FORMATION OF STEP-TERRACED GaAs SURFACES IN EQUILIBRIUM CONDITIONS: MONTE CARLO SIMULATION

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Atomically flat crystal surfaces are needed for fundamental surface science, reproducible fabrication of nanoscale structures, and device applications. It was experimentally shown in [1,2] that GaAs(001) surfaces, which consist of atomically flat terraces separated by steps of monatomic height, can be obtained by annealing in the conditions close to equilibrium between the surface and the vapors of the III and V components, when neither growth, nor sublimation take place. At present the mechanisms of surface flattening and formation of step-terraced morphology are understood only qualitatively. This work is aimed to clarify the microscopic mechanisms of surface smoothing by comparison of experimental results obtained on GaAs(001) [1,2] with Monte Carlo simulations [3]. Kinetic Monte Carlo simulations were performed for a Kossel crystal in the standard solid-on-solid model with surface diffusion peculiarities typical for real surfaces [3]. The kinetics of surface smoothing was simulated by allowing only the surface diffusion, without deposition or sublimation. The key parameters of the simulation, i.e. the energy of lateral surface bonds $E_b \sim 0.34$ eV and the activation energy of the surface diffusion $E_d \sim 1.2$ eV are selected to fit the characteristic experimental durations of smoothing. To characterize quantitatively the formation of step-terrace morphology, we used the total length of monatomic steps L_S normalized to the length characteristic of the ideal vicinal surface L_0: $l_S = L_S/L_0$. This parameter is more adequate for characterization of step-terrace morphology formation than the mean root square roughness [2]. Despite the simplicity of the Kossel crystal model the calculated kinetics of step length l_S describes the experiment reasonably well. The microscopic mechanisms of surface smoothing consist in recombination of adatoms and vacancies, islands and pits, Ostwald ripening of islands and pits, their incorporation into the vicinal steps, and straightening the steps. It should be noted that the parameters extracted from the comparison of experimental data and Monte Carlo simulation should be treated with caution. The work is under way to take into account, along with the surface diffusion, the transfer through the gas phase via evaporation and readsorption and a more realistic model of a reconstructed GaAs surface.

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