Modeling the phase transition kinetics in lattice systems

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For considering the density evolution of a lattice fluid the non-equilibrium distribution in a local equilibrium representation is used. The non-equilibrium distribution function is determined by local values of the chemical potential at lattice sites. The expressions in terms of the transition probabilities for microscopic fluxes between lattice sites and the balance equations are used for formulating the evolution equations of inhomogeneous systems in finite differences. The simplest Euler's numerical algorithm is used for integrating these equations over time. This algorithm ensures stable solution of the equations at little requirements for computational resources that permitted to investigate phase transition kinetics at various thermodynamic, initial and boundary conditions.

The lattice fluid with nearest neighbor interparticle attraction on square and simple cubic lattices below critical temperature is considered. The initial density distribution is taken to consist of two regions: the high density region around the center of the system with density slightly lower equilibrium liquid density and the low density region outside the central region with density slightly higher the equilibrium gas density at a given temperature. The average system density corresponds to thermodynamically unstable state at subcritical temperature and the high density region serves as a region for the liquid density phase formation (inoculating area).

In two-dimensional systems the second high density region on the system periphery appears that disappears at bigger times. The inoculating area critical size is approximately equal to the double width of the phase transition region. Several complementary condensed areas in three-dimensional systems are observed. Number of areas depends on initial conditions. However, as opposed to two-dimensional systems, phase stratification takes place with arbitrary inoculating area size.

For the charging process imitation of a battery the first two lattice layers are initially filled above the condense phase concentration and the other layers are empty. The concentration profile kinetics in the system with and without external electric field are investigated.