdenum. In this work we will present a review of approaches for a determination of critical parameters of refractory metals. Also we are going to discuss our results of quantum molecular dynamics simulation for the interpretation of experimental data and the estimation of critical parameters of tantalum, tungsten and molybdenum.

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