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Monte Carlo simulation of GaAs smoothing in equilibrium conditions

D.M. Kazantsev[1,2], I.O. Akhundov[1], A.N. Karpov[1], N.L. Shwartz[1,3], V.L. Alperovich[1,2] and A.V. Latyshev[1,2]

[1] Institute of Semiconductor Physics, 630090 Novosibirsk, Russia
[2] Novosibirsk State University, 630090 Novosibirsk, Russia
[3] Novosibirsk State Technical University, 630073 Novosibirsk, Russia

Abstract. Experimental results on the step-terraced surface morphology formation under annealing GaAs(001) substrates in equilibrium conditions are compared with Monte Carlo simulations in a simple model of a Kossel crystal. The Monte Carlo simulations describe qualitatively the formation of atomically flat terraces separated by straight monatomic steps. The opportunities and restrictions of these simulations for extracting microscopic parameters of the surface are discussed.

Introduction

Atomically flat crystal surfaces are needed for fundamental surface science, reproducible fabrication of nanoscale structures, and device applications. Almost perfect silicon surfaces, which consist of atomically flat regular terraces separated by steps of monatomic height can be obtained by annealing in vacuum [1]. Preparation of ordered step-terraced surfaces of III–V semiconductors by vacuum anneals is hindered by high and different evaporation rates of the III and V components. It was experimentally shown in [2,3] that step-terraced surfaces of "epi-ready" GaAs(001) substrates can be obtained by annealing in the conditions close to equilibrium between the surface and the vapors of the III and V components. At present the mechanisms of surface flattening and formation of step-terraced morphology are understood only qualitatively. In order to clarify these mechanisms on a microscopic level and to obtain the parameters which govern the smoothing process one should compare the experimental results with a microscopic theory. This work is aimed at studying the microscopic mechanisms of surface smoothing by comparison of experimental results obtained on GaAs(001) [2,3] with Monte Carlo simulations [4].

1. Experimental

The samples were cut from "epi-ready" GaAs(001) substrates. The anneals were performed in a quartz tube, under the flow of pure molecular hydrogen. The equilibrium conditions were provided in a quasi-closed volume by the presence of the saturated Ga-As melt. The morphology of the initial and annealed GaAs surfaces was studied ex situ by the atomic force microscopy (AFM). The details of annealing and AFM measurements are described in [2]. 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 [4].

2. Results and discussion

In Fig. 1 the left column shows the AFM image of the initial "epi-ready" GaAs(001) substrate (a) and the AFM images after annealing at 625 °C for various durations (b–e). Although the initial surface has a small root mean square roughness $\rho \approx 0.12$ nm, it is disordered on a microscopic level and shows no traces of atomic steps. After a 15-min anneal distinct "step and terrace" morphology is revealed, with meandered steps. Two-dimensional islands and pits of monatomic height and depth, respectively, are clearly seen on terraces (Fig. 1b). With increasing duration of the anneals, the average lateral size of the islands increases, the islands merge with the steps, and the steps become more and more straight. Eventually, the surface approaches the morphology of an ideal vicinal surface with atomically flat terraces separated by monatomic steps (Figs. 1b–e).

The right column in Fig. 1 shows the results of Monte Carlo simulation of surface flattening. The initial "rough" surface (Fig. 1f) was prepared by allowing surface diffusion at the ideal vicinal surface at sufficiently high temperature $T = 625$ °C and low energy of lateral surface bonds $E_b \approx 0.1$ eV during 3 hours, followed by random deposition of 1.5 atomic layers. The kinetics of surface smoothing was simulated by allowing only the surface diffusion, without deposition or sublimation. Each row in Fig. 1 corresponds to the same duration of the experimental and simulated anneal. The key parameters of the simulation, i.e. the energy of lateral surface bonds $E_b \approx 0.34$ eV and the activation energy of the surface diffusion $E_d \approx 1.75$ eV are selected to fit the characteristic experimental durations of smoothing. It is seen from Fig. 1 that despite the simplicity of the model the simulation qualitatively describes the step-terraced morphology formation. The driving force for surface smoothing is the minimization of the surface free energy and the microscopic mechanisms 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.

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] and its usage has a clear thermodynamic meaning because the contribution of steps to the free energy of the surface is proportional to the step stiffness multiplied by the step length. Fig. 2 shows the kinetics of the measured (triangles) and calculated (circles) step lengths l_S. It is seen that the calculated kinetics of l_S describes the experiment reasonably well.

Calculated kinetics of l_S allows us to trace different stages of surface smoothing. These stages are illustrated in Fig. 2 by typical images of the surface relief. Initial fast decrease of l_S at $t < 10$ min corresponds, presumably, to recombination of adjacent small islands and pits. Slower decrease at $10 < t < 150$ min is due to Ostwald ripening of islands and pits