A Molecular Dynamics Simulation of the Electric and Thermodynamic Properties in Molten ($Nd_{1/3}$, Na or K)Cl Mixtures

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Molecular dynamics simulations have been carried out on molten ($Nd_{1/3}$, K)Cl at 1065 and 1073 K and ($Nd_{1/3}$, Na)Cl at 1124 K for various compositions. The calculated self-exchange velocity (v), self-diffusion coefficient (D), electrical conductivity (κ) and enthalpy of mixing (ΔH_{mix}) were compared with the corresponding experimental values. The calculated results revealed that v and D of potassium decrease with increasing anmount of neodymium, as expected from the experimental internal mobility (b). The decrease of b_{K}, v_{K}, and D_{K} are attributed to the tranquilization effect by Nd^{3+} which strongly interacts with Cl^- as well as Dy^{3+}. On the contrary, b_{Nd}, v_{Nd}, and D_{Nd} increase with increasing concentration of Nd^{3+}. This might be ascribed to the stronger association of Nd^{3+} with Cl^- due to the enhanced charge asymmetry of the two cations neighboring Cl^-. In addition, the sequences of the calculated v's, D's and κ's for the various compositions were consistent with those of the known experimental results. The experimental enthalpy of mixing with its negative dependence on the cation size was qualitatively reproduced.

Key words: Electric Conductivity, Enthalpy of Mixing; Internal Mobility; Molten $NdCl_3$-Alkali Chloride; Molecular Dynamics Simulation; Self-exchange Velocity; Self-diffusion Coefficient.