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

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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, 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.