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Elastic strains influence during GaSb/InAs heteroepitaxy from liquid phase

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Abstract. Influence of strains that appear in GaSb/InAs heterosystem on heteroepitaxial layer planarity is considered. It is shown that minimal supercooling of solution-melt at the saturation temperature of gallium antimonide in gallium melt 450 °C is 7.8 °C for [111] and 5.8 °C for [100] growth directions. Calculated are the minimal growth rate 22 nm/s that is necessary for prevention of distortion appearance of epitaxial layer surface caused by elastic strains and the critical thicknesses of misfit dislocation formation – 50 and 54 nm for the [100] and [111] growth directions, respectively. It is shown experimentally that the lack of minimal supercooling leads to the island growth mode.

Keywords: liquid phase epitaxy, strain, growth rate, GaSb, InAs.

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1. Introduction

Recently the properties of type-II broken gap heterojunction based on InAs and GaSb are widely used for different optoelectronic devices manufacturing [1]. At present, the basic methods used for obtaining GaSb/InAs are molecular beam epitaxy (MBE) and metal organic chemical vapour deposition (MOCVD) [2, 3].

Most close to equilibrium growth conditions are provided with methods of liquid phase epitaxy (LPE) [4]. At the same time, there are several specific problems in the course of obtaining GaSb/InAs with the LPE methods. One of the problems is related with interaction between the substrate and liquid phase with non-equilibrium composition. It leads to substrate erosion, non-planarity and uncontrolled composition of the epitaxial layer [5, 6]. Such problem can be solved by LPE from an initially supercooled liquid phase [6]. The second type of problems is connected with availability of elastic strains in the GaSb/InAs heterostructure owing to lattice constants mismatch (0.74 % at the epitaxy temperature 450 °C).

The availability of elastic strains in the epitaxial layer, when it grows isomorphously until appearance of misfit dislocations, imposes a requirement on minimal solution-melt supercooling ΔT_{\min} due to increasing the solid phase chemical potential. When ΔT values of supercooling are smaller than ΔT_{\min} the epitaxial layer

grows in accordance with the Stranski-Krastanov mechanism [7]. As a result, layer planarity can be broken, to avoid the epitaxial layer non-planarity the supercooling that is sufficient for suppression of Stranski-Krastanov growth mechanism must take place until the layer thickness reaches a critical value of misfit dislocation formation. The elastic strains are driving forces for surface distortion of epitaxial layer, too [8, 9]. Process of suppression of such distortion development can be provided due to the sufficient epitaxial layer growth rates.

In this connection, the aim of this work is calculation of minimal supercooling ΔT_{\min} and necessary growth rate for optimization of GaSb growth on InAs substrate from liquid phase as well as providing continuous character of the epitaxial layer and its planarity.

2. Calculation model and results

GaSb/InAs heteroepitaxial layer critical thickness calculated using the Matthews and Blakeslee method [10] is significantly less than the experimental ones [11-13]. That is why, to determine the epitaxial layer critical thickness, used was a two-dimensional simulation of elastic strains and deformation energy distribution in the strained structure with an available network of misfit dislocations.

Simulation by the finite-element method was based on the Van-der-Merwe heteroepitaxial layer growth model [14]. But use of any adequate forces model on the substrate-epitaxial layer interface (such as the Peierls-Nabarro potential) leads to nonlinear or transcendent combined equations in the course of simulation. To solve this system the intermediate layer was introduced. The initial structure for simulation (Fig. 1) consisted of the unstrained epitaxial layer, unstrained substrate and strained intermediate layer, one side of which was fitted to the substrate lattice parameter and other one – to the unstrained epitaxial layer lattice parameter. Physical properties of this intermediate layer were defined by averaging those of the substrate and epitaxial layer. From [14], an atom located at the central line of symmetry can be considered as horizontally undisplaced. The misfit dislocation appears when the displacement between the substrate and layer atoms reaches a half of the lattice parameter.

