QUANTUM GROWTH MODELS OF THIN FILMS ON SUBSTRATES

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There is a problem of constructing models of the kinetics of phase transitions in two-phase gas-crystal or liquid-crystal systems, and it is desirable that they are free from uncontrolled use of macroscopic characteristics in them that are not applicable to nanostructures. The process of film formation as a result of gas or liquid epitaxy on a crystal substrate, which we simulate by the pseudopotential of the crystal field with the symmetry of the crystal of the substrate, is considered. A set of particles of an unordered phase is considered as a dynamic system of particles in a state of thermodynamic equilibrium with a crystal substrate. At temperatures below critical, a part of the system particles are deposited on a substrate in a state with zero translational momentum. As a result of the interaction of adatoms, nuclei of a new phase are formed on the crystalline surface.

To study the process of deposition of a substance on a substrate, we use the Hamiltonian of the Bose-particle system in the representation of the second quantization a_k^+, a_k and pseudopotential of the form of the substrate field. The no conservation of the number density of particles $\left\langle a_{k_1}^+ a_{k_2} \right\rangle$ in an unordered system is due to the presence of a substrate field, which leads to the appearance of nonzero anomalous means $\left\langle a_{k_1} a_{k_2} \right\rangle$, which, at $k = 0$, determine the concentration of precipitated particles.

To determine the concentration of condensate, we use the method of quasi-averages and two-time Green functions. Solving together the system of equations for the normal and anomalous one-particle Green functions in the mean field approximation, we find ε – the energy of single-particle excitations, and Δ – the gaps in the excitation spectrum of the monolayer of crystalline condensate on the substrate. The appearance of $\Delta \neq 0$ is a criterion for the onset of condensation of a disordered phase on a substrate. Solving together the system of equations for the Green's functions, we find the equation for determining the gap Δ in the excitation spectrum of the precipitated crystal lattice.

$$\Delta = -\sum V\left(kk\right)\frac{\Delta}{\sqrt{\varepsilon^2+\left|\Delta\right|^2}}th\frac{\sqrt{\varepsilon^2+\left|\Delta\right|^2}}{2\Theta}. \tag{1}$$

Using equation (1), spinodal of the appearance of thin films on a crystalline surface can be obtained. The energy of single-particle excitations ε is determined by the kinetic energy of the particles and the potential of the substrate field *U*. The numerical solution of equation (1) was carried out using the Mathcad package. Determining the conditions for the appearance of a nonzero solution of equation (1), spinodals of the appearance of thin films on the substrate surface are obtained for various values of the pair interaction parameters, different substrate potentials *U*, and also for different substrate temperature.

For the probability density of the distribution of adatoms over levels $\left\langle a^{+}a \right\rangle = n$ from the system of Heisenberg equations of motion for the order parameter of the problem – the shear component of the structural transformation and average level populations; after averaging, we can obtain a nonlinear equation

$$n(t) = \frac{1}{2\mu} - \eta th\left(\mu\eta\frac{t-t_0}{\tau_0}\right), \qquad (2)$$

here τ is the growth delay of the film. This equation is known in the “super radiation” theory as the Rehler–Eberle equation, which at short times has a solution in the form of a kin-like inhomogeneous distribution of adatoms at the boundary of a flat film. Equation (2) was obtained as a solution of the system of equations for the order parameter and conjugate field in the case of a first-order structural phase transition “no structured phase — crystalline film» on the substrate [1]. Expression (2) describes the process of formation of an inhomogeneous kink-like distribution of atoms, which represent the domain wall of the edge of a thin growing film.

1. Lebedev, V. I. Quantum Models of Thin-Film Formation // High-Tech Technologies, Radio Engineering, Moscow, №7, 2012, v.13, p 97-102.