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Influence of interface dislocations on surface kinetics during epitaxial growth of InGaAs

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Abstract

The correlation between surface striations and misfit dislocations at the interface has been studied on $In_xGa_{1-x}As$ single layers ($x < 0.25$), as a function of the growth parameters (substrate temperature and deposition rate), by means of atomic force and transmission electron microscopies. It is concluded that both features may be initially linked by mechanical causes (elastic displacement fields), but eventually evolve in a different way due to the surface kinetic effects. The range of growth conditions for an optimum surface quality is determined. A simplified treatment of the diffusion equation, in which the effect of the surface on the dislocation stress field is included, has allowed an estimation of the effective mean free path between collisions for the group III adatoms in the range of a few Å. © 1998 Elsevier Science B.V.

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1. Introduction

The surface roughness that usually appears during the epitaxial growth of semiconductor strained layers may exhibit several shapes (islands, ripples, striations) each obeying to different causes. Eventually, these features usually become faceted in sufficiently thick layers. The appearence of an island-like, nonplanar growth front depends on a balance among several factors: (i) the surface tension (mainly from the contribution of the surface reconstructions between homospecies); (ii) the residual strain, which suffers strong fluctuations at the terrace edges; and (iii) the kinetics of the surface adatoms, which can be partially controlled by the growth conditions: flux ratio, deposition rate (v), substrate temperature (T_s) and orientation.

When the deposition conditions are such that a layer-by-layer (2D) growth is guaranteed, the strained epilayer will go through a metastable regime (pseudomorphic), until its thickness allows the dislocation nucleation barrier to be overcome. Even under these conditions, the development of a striated relief (generally along directions of the ⟨110⟩ family in zincblende compounds) cannot be avoided. Recently, a thermal instability of the surface has been rather discarded as a possible origin for these striations in typical III–V semiconductors [1].

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Table 1
Growth parameters for each sample, together with the average roughness amplitude, the density of surface striations ρ_{str} (evaluated by AFM), and the density of dislocations at the interface ρ_{MD} (determined by TEM). Two values are given wherever the features along the [110] and [−110] directions can be resolved, respectively

Sample	T_s (°C)	v (μm h^{-1})	ρ_{MD} (10^4 cm^{-1})	ρ_{str} (10^4 cm^{-1})	Amplitude $\langle a \rangle$ (nm)	ρ_{MD}/ρ_{str}
#513	520	0.2	6:7	1.7	1.8	3.8
#515	520	1.5	24:27	7.4	1.95	3.4
#516	400	1.5	22:24	7.2:6.2	0.6	3.2
#517	520	0.2	thicket	—	5.1	—
#518	400	0.2	thicket	2.9:6.9	1.3	—
#519	520	0.8	16:18	4.2	4.1	4.0
#520	450	0.8	—	7.1	0.74	—
#521	400	0.8	25:23	7.1:6.1	0.75	3.4

The present work focuses on the correlation between the striated patterns on the surface and the misfit dislocations at the interface of InGaAs/GaAs epitaxial layers. This correlation was previously analysed by transmission electron microscopy (TEM) in thick films with large surface striations [2]. However, the weak contrast associated with the striations has prevented a simultaneous study of both features in thin layers (tens of nm).

2. Experimental

In order to study these phenomena at their origin, several series of $In_xGa_{1-x}As$ single layers ($0.10 < x < 0.25$) have been grown on GaAs (001), on-axis substrates, by molecular beam epitaxy. The epilayer thicknesses (t) are below and above the critical value for the activation of the dislocation multiplication processes (t_{cr}). T_s was ranged from 400 to 520°C, and v within the interval 0.2–1.5 μm h^{-1} (see Table 1 for details), for a constant V/III equivalent pressure ratio of 40.