As a critical epitaxial layer thickness, we assumed such thickness value that provides the equality of energies between two-dimensional strained epitaxial layers without dislocations and that with misfit dislocations. The energy of the elastically strained two-dimensional epitaxial layer is determined as follows:

$$F = \frac{1}{2} \frac{EU_{xx}^2}{(1-\mu^2)} \frac{a_l a_s}{a_l - a_s} h, \quad (1)$$

where E , μ , U_{xx} are Young's modulus, Poisson's ratio and epitaxial layer strain, respectively; a_l , a_s are the lattice parameters of the epitaxial layer and substrate, respectively, h is the epitaxial layer thickness. The factor $a_l a_s / (a_l - a_s)$ is the misfit dislocation period [14]. The obtained critical thickness (Fig. 2) is 50 nm for growth on (100) InAs substrate and 54 nm in the case of (111) substrate orientation. These values are in a good agreement with the experimental results from [12] based on X-ray scattering analysis of misfit dislocation density.

Minimal supercooling related with the necessity to compensate the influence of elastic strains can be defined from the equality of chemical potentials of solid

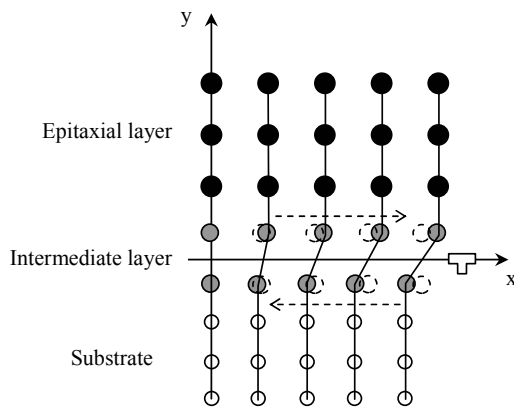


Fig. 1. Initial GaSb/InAs heterostructure for simulation.

and liquid phases in the regular solution approach. When considering $\Delta T_{\min} \ll T_0$, one can obtain

$$\frac{1}{2} \frac{EU_{xx}^2}{(1-\mu)} \Omega = k_B T_0 \ln \left(\frac{\gamma(T_0) C(T_0)}{\gamma(T_0 - \Delta T_{\min}) C(T_0 - \Delta T_{\min})} \right), \quad (2)$$

where Ω is the atomic volume, k_B is the Boltzmann constant, T_0 is the temperature of solution-melt saturation, $C(T)$, $\gamma(T)$ are the concentration and activity coefficients of GaSb in gallium melt at the temperature T . Based on dependence [15],

$$RT \ln \gamma = \alpha_{\text{GaSb}} (1 - x_{\text{GaSb}})^2, \quad (3)$$

where R is the absolute gas constant, α_{GaSb} , x_{GaSb} are the parameters of interphase interaction and mole fraction of GaSb in gallium melt and assuming $x_{\text{GaSb}} \ll 1$, Eqs (2), (3) lead to the transcendent equation with respect to ΔT_{\min} :

$$\frac{1}{2} \frac{EU_{xx}^2}{(1-\mu)} \Omega = k_B T_0 \left(\ln \frac{C(T_0)}{C(T_0 - \Delta T_{\min})} + R^{-1} \left[\frac{\alpha_{\text{GaSb}}(T_0)}{T_0} - \frac{\alpha_{\text{GaSb}}(T_0 - \Delta T_{\min})}{T_0 - \Delta T_{\min}} \right] \right), \quad (4)$$

Using the approximation of antimony atomic fraction dependence in gallium melt [16] on the temperature close to the saturation one $T_0 = 450^\circ\text{C}$, $x_{\text{Sb}} = 1.01 \cdot 10^{-9} + 10^{0.00987}$ and the parameter of interphase interaction dependence $\alpha_{\text{GaSb}} = (14738 - 21.48T) \text{ J/mol}$ [15], it can be found from (4) that the minimal supercooling temperatures are 7.8 and 5.8 °C for (111) and (100) orientations, respectively. These values are quite reachable during the epitaxy of GaSb layers, because the critical supercooling values of transition to labile region for antimony solution in gallium melts is about 12 °C [17].

