Functional Materials 10, No.4 (2003)

Effect of directional atomic interaction parameters on properties of melted halide compounds

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Received June 20, 2003

The role of a directional chemical bond in shaping make-up both properties of halides and their melts is parsed. Usage of parameters of a physico-chemical model of ionic melts with disordered bcc-similar structure for the assaying of change of physical and physico-chemical properties of halides and their melts has allowed to fix linkages with change properties of integral models parameters as semiempirical models. Usage of these models allows at a numerical level to forecast properties of melts of halides depending on their make-up.

Проанализирована роль направленной химической связи в формировании структуры и свойств галоидных соединений и их расплавов. Использование параметров физико-химической модели ионных расплавов с разупорядоченной ОЦК-подобной структурой для анализа изменения физико-химических свойств галоидных соединений и их расплавов позволило установить связи свойств с изменением интегральных модельных параметров в виде полуэмпирических моделей. Использование этих моделей позволяет на численном уровне прогнозировать свойства расплавов галоидных соединений в зависимости от их состава.

In connection with more and more wide use of halide compounds as scintillation materials, the interest to interpretation of the atomic interaction part in formation of properties of such compounds, mixtures, solutions, and melts thereof increases continuously [1, 2]. The simplified concepts of electron structure of those materials based on ionic model of chemical bond and valence theory impede considerably the development of fundamental investigations in this field of physical materials science. In this connection, authors of numerous works [3–5] establish with regret that most of researchers studying salt systems continue to consider interacting ions as rigid spherical particles, thus excluding their mutual polarizing effect that may cause unpredictable consequences.

The fact that such situation is kept up to date is associated with no efficient alternative has been proposed to concepts of the ionic model of halide compound structure.

The use of directional chemical bond model [6, 7] to analyze the atomic interaction part in formation of structure and properties of oxide compounds including non-equivalent crystallographic positions allowed to consider the complex of problems concerning the matter from a novel untraditional point of view [8]. In particular, it has been shown taking borate compounds as an example that the refuse of postulated integer charge values of boron, oxygen, and