Strongly coupled plasma in refractory metals near the liquid-gas coexistence curve and critical point: first-principle study

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Dense metallic plasma is a complicated object for both theoretical and experimental study. Due to very high coupling and degeneracy parameters traditional chemical picture and perturbation approaches are of questionable applicability for such plasma. Strong correlation effects hamper the usage of average atom models. Expanded states of a liquid metal can be obtained in shock-wave experiments with porous samples. In this case a porous sample unloads into some obstacle after the shock-wave compression and the expansion velocity can be registered. Such experiments are quite complicated and rare. Another example is an isobaric expansion (IEX) of wires under heating by a powerful current pulse. IEX experiments are also sparse and contradictory. The challenge of the current work is to describe both isobaric and isentropic expansion experiments for a number of metals by one and the same theory. Also it is of importance to estimate the liquid-gas phase transition boundary and critical point. A very important question - a probable existence of metal-to-nonmetal transition predicted in liquid iron - is also discussed.

We use quantum molecular dynamics to calculate thermodynamic properties and electrical conductivity of expanded liquid aluminum, molybdenum, tungsten, iron and uranium. Various shock-compression experiments are reproduced for porous tungsten [1] and molybdenum as well as subsequent isentropic expansion. Special attention is paid to available isobaric expansion experimental data for theoretical estimations of critical points. We succeeded in reconciliation of several types of experiments for refractory metals. Thorough analysis of experimental data will be presented. A special Monte Carlo procedure is applied for the estimation of the liquid–gas coexistence curve and critical point parameters of tungsten and molybdenum. The result is close to an estimation obtained with Likalter's similarity relation. Also we apply a new criterion of mean ion charge estimation in strongly coupled plasmas. This work is supported by RSF grant No. 18-79-00346.

1. Minakov, D. V., Paramonov, M. A., & Levashov, P. R. Phys. Rev. B **97**, 024205 (2018).