Molecular Dynamics Simulation of the Internal Mobilities in Molten (Dy$_{1/3}$, K)Cl

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Z. Naturforsch. 56a, 273–278 (2001); received January 22, 2001

Molecular dynamics simulations have been performed on molten (Dy$_{1/3}$, K)Cl at 1093 K in order to compare the calculated self-exchange velocity (SEV), self-diffusion coefficient (D) and electrical conductivity with the corresponding experimental results. It was found that SEV, $v_k$, and $D$ of potassium decrease with increasing concentration of dysprosium, as expected from the internal mobility, $b$. The decrease of $b_k$, $v_k$, and $D_k$ are ascribed to the tranquilization effect by Dy$^{3+}$ which strongly interacts with Cl$^-$. On the contrary, $b_{Dy}$, $v_{Dy}$, and $D_{Dy}$ increase with increasing concentration of Dy$^{3+}$. This may be attributed to the stronger association of Dy$^{3+}$ with Cl$^-$ due to the enhanced charge asymmetry of the two cations neighboring to the Cl$^-$. In addition, the sequence of the calculated SEV’s, D’s and electrical conductivities for the various compositions were consistent with those of the referred experimental results.

Key words: Electrical Conductivity; Internal Cation Mobility; Molten DyCl$_3$-KCl; Molecular Dynamics Simulation; Self-exchange Velocity; Self-diffusion Coefficient.