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P5.3009 The thermodynamic and transport properties of metals in warm dense matter regime

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In this work, using the chemical model of the atomic plasma "3+" proposed in [1], we present a joint calculation of the composition, equation of state and transport properties of metal vapors in warm dense matter regime within the unified approach 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. 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 warm dense matter regime for various group of metals: from low-melting posttransition (Al, Pb, Ga) to refractory metals (Be, Mo, Ta, W). 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

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