Equation of state and transport properties of supercritical fluid of refractory metals

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In this work, we propose a generalized model to describe the thermodynamic and transport properties of supercritical fluid of metals, based on the "3+" model of plasma fluid proposed by us in [1, 2]. The Helmholtz free energy of dense atomic metal vapors describe the mixture 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 lying outside the Wigner–Seitz cell (WS). Jellium provides the appearance of collective quantum energy—cohesion. According to our hypothesis, the ion cores together with the jellium form a "gas-metal" state that exists at any density. The concentration of thermal electrons is determined by the Saha formula. The interaction between free charges is described in nearest neighbor approximation (NNA). The equation of state and electrical conductivity were calculated in supercritical fluid regime for refractory metals (Be, Ta, Mo, Zr) in wide range of densities and temperatures. The obtained results are compared with available data of numerical experiments [3, 4]. Calculations in the framework of the "3+" model show a good agreement with available data and describes the continuous transition from gas-plasma to metallic conductivity.

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[4] French M and Mattsson T R 2014 *Phys. Rev. B* **90** 165113