A polydisperse hard spheres model for interatomic correlations in multicomponent metallic melts

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Since the ions behave as a classical liquid in metallic melts, the influence of different contributions of the interionic pair potential to the structure and properties of such systems is considered next way: it is now generally accepted that the structure of simple liquids, at least at high density, is largely determined by geometric factors associated with the packing of the particles caused by strong short-range interionic repulsion and, in contrast, the long-range attractive interactions may, in a first approximation, be regarded as giving rise to a uniform background potential, that provides the cohesive energy of the liquid, but has little effects on its structure formation. So, ion-ion repulsion in a liquid metal may be regarded as the principal factor determining the ionic arrangement and interionic correlations consequently.

Now we propose another way of constructing correlation functions (SF, PCF) of liquid metal using exact HS solutions of OZ, but PCF would keep its natural smoothness at short-range distances. So, in this work, we regard metallic melt as fluid in which the size of particles is characterized by some random HS diameter distributed by a continuous function, that may also be interpreted as a probability density function of sizes. The other properties (like mass, charge etc.) of particles are constant and associated to the geometric center of such particles. Such a model is based on presentation of metallic system as a polydisperse hard sphere mixture and real interatomic interactions are included implicitly and may be regarded as effective macroscopic forces, that transform HS fluid to soft-core one.

The ultimate results show us an increasing of the isothermal compressibility and decreasing of height of the first maximum of the SF of the model fluid vs. a simple HS approximation. Simultaneously we achieved the smooth PCF instead of a sharp one for HS.