THERMODYNAMIC CHARACTERISTICS OF MOLTEN SALTS CONSIDERING POLARIZATION EFFECTS

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The study of thermodynamic characteristics and phase equilibria in various systems is an important part of most of the studies related to materials science, since in considering particular properties of the material, it is first necessary to have information about the stability boundaries of each phase in the system. There are various theoretical approaches to solving this problem, based on ab initio methods, molecular modeling, thermodynamic modeling and their combination, while the statistical-thermodynamic theory applied to these problems is less developed.

One of the directions in this field is the study of thermodynamic properties and interphase boundaries in molten salts. Therefore, a theoretical description of the various effects observed in these systems is an important issue. This investigation is related to the study of the influence of polarization effects between ions on the thermodynamic properties and the melting process of halide melts of alkali metals. The difficulty here is that polarization effects always arise not only between neighboring particles, but also in subsequent coordination spheres. Therefore, to consider the polarization effects, it is necessary to introduce a dielectric constant.

In this report, we will present a simple statistical-thermodynamic model to take into account the polarization contribution to the pair potential of the ion interaction in a molten salt. Such a model is realized using thermodynamic perturbation theory, where the reference system is the potential of charged hard spheres. Thus, the weaker polarization effect of ions can be considered as a perturbation.

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