The surface roughness of several (001) samples with identical structure ($t = 78$ nm and $x = 0.21$) as revealed by ex situ atomic force microscopy (AFM) is shown in Fig. 1. These layers were grown using different temperatures at a fixed $v = 0.8$ μm h^{-1}. As T_s increases, the roughness evolves from a crossed

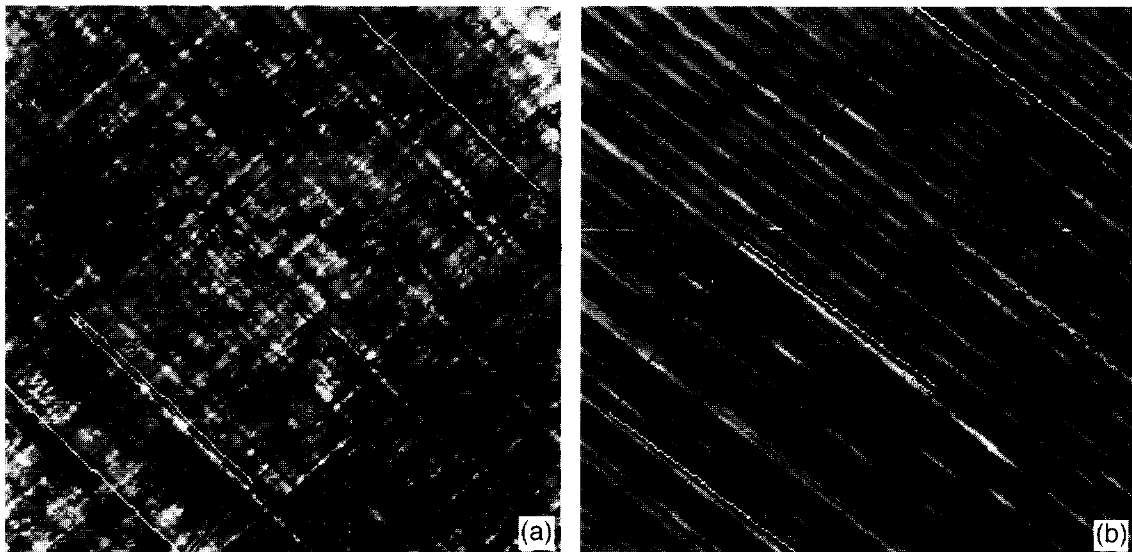

Fig. 1. AFM images (10 × 10 μm) of two $In_xGa_{1-x}As$ samples with identical thicknesses (78 nm) and compositions ($x = 0.21$), grown at the same deposition rate (0.8 μm h^{-1}), but different temperatures: 400°C (a) and 520°C (b).

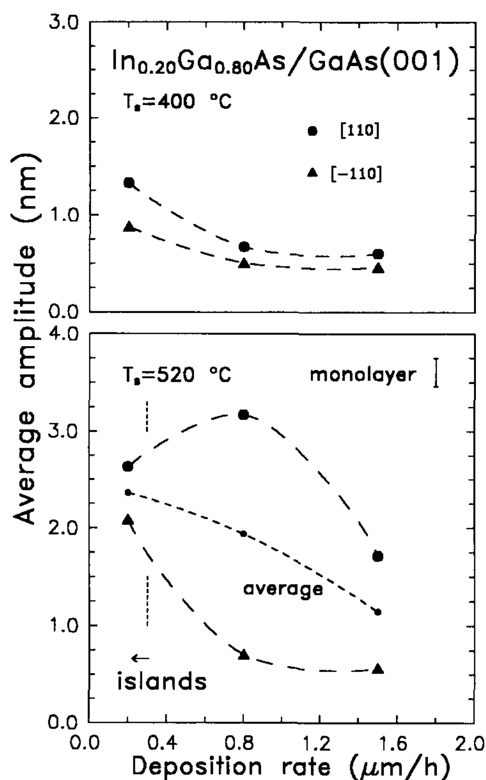

Fig. 2. The amplitude of the surface roughness along the [−110] and [110] directions is plotted vs growth rate (v), for $In_{0.20}Ga_{0.80}As$ layers with $t \approx 90$ nm, grown at $T_s = 400°C$ and $T_s = 520°C$. The range for which 3D growth is expected has been pointed out. Dashed lines are to guide the eye.

pattern to a striated one, along the [110] direction. In addition, the amplitude and width of the striations become larger. As it is well known, both characteristics also increase for longer growths, i.e., thicker layers [3]. This behaviour was elsewhere related to the appearence of bunches of dislocations slightly above the interface [2]. However, very different surface patterns may be observed in layers with similar dislocation densities at the interface by only varying the growth conditions (see Table 1). This suggests that the roughness is mainly determined by the surface kinetics rather than the mechanical effects, under certain growth conditions.

