Applied Surface Science 333 (2015) 141–146

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Monte Carlo simulation of GaAs(0 0 1) surface smoothing in equilibrium conditions

D.M. Kazantsev[a], I.O. Akhundov[a], A.N. Karpov[a], N.L. Shwartz[a,c], V.L. Alperovich[a,b,*], A.S. Terekhov[a], A.V. Latyshev[a,b]

[a] Rzhanov Institute of Semiconductor Physics, 630090 Novosibirsk, Russia
[b] Novosibirsk State University, 630090 Novosibirsk, Russia
[c] Novosibirsk State Technical University, 630073 Novosibirsk, Russia

ARTICLE INFO

Article history:
Received 27 October 2014
Received in revised form 28 January 2015
Accepted 29 January 2015
Available online 7 February 2015

Keywords:
Surface smoothing
GaAs
Monatomic steps
Step-terraced morphology
Monte Carlo simulation

ABSTRACT

Monte Carlo simulation of smoothing and step-terraced morphology formation on the Kossel crystal surface is carried out. The simulation results are compared with the experimental data on GaAs surface smoothing in equilibrium conditions. Despite the simplicity of the Kossel crystal model, the simulation qualitatively describes the experiment. The full length of monatomic steps and the mean size of islands on terraces are explored for quantitative characterization of the surface relief evolution. The comparison of the simulation and experiment yields surface diffusion activation energy $E_d = 1.3 \pm 0.05$ eV, lateral bond energy $E_b = 0.32 \pm 0.02$ eV and adatom desorption energy $E_{des} = 2.1 \pm 0.05$ eV, which are in reasonable agreement with the values obtained earlier from GaAs growth experiments and *ab initio* calculations.

1. Introduction

Atomically flat crystal surfaces are needed for fundamental surface science, reproducible fabrication of nanoscale structures and device applications [1,2]. A standard method of crystal surface smoothing consists in chemo-mechanical polishing (CMP) [3]. By means of CMP, one can obtain surfaces with extremely low values of root mean square (rms) roughness, comparable with the interatomic distance. However, due to mechanical impact, after CMP the uppermost surface layer is disordered, with a large concentration of structural defects and disrupted lateral correlations in the positions of surface atoms. This atomic-scale disorder can be reduced by allowing surface migration at elevated temperatures. Almost perfect silicon surfaces, which consist of atomically flat regular terraces separated by steps of a monatomic height, can be obtained by annealing in vacuum [4–6]. The 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. This problem can be circumvented by annealing in the conditions close to equilibrium between the surface and the vapors of the III and V components, at which the mean fluxes of atoms desorbed from the surface into the gas phase and adsorbed from the gas phase to the surface are equilibrated, so that neither growth, nor sublimation occurs [7]. It was experimentally shown that *in situ* annealing of MBE-grown GaAs(0 0 1) films at a sufficiently high As_4 vapor pressure and moderate temperature, as well as annealing of GaAs(0 0 1) substrates in a MOCVD setup in the mixture of arsine and hydrogen, yielded flat step-terraced surfaces [8,9]. A more simple and cost-effective technique for GaAs surface smoothing was developed in Refs. [10,11]. In this technique the conditions close to equilibrium between the surface and Ga and As vapors were provided by the presence of a saturated Ga–As melt.

From the thermodynamic point of view, the transformation of a smooth (in terms of small rms roughness) but microscopically disordered surface into an ordered one with step-terraced morphology corresponds to the surface free energy minimization [7]. However, the mechanisms that determine the kinetics of this conversion are understood only qualitatively. To clarify these mechanisms on a microscopic level and to obtain the parameters that govern the step-terraced morphology formation, one should compare the experimental results on smoothing kinetics with a microscopic theory. However, to our knowledge, an analytical microscopic theory which could adequately describe the kinetics of the step-terraced morphology formation is not yet available. In the absence of an analytical theory, direct Monte-Carlo

* Corresponding author at: Rzhanov Institute of Semiconductor Physics, 13 Lavrentieva, 630090 Novosibirsk, Russia. Tel.: +7 383 330 9874.
E-mail address: alper@isp.nsc.ru (V.L. Alperovich).

http://dx.doi.org/10.1016/j.apsusc.2015.01.226
0169-4332/