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Formation and interaction of dislocation-induced and vicinal monatomic steps on a GaAs(001) surface under stress relaxation

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ABSTRACT

Formation and interaction of curved vicinal and straight dislocation-induced steps of monatomic height on smooth GaAs(001) surface is studied under thermo-mechanical stress relaxation in GaAs/AlGaAs heterostructures bonded to glass. Typical dislocation phenomena, like transverse glide, are revealed in the slip steps patterns. At elevated temperatures, slip steps keep their straight shape, while curved vicinal steps acquire distinct small-scale (~10 nm) undulations caused, presumably, by kink bunching. Annihilation of steps with opposite signs and anticrossing of slip steps with each other and with vicinal steps are studied.

Semiconductor surfaces with atomically flat terraces separated by steps of monatomic height are needed for fundamental surface science, device applications and reproducible fabrication of nanoscale structures [1]. In particular, straight monatomic steps are highly desirable for assembling adatoms into one-dimensional “quantum wires” [2]. Step-terraced surfaces with monatomic vicinal steps can be prepared at elevated temperatures by allowing surface diffusion on chemo-mechanically polished substrates with small root mean square (rms) roughness, comparable to or smaller than inter-atomic distance. Nearly perfect step-terraced silicon surfaces are prepared by annealing in a vacuum [3,4]. Step-terraced GaAs surfaces can be obtained by annealing at sufficiently high pressure of arsenic-contained vapor components to avoid surface depletion with arsenic [5–8]. However, at real surfaces, vicinal steps are not perfectly straight because their shape is determined by long-period undulations of the surface relief, which cannot be reduced at reasonable temperatures and durations of annealing.

In principle, a straight monatomic step — a slip step — can be produced on a crystal surface by generation of a dislocation half-loop under relaxation of mechanical tensions. Generation and subsequent motion of slip steps are believed to be the mechanisms underlying “cross-hatched” morphology formation during epitaxial film growth on lattice-mismatched substrates [9]. However, in most cases, the cross-hatched relief of grown films is relatively rude, with typical roughness heights much larger than interatomic distance. Generation of monatomic slip steps due to introduction of single dislocation loops was found by Lutz et al. [10] in AFM images of the partially relaxed 80-nm GeSi film grown on a Si substrate at early stages of cross-hatched relief formation, but distinct step-terraced morphology was not observed.

In the present study we experimentally proved the opportunity of forming a rectangular grid of straight monatomic slip steps induced by generation of dislocations due to thermo-mechanical stress relaxation in GaAs/AlGaAs heterostructures bonded to glass substrates.

We used $Al_xGa_{1-x}As/p\text{-}GaAs/Al_xGa_{1-x}As$ double heterostructures with the GaAs and $Al_xGa_{1-x}As$ layer thicknesses in the range of 0.5–2 μm and Al content $x \sim 0.5$, which were epitaxially grown on GaAs(001) substrates. The heterostructures were bonded to glass plates by means of thermocompression bonding. The GaAs substrate and AlGaAs stop layer were removed by selective wet etching [11]. Such glass-bonded *p*-GaAs/AlGaAs heterostructures with the surface of *p*-GaAs activated by cesium and oxygen to the state of negative effective electron affinity are used as transmission-mode photocathodes in image intensifiers and in the sources of ultra-cold and spin-polarized electrons [11–13]. Due to the AlGaAs interlayer, which is lattice-matched to the GaAs emitting layer (the relative mismatch is below 10^{-3}), electron recombination velocity at the back *p*-GaAs/AlGaAs interface of the emitting *p*-GaAs layer is substantially reduced as compared to a free *p*-GaAs surface or direct GaAs/glass interface, and this facilitates the increase of photocathode quantum efficiency [11,12]. The dislocation network in the structure after bonding, chemical etching and anneals was monitored by photoluminescence (PL) intensity

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topography. The anneals of glass-bonded structures were performed in the conditions close to equilibrium with As and Ga vapors, when neither growth, nor sublimation takes place [7]. The equilibrium conditions were provided by the presence of the saturated Ga–As melt in the vicinity of GaAs surface. The morphology of the surface was studied ex situ by atomic force microscopy (AFM). The details of annealing and AFM measurements were described earlier [7].

To study the GaAs surface morphology evolution under stress relaxation, isochronous one-hour anneals were performed at successively increased temperatures. Stresses in the semiconductor structure build up under heating due to the difference in the thermal expansion coefficients of the structure and glass. Partial plastic stress relaxation takes place above the dislocation generation threshold, which depends on the magnitude of stress and temperature. The AFM images of the GaAs surface before and after anneals at various temperatures are shown in Fig. 1a-e. The initial chemo-mechanically polished surface is characterized by a small rms roughness ($\rho \leq 0.2$ nm over areas of about 1 μm^2, but it is disordered on a microscopic level, with no step-terraced morphology (Fig. 1a). Distinct islands and pits bounded by steps of one or two-monolayer (ML) height are formed as a result of annealing at 57 °C (Fig. 1b). It is seen that the increase of the annealing temperature, which facilitates surface diffusion, leads to the increase of the island mean size (Fig. 1c) and, eventually, to the formation of the step-terraced morphology, which consists of atomically flat terraces separated by curved monatomic steps (Fig. 1d and e). The widths of terraces and steps curvature are determined by the miscut angle from the singular (001) crystal face and by the variations of this angle along the surface, respectively.

