The dissociation and thermodynamics of dense fluid oxygen by self-consistent fluid variational theory

Q.F. CHEN, Y. ZHANG, L.C. CAI, Y.J. GU — The dissociation, pressure, internal energy, and entropy of dense fluid oxygen at high temperatures and densities have been calculated from the free-energy functions using the self-consistent fluid variational theory. The accurate high-pressure and high-temperature effective pair potentials are adopted to describe the intermolecular interactions, which are made to consider molecular dissociation. In this paper, we focused on a mixture of oxygen atoms and molecules and investigated the phenomenon of pressure dissociation at finite temperature. The single-shock Hugoniot derived from this equation of state agrees well with gas-gun experiments for pressure vs density. As density and pressure increase along the Hugoniot, the system appears to undergo a continuous transition from a molecular to a partially dissociated fluid containing a mixture of atoms and molecules. The equation of state and dissociation degree are predicted in the ranges of temperature of 5000-16 000 K and density of 0.1-4.5 g/cm$^3$. These data are formulated in the analytical form of dissociation degree-density-temperature and pressure-density-temperature equation of state.

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