

Thermal smoothing and roughening of semiconductor surfaces: experiment on GaAs and Monte Carlo simulation

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Abstract. GaAs thermal smoothing at temperatures $T \leq 650^\circ\text{C}$ in the conditions close to equilibrium yields surfaces with atomically smooth terraces separated by steps of monatomic height. At higher temperatures surface smoothing is changed to roughening. Possible reasons of surface roughening at elevated temperatures are studied by means of Monte Carlo simulation and compared with the experimental results on GaAs. It is proved that GaAs roughening at elevated temperatures is caused by kinetic instabilities due to deviations from equilibrium towards growth or sublimation. The microscopic mechanisms of kinetic-driven roughening are discussed.

Introduction

Fundamental surface science, nanostructures fabrication and device applications require high-quality, atomically flat crystal surfaces. Surfaces with atomically smooth terraces separated by steps of monatomic height can be obtained by annealing in vacuum [1,2]. The application of vacuum annealing to GaAs and other III-V semiconductors is hindered due to the preferential evaporation of a more volatile V component. To avoid surface depletion with more volatile component and possible kinetic instabilities, thermal smoothing should be made in the conditions close to the thermodynamic equilibrium, when neither sublimation, nor growth occurs [3]. Ding *et al.* [4] proved that annealing MBE-grown GaAs(001) films at a sufficiently high As₄ vapor pressure and moderate temperature yielded flat surfaces, while, at lower As₄ pressures and higher temperatures, the preroughening and roughening transitions occurred. Step-terraced surfaces were also obtained by annealing GaAs(001) substrates in MOCVD setups in the mixture of arsine and hydrogen [5]. Another technique for GaAs surface smoothing by annealing in conditions close to equilibrium between the surface and Ga and As vapors was developed in [6]. This technique yields step-terraced GaAs(001) surfaces with atomically smooth terraces (Fig. 1a–c).

Increasing the annealing temperature speeds up surface mass transport and, thus, facilitates the smoothing process. However, at temperatures $T \geq 700^\circ\text{C}$ GaAs surface smoothing is changed to roughening, which consists in the formation of multilayer islands and pits, step bunches, and destruction of step-terraced morphology (Fig. 1d) [6]. This roughening restricts the annealing temperature and, thus, the maximal initial surface roughness that can be smoothed at reasonable annealing durations. In principle, surface roughening can be caused by the thermodynamic roughening transition, when step line tension decreases down to zero due to the entropy term in surface free energy, and spontaneous step generation becomes energetically favorable [3,7]. The roughening temperature, however, is typically close to or above the crystal melting point [3,7], so the roughening transition does not occur in real experimental conditions. Alternatively, surface roughening can be caused by kinetic instabilities, which, in their turn, may arise due to deviations of annealing condition from equilibrium towards growth or sublimation. This paper is aimed at elucidating the mechanism of GaAs surface roughening at elevated temperatures by

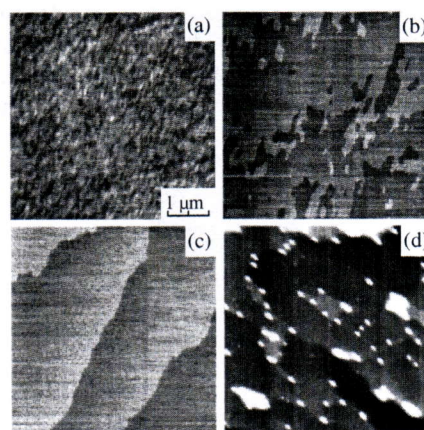


Fig. 1. AFM images of an epi-ready GaAs substrate before (a) and after anneals for 2 h at 575°C (b), 650°C (c) and 775°C (d) [6]. The rms roughness of the substrate (a) is of ~ 0.12 nm. The steps in (b) and (c) are of ~ 0.3 nm, which is equal to the period of GaAs lattice in (100) direction. The height of islands in (d) ranges from 1.5 to 6 nm.

means of both experiment and Monte Carlo simulation.

1. Method

Initial step-terraced GaAs(001) surfaces used in these experiments were obtained by means of annealing “epi-ready” substrates at $T = 600\text{--}650^\circ\text{C}$ in the conditions close to equilibrium provided in a quasi-closed container by the presence of the saturated Ga-As melt. The anneals at higher temperatures $T = 700\text{--}775^\circ\text{C}$ were performed in the same experimental setup. Prior to annealing, the substrates were treated in the solution of HCl in isopropyl alcohol to remove the surface oxides. The morphology of the initial and annealed GaAs surfaces was studied *ex situ* by atomic force microscopy (AFM). The details of surface wet treatment, annealing and AFM measurements are described in [6].

Monte Carlo simulations of surface roughening were performed in the model of the Kossel crystal [8,9]. The model was extended to artificially maintain the equilibrium or a specified deviation from equilibrium between atomic fluxes from and to the surface. The model parameters, which include diffusion activation energy $E_d = 1.3$ eV, lateral bond energy $E_b = 0.32$ eV and adatom desorption energy $E_{des} = 1.9$ eV