Peculiarities of diffusion of particles on disordered lattices

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A system of particles on periodic two- or three dimensional lattices with uniform site energies is considered. Particle jumps to nearest neighbor vacant sites are thermally activated with randomly distributed intersite barriers. The statistical mechanics expressions for the kinetic diffusion coefficient that take into account interparticle interactions are derived for dynamically disordered systems.

The lattice systems with uniform, exponential and Gaussian probability distributions of the barriers are investigated.

The comparison between analytical results and Monte Carlo simulation data shows that the equilibrium characteristics of the model (the chemical potential and the probability for two nearest neighbor lattice sites to be vacant) are represented by the diagram approximation with high accuracy.

For the systems with static disorder the analytical expressions for the kinetic diffusion coefficient at low and high temperatures are proposed and investigated. The interpolation expression for the case of intermediate temperatures is considered.

The activation energy U_J for the kinetic diffusion coefficient is suggested to be described by the following expression

$$U_J = \epsilon_0 - (\epsilon_0 - \epsilon_p)\exp(-k_{\rm B}T/\epsilon_J), \qquad (1)$$

where ϵ_J depends on the type of lattice system and probability distribution functions $\nu(\epsilon)$ of the barriers and can be determined from MCS data; T is temperature; $k_{\rm B}$ is the Boltzmann constant; ϵ_0 is the average barrier energy; ϵ_p is the percolation energy that is calculated in accordance with the following expression

$$\int_0^{\epsilon_p} \nu(\epsilon) d\epsilon = p_c, \qquad (2)$$

where p_c is the threshold for the bond percolation problem.