DIFFUSION OF ADPARTICLES FAR FROM EQUILIBRIUM CONDITIONS.

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The generalized (frequency ω and wave-vector **q** dependent) diffusion coefficient D(**q**,ω) is determined for the system of interacting adsorbed particles under non-equilibrium conditions, characterized particularly by the strong gradient of coverage. The interaction of adparticles at low temperatures results in the memory effects and in the complex dependence of D on ω. Our contribution, based on the general theory published in [1], links to the paper [2], where diffusion coefficient in hydrodynamic limit was studied under such conditions. The deviations of Green - Kubo formula (derived for the relaxation of fluctuations around the equilibrium state) from the non-equilibrium results reflect the influence of the gradient of coverage on the collective behavior of adparticles.

Another system with the non-equilibrium effects are adatoms on stepped surface. We study non-equilibrium effects in spreading and collective diffusion of adatoms on stepped surfaces through Monte Carlo simulations of a lattice-gas model. The spreading density profiles are analyzed by the Boltzmann-Matano method to determine the temporal behavior of the effective collective diffusion coefficients. We find that the presence of steps induces considerable non-equilibrium effects in diffusion. For spreading along the steps, we find that these deviations can be explained by the slow approach of the different adparticle concentrations on terraces and at step edges towards equilibrium. For spreading across the steps, however, we find no such dependence, indicating the breakdown of the linear response theory at early times. We consider the case of nearest--neighbor repulsive and atractive interactions and different binding energies at the step edges [3].

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