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LiF-KF熔盐溶液局部结构的计算机模拟研究

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摘要 本文用Monte Carlo法对同离子系LiF-KF熔盐溶液的局部结构进行了计算机模拟,
介绍了计算方法和模型。计算了LiF, KF及Lif-KF混合前后正-正离子, 正-负离子, 负-负离子间位能变化,
各类离子的近邻离子排布规律,
以及各种形式离子团的组成比例。本文还讨论了在熔盐瞬时结构中存在的静电场的微区涨落。

关键词 计算 计算机模拟 氟化钾 氟化锂 熔盐 蒙特卡罗模拟 同离子系 位能

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Computerized simulation of local structure of molten LiF-KF solution by Monte Carlo method

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Abstract The local structure of LiF-KF solution (as a typical common-anion system) has been simulated by Monte Carlo method. The change of potential energy between anions, anions and cations as well as cations during the mixing between molten LiF and KF has been calculated The distribution regularity of neighbors of various ions and the content of ionic clusters of different types have been studied. By means of simulated model of the solution the fluctuation of electrostatic field in instantaneous local structure in the mixture has been discussed.

Key words CALCULATION COMPUTERIZED SIMULATION POTASSIUM FLUORIDE LITHIUM FLUORIDE FUSED SALTS MONTECARLO SIMULATIONS POTENTIAL ENERGY

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