

Short-range ordering in crystallized mixtures of atomic nuclei and phase diagram of C/O mixture

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Mixtures of bare atomic nuclei on a nearly uniform degenerate electron background are a realistic model of matter in the interior of white dwarfs. Despite tremendous progress in understanding their phase diagrams achieved mainly via first-principle simulations, structural, thermodynamic, and kinetic properties of such mixtures are poorly understood. We develop a semi-analytic model of the crystal state of binary mixtures based on the concept of mutual short-range ordering of ions of different sorts. We derive analytic formulas for electrostatic energy of crystal mixtures, including the effect of static ion displacements from the lattice nodes, and estimate their residual entropy. Then we perform free energy minimization with respect to the order parameters for a C/O mixture at all relevant compositions and temperatures. The resulting C/O phase diagram is in a reasonable agreement with that obtained in the most recent first-principle study. The equilibrium microstructure of a crystallized mixture is shown to evolve with decrease of temperature which, in principle, can induce structural transitions. The latter will be accompanied by thermal energy release. The proposed theory opens up a path to analyze ordering and construct phase diagrams of ternary mixtures, which are of great practical interest in astrophysics, as well as to improve calculations of electron-ion scattering rates and kinetic properties of dense crystallized matter.