Thermodynamic and kinetic roughening: Monte Carlo simulation and experiment on GaAs

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Abstract. GaAs thermal smoothing at temperatures $T \leq 650$°C in the conditions close to equilibrium yields surfaces with atomically smooth terraces separated by steps of monatomic height. At higher temperatures $T \geq 700$°C, surface smoothing is changed to roughening. In the present paper, 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 the thermodynamic roughening transition, which consists in spontaneous generation of atomic steps due to decrease in the step line tension down to zero, cannot explain the experiment because it should occur at temperatures $T \sim 1800$ - 2000°C, i.e. much higher than in the experiment. Kinetic instabilities caused by deviations from equilibrium towards growth or sublimation are shown to cause GaAs roughening at elevated temperatures. The microscopic mechanisms of kinetic-driven roughening are discussed.

1. Introduction

Fundamental surface science, nanostructures fabrication and device applications require high-quality, atomically flat crystal surfaces [1-5]. A technique for GaAs surface smoothing by allowing mass transport at elevated temperatures was developed in [6,7]. To avoid surface depletion with arsenic, the anneals were performed in conditions close to equilibrium between the surface and Ga and As vapors, when neither growth nor sublimation takes place. This technique yields GaAs(001) surfaces with atomically smooth terraces separated by steps of monatomic height (figure 1(a-c)).

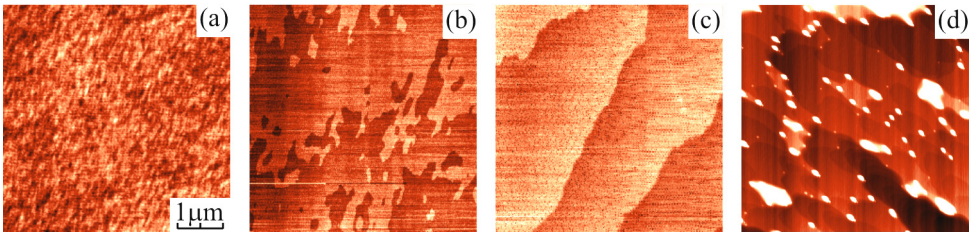

Figure 1. AFM images of an epi-ready GaAs substrate before (a) and after anneals for 2 h at 575°C (b), 650°C (c) and 775°C (d) [6].

Increasing the annealing temperature speeds up surface mass transport and, thus, facilitates the smoothing process. However, at temperatures $T \geq 700$°C, GaAs surface smoothing is replaced by roughening which consists in the formation of step bunches, multilayer islands and pits, and

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