# MOLECULAR DYNAMICS STUDY OF ISOTHERMAL COMPRESSIBILITY OF BINARY MOLTEN POTASSIUM HALIDES

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The calculation of the isothermal compressibility of binary molten potassium halides (KBr-KI, KCl-KI, KF-KI) in the entire concentration range at a temperature of 1200 K was carried out using the classical molecular dynamics simulation. The cubic cell, containing 3456 particles, was simulated in the NVT-ensemble under periodic boundary conditions. The interionic interactions used in this work were based on the simple Born-Mayer potentials derived by Fumi and Tosi. Long-range forces were calculated by the Ewald method. Experimental densities were used for the pure binary melts and the additivity of molar volumes was assumed for the mixtures. The simulations were typically $10^6$ steps in length, with a timestep of 4 fs.

The isothermal compressibility is calculable as the infinite wavelength limit of the static structure factor. The results from proposed model would assign the patterns of variation of the isothermal compressibility observed in the experiment as a function of the concentration. Namely, an increase in the positive deviations of the isothermal compressibility from additivity upon replacement of the anion of the second component in the Br-Cl-F series.

Analysis of the structural characteristics of the binary mixtures as a function of the concentration of the components demonstrates that the local environment of the potassium cation significantly changes in the KF-KI system upon addition of the fluoride ion. In the bulk of the binary molten mixture KF-KI, regions predominantly containing cation-anionic pairs corresponding to the pure salts are formed. In contrast, in the binary mixtures KBr-KI and KCl-KI, a natural change in the composition of the nearest cation-anionic environment is observed with the addition of the second component.