It is seen from Fig. 1, that along with these curved vicinal steps, a rectangular grid of straight steps is formed on the surface. Like cross-hatch patterns on the surfaces of the epitaxial films grown on lattice mismatched Si(001) and GaAs(001) substrates [10,14], these steps are directed along the [110] and $[1\bar{1}0]$ crystal axes and, apparently, have the same origin arising from plastic relaxation of mechanical stresses by generation of misfit dislocations. However, unlike typical cross-hatch patterns, which are usually rough and visible with an optical microscope or even with a naked eye, we observe here the dislocation-induced slip steps of monatomic height. This is confirmed by the height distribution function (Fig. 1f) determined for the surface area which contains flat terraces on both sides of a slip step. Also, the cross-section shown in Fig. 1g proves that, within the experimental accuracy, both the vicinal and slip steps have the same height of approximately 0.3 nm corresponding to the period of the GaAs lattice in the [001] direction.

Slip steps originate from partial plastic relaxation of thermo-mechanical stress in the GaAs/AlGaAs(001) heterostructure. This relaxation occurs preferentially via the formation of dislocation half-loops in {111} glide planes. Each half-loop consists of a 60° misfit dislocation (MD), which lies in the (001) plane, and two threading dislocations (TDs) which cross the surface [9,10,14,15]. A dislocation half-loop produces a step of monatomic height along the straight line connecting the threading segment intersections with the surface. The misfit dislocation and the corresponding slip step develop due to the half-loop extension by the glide of threading segments in the opposite directions towards the sample edges. For a thin film, the surface displacement profile has an asymmetric "dipole" shape with a sharp step separating a larger ridge from a smaller trough [10,14]. The profile lateral width is approximately equal to the layer thickness. In our case, the surface displacement profile has the shape of a rectangular step of monatomic height (see Fig. 1) because the film thickness exceeds the mean distance between the dislocations. To our knowledge, this is the first distinct observation of step-terraced morphology with dislocation-induced monatomic steps produced due to plastic relaxation in a stressed semiconductor film. This observation was facilitated by the use of GaAs surfaces with a small initial rms roughness and by the technique of atomic smoothing in equilibrium conditions [7].

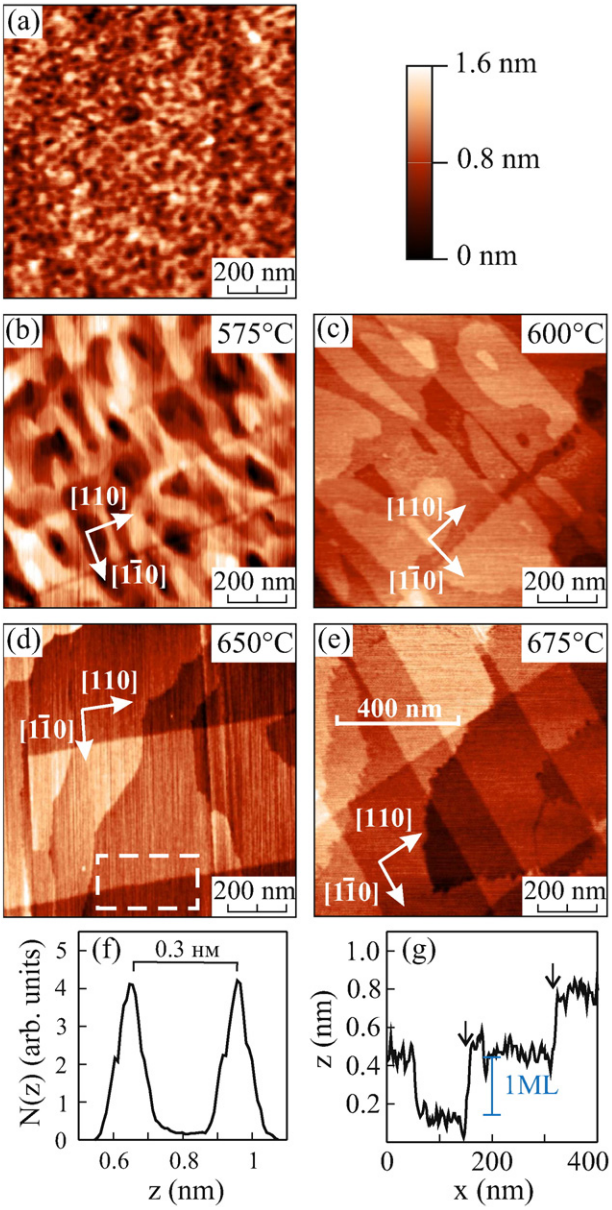

Fig. 1. AFM images of the GaAs(001) surface of the GaAs/AlGaAs heterostructure bonded to glass before (a) and after one-hour anneals at increasing temperatures (b–e). (f) height distribution function calculated over the rectangular region shown by the dashed line in (d). (g) z–x cross-section of the 400-nm segment shown in (e). Slight angle distortions are due to incomplete correction of AFM scanner nonlinearities.

The observation of slip steps allowed us to reveal typical dislocation phenomena like transverse glide of dislocations [16]. Shown in Fig. 2a is the AFM image with three distinct Γ-turns of slip steps indicated by arrows. Slip step Γ-turns originate from the transverse glide of dislocation half-loops, as illustrated schematically in Fig. 2b. The change of the gliding plane from (111) to $(1\bar{1}1)$ is possible because the Burger's vector direction $\vec{b}$ is close to the line of intersection between these planes.

Apart from the same monatomic height, vicinal and slip steps are qualitatively different in a few important respects. The first apparent difference is that the dislocation steps are straight and have definite crystallographic directions, while the vicinal steps are curved, with their shape and direction determined by uncontrollable smooth surface relief undulations. Second, in the surface fragment with a certain sign of the miscut angle, the vicinal steps have the same sign and, thus, form a monotonically descending (or ascending) staircase. On the contrary, as