The equation of state and transport properties of metal vapors in supercritical fluid regime

A.L. Khomkin, A.S. Shumikhin

Joint Institute for High Temperatures of RAS, Moscow, Russia

In this work, using the chemical model of the atomic plasma "3+" proposed in [1], we present a joint calculation of the equation of state and transport properties of supercritical fluid of metal vapors within the unified approach. It consists of free non-ideal electrons and ions and atoms immersed in jellium. Given the presence of jellium, we named this model the "3+" model. Jellium is constituted by tails of wave functions of bound electrons. Jellium provides the appearance of collective quantum energy—cohesion. Jellium does not change the balance and the electroneutrality equations. The main feature of jellium is its collectivity and the ability to conduct the current. The interaction between free charges is described in nearest neighbor approximation (NNA). We show that the corrections for the charge-charge interaction and interatomic interaction compensate each other by calculating the composition and the equation of state. The equation of state and electrical conductivity were calculated in supercritical regime and for binodal for various group of metals: alkali (Cs, Rb, Na), alkali earth (Be), transition (Cu, Fe, W etc.) and posttransition (Al, Pb etc.). The obtained results are compared with data of physical and numerical experiments [2-5]. Calculations in the framework of the "3+" model show a good agreement with both physical and numerical experiments. We calculated also the critical point parameters (density, temperature, pressure and electrical conductivity) for various groups of metals.

References

1. A.L. Khomkin, A.S. Shumikhin, J. Exp. Theor. Phys. **124**, 1001 (2017).

2. A.W. DeSilva, A.D. Rakhel, Contrib. Plasma Physics **45**, 236 (2005).

3. J. Clerouin, P. Noiret, V.N. Korobenko, A.D. Rakhel, Phys. Rev. B **78**, 224203 (2008).

4. F. Hensel, J. Phys.: Condens. Matter **2**, SA33 (1990).

5. D. Li et al, Sci. Rep. **4**, 5898 (2015).