熔融**ZnCl2**结构的分子动力学模拟研究

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摘要　熔融ZnCl2作为一种离子性共价性参半的典型熔盐,
其近邻结构在实验测量和分子动力学模拟方面均作过一些研究。本文依据新近EXAFS实验结果,
比较了不同的有效势下模拟得到的径向分布函数,
表明KDR势可作为一种实用势。并进一步在KDR势模拟产生的瞬态构型基础上,
使用键序参数方法研究了晶态和熔融态ZnCl2中的近邻结构。结果表明, 和晶态ZnCl2一样, 在熔融ZnCl2
中存在稳定的Zn/Cl正四面体结构, 但熔态和晶态Zn/Cl近邻结构热波方差σ不同。计算表明300K晶态σ=5.0℃,
613K熔融态σ=12.2℃。也对熔融ZnCl2的网络状结构和宏观输运性质进行了讨论。

关键词　晶体结构　氯化锌　径向分布函数　动力学模拟

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Molecular dynamics study on the structures of molten ZnCl2

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Abstract　The local structure of a typical molten salt ZnCl2, in which the chemical bonds can be viewed as half ionic and half covalent, has been studied by molecular dynamics simulations. Comparing with the recent EXAFS experimental results in the radial distribution functions simulated from different different effective potentials, we found that KDR potential is a useful one and able to give a more realistic representation of ZnCl2 melt. Based on the instantaneous configurations given by the simulations with KDR potential, the near-neighbor structures in the crystalline and molten states of ZnCl2 have been studied by using the bond-order-parameter method. The results indicates that there exist the same stable Zn-Cl tetrahedral structures in molten ZnCl2 as in crystalline state while the square deviations of thermal fluctuation σ of Zn-Cl units are different from each other. The calculations show $\sigma=5.0℃$ in crystalline, 300K and $\sigma=12.2℃$ in molten, 613K. In addition, the network-like structures and the transprot properties of molten ZnCl2 were discussed in this paper.

Key words　CRYSTAL STRUCTURE　ZINC CHLORIDE　RADIAL DISTRIBUTION FUNCTION

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