

# MELTING CHARACTERISTICS OF SODIUM HALIDES: A MOLECULAR DYNAMICS SIMULATION

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A theoretical study of the of melting and crystallization phase transitions characteristics in classical ionic systems was carried out using molecular dynamics. In order to trace the role of the Born-Mayer repulsion on temperature, entropy, and density jump during melting a primitive electrolyte model with charges of opposite sign and identical radii is considered. The main attention will be focused on the description of the characteristics of the melting and crystallization phase transitions as a function of the Born-Mayer pair potential parameters. The melting of crystal cell containing 512 particles is modeled with NPT ensemble with a timestep of 0.005 ps and the total number of steps  $4 * 10^6$ , which in our opinion is enough to achieve the equilibrium state of the system. The simulation results show that the pre-exponential factor of the Born repulsion influences only the density of the system under consideration, while the temperature of the phase transition remains constant. The decrease in the characteristic length of the pair potential leads to a decrease in the melting temperature of the model system. Estimations of the vacancies effect on the melting point on the example of sodium halides are carried out. The proposed theoretical approach to the description of the liquid-solid phase transition is applied to sodium halides. In particular, for sodium chloride, having an experimental melting point of 1074 K, it is shown that the simulated crystal overheats by about 50 K above the melting point. The calculated temperature and heat of fusion are 1112 K and 38.4 kJ / mol respectively, and the density jump was 0,44 g/cm<sup>3</sup>. The report will provide a comparison of the calculated and experimental melting characteristics for all sodium halides. The study was supported by the Russian Foundation for Basic Research, project no. 18-03-00606.