STRUCTURAL TRANSITION IN STRONGLY COUPLED COULOMB CLUSTERS

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The equilibrium states of Coulomb clusters containing up to 5000 particles at high values of the Coulomb coupling parameter Γ are studied by the molecular dynamics method. It is shown that at the number of particles exceeding 2000, a crystallized core with the dominant hcp structure appears in the Coulomb clusters, which melts at the value of Γ close to that characteristic of an infinite single-component plasma [1]. In general, a large cluster is a crystalline core surrounded by spherical shells, the number of which does not depend on the total number of particles, but depends on the coupling parameter. The high value of the structural transition threshold is explained by the proximity of the potential energies of the crystalline structure and the system of nested spherical shells. An expression for the compressibility factor of the system is obtained,

$$Z_c = 1 + \frac{\Gamma}{3}(u_p - 2u_b - 3N^{2/3}),$$

where u_p and u_b are the energy of interparticle interaction per particle and the energy of interaction of particles with the background, respectively. The particle compressibility factor, determined both by the force virial and by the energy, turns out to be close to zero in a wide range of particle numbers, which allows extrapolating this result to a classical single-component plasma. An explanation for this result is proposed based on the Wigner–Seitz cell model.

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1. Zhukhovitskii D. I., Perevoshchikov E. E. // Teplofiz. Vys. Temp. 2024. V. 62. No. 4. (in press).