The roughness amplitude for those samples grown at 400°C and 500°C has been plotted vs growth rate in Fig. 2. In general, the surface smooths as v increases. This indicates that the lifetime for the adatoms to reach their equilibrium positions is limited by the monolayer covering time. The behaviour of the sample grown at 520°C and $v = 0.2$ μm h^{-1} seems to deviate from the tendency observed in the other samples. This is attributed to the qualitative change of the surface morphology (island-type). Anyway, the average between both directions does conserve the tendency (Fig. 2, lower plot). The striation amplitude has been plotted vs T_s, for an intermediate $v = 0.8$ μm h^{-1}, in Fig. 3. As the substrate temperature increases, the striations behave like in the case when the growth rate is reduced.

In all the cases, the grooves along the [−110] direction are lower than those along [110], as well as considerably less sensitive to the variations of the growth conditions. At the beginning of the relaxation, the difference of amplitude between both directions is minimum (of the order of one monolayer), so that a cross-hatched pattern is observed. At this stage, the roughness height (around two monolayers) is close to the value expected from the displacement fields associated with a misfit dislocation. Moreover, the density of these dislocations appears to be just a few times higher (around three) than that of the striations (see Table 1).

Later, the distribution of the grooves evolves in the opposite sense to that of the dislocations at the interface. The former extends along the preferential

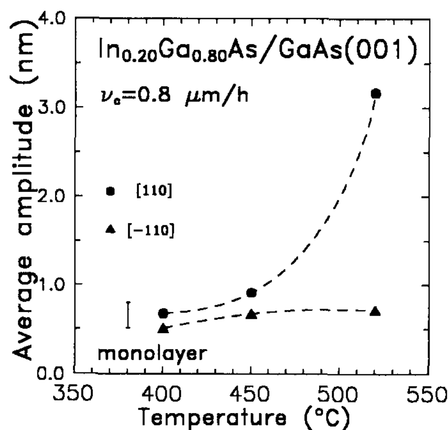

Fig. 3. The amplitude of the surface roughness along both [−110] and [110] directions is plotted vs substrate temperature T_s, for $In_{0.20}Ga_{0.80}As$ layers ($t \approx 90$ nm), grown at a fixed $v = 0.8$ μm h^{-1}. Dashed lines are to guide the eye.

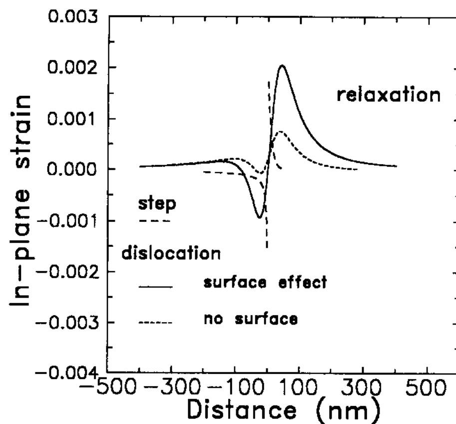

Fig. 4. The ε_{xx} strain component induced at the surface by two reticular defects. Dashed line: a surface step 1 nm high. Dotted and solid lines: a 60° dislocation at a depth of 60 nm, excluding and including the effect of the surface on the stress field, respectively. Both defects are aligned perpendicularly to the figure plane, so that the x-coordinate indicates the horizontal distance.

direction [110], reducing gradually its density. The latter becomes similar for both directions, and rises until the hardening regime. This difference can be considered also a consequence of surface kinetic effects.

3. Theoretical considerations

The in-plane strain component (ε_{xx}) associated with both the edge of a forming terrace (1 nm thick), and a 60° dislocation (located at $x = 0$ and a depth of 60 nm) has been evaluated at the surface plane ($z = 0$), and it is plotted vs the horizontal distance x in Fig. 4. A step of compressed material induces a non-uniform tensile stress in the portion of substrate beneath it, as well as a compressive stress to the other side [4] (dashed line). The strain field is maximum at the edge position, so that a barrier for the incorporation of surface diffusive atoms to the step is created. Such a mechanism is considered to drive the irruption of the 3D growth [5]. The dotted line in Fig. 4 represents the $\varepsilon_{xx}(x)$ field for a 60° dislocation in an infinite medium with $In_xGa_{1-x}As$ equivalent properties. However, the stress fields are strongly modified in the vicinity of a surface due to the boundary conditions. As a result of including this effect, the increment of the peak-to-valley strain fluctuation results to be around five times greater than that in an infinite medium (solid line).

In order to account for the consequences of this perturbation on the surface morphology, a simple diffusion calculation may be performed. For simplicity, the driving force for the mass transport will be considered to arise only from those variations of the surface effective chemical potential due to the strain fluctuations, $\mu[\varepsilon(s)]$. This function may be roughly estimated as the increment of elastic energy associated with the incorporation of the new strained cells. Using the strain fields obtained in Fig. 4, $\varepsilon(s)$ is determined and introduced in the surface diffusion equation,

$$\mathrm{d}n/\mathrm{d}t = -\nabla \cdot \boldsymbol{J}. \tag{1}$$

The surface flux $\boldsymbol{J} = n(s) \cdot v(s)$ is simplified to $\boldsymbol{J} = \rho_s \cdot \langle v(s) \rangle$, where ρ_s is the density of surface sites, and $\langle v(s) \rangle$ is the average velocity along the x-direction for those adatoms at the position s. This function has been averaged assuming a collision rate identical for all the atoms, according to

$$\langle v(s) \rangle = \langle x \rangle / \langle t \rangle, \tag{2}$$

where $\langle x \rangle = \lambda$ is the mean free path between collisions, and where

$$\langle t(s) \rangle = \int_s^{\infty} t(x,s) \frac{\mathrm{e}^{-(x-s)/\lambda}}{\lambda} \mathrm{d}x,$$

and

$$t(x,s) = \sqrt{\frac{m}{2}} \int_s^x \frac{\mathrm{d}r}{\sqrt{\mu(s) - \mu(r)}}$$

(see Ref. [6]).

The first member of Eq. (1) is thus interpreted as the increment of roughness amplitude per unit time, due exclusively to the flux of the adatoms towards the lower energy zones. In a previous work [7], it was concluded experimentally that this rate can be considered approximately linear at the initial stages of the roughness, i.e., $\mathrm{d}z/\mathrm{d}t = z/\tau$ (where τ is equivalent to the inverse of the growth rate). This experimental determination, together with the evaluation of Eq. (1), allows a rough estimation of the mean free path between collisions for the group III atoms, which results in the range of a few angstroms for our growth parameters.

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References

[1] C. Lavoie, T. Pinnington, E. Nodwell, T. Tiedje, R.S. Goldman, K.L. Kavanagh, J.L. Hutter, Appl. Phys. Lett. 67 (1995) 3744.
[2] R. Beanland, T.B. Joyce, P.J. Goodhew, M. Aindow, P. Kidd, M.A. Lourenço, J. Cryst. Growth 149 (1995) 1.
[3] S.F. Yoon, J. Vac. Sci. Technol. B 11 (1993) 562.
[4] S.M. Hu, J. Appl. Phys. 50 (1979) 4661.
[5] C.W. Snyder, B.G. Orr, D. Kessler, L.M. Sander, Phys. Rev. Lett. 66 (1991) 3032.
[6] K.V. Shalímova, Physics of Semiconductors, Mir, Moscow, 1975.
[7] A.L. Álvarez, F. Calle, A. Sacedón, E. Calleja, E. Muñoz, R. García, L. González, Y. González, H.G. Colson, P. Kidd, R. Beanland, P. Goodhew, Solid-State Electron. 40 (1996) 647.