Let us consider the influence of mechanical strains on growing epitaxial layer surface. In [8], the surface distortions induced by mechanical strains are considered with the harmonic approach. The highest rate of amplitude increasing is

$$\omega_m = \frac{27 D n_0 \Omega^2 \sigma_0^8 q_m^3}{2 E^4 \alpha^3 k_B T}, \quad (5)$$

where σ_0 is the epitaxial layer strain, D is the adatom diffusion coefficient, n_0 is the density of surface defects, α is the surface energy. Estimation of ω_m value by (5) shows that $\omega_m = 0.4 \text{ s}^{-1}$ (it was assumed that $n_0 = 1.46 \cdot 10^{10} \text{ cm}^{-2}$, $\alpha = 0.364 \text{ J/m}^2$, $D = 2.8 \cdot 10^{-5} \text{ cm}^2/\text{s}$, $\sigma_0 = 8.7 \cdot 10^8 \text{ Pa}$). As a characteristic time of process the value $1/\omega_m$ can be used [8]. Hence, for suppression of dislocations, it is necessary that the time of achieving the critical thickness, which leads to relaxation of considerable part of elastic strains due to misfit

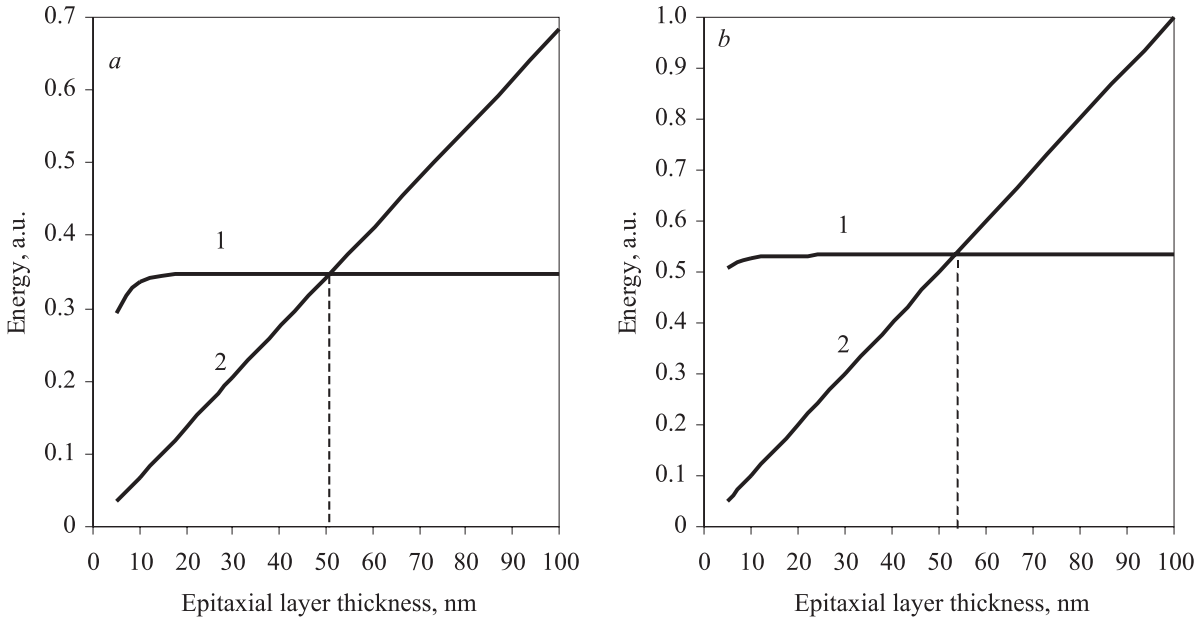


Fig. 2. Dependences of energy of structures that contains misfit dislocation (curves 1) and elastically strained dislocation-free epitaxial layer (curves 2) on the layer thickness, the layer being grown on the substrates with orientations (111) (a) and (100) (b).

dislocation formation, must be less than $1/\omega_m = 2.5$ s, hence, the growth rate must be higher than 22 nm/s.

3. Experiment

Calculated values of minimal supercooling and growth rate were used for GaSb heteroepitaxy on the (111) InAs substrate. The conditions for obtaining the planar layer were as follows:

$$\begin{cases} 7.8^\circ\text{C} \leq \Delta T < 12^\circ\text{C}, \\ h(2.5\text{ s}) > 55\text{ nm}. \end{cases} \quad (6)$$

Morphology of epitaxial layers obtained by (6) and at $\Delta T = 5^\circ\text{C}$ are shown in Fig. 3a and b, respectively. In Fig. 3a shown are the continuous heteroepitaxial layer obtained under fulfillment of the conditions (6). The layer roughness was less than $0.3\ \mu\text{m}$ (layer thickness was about $3\ \mu\text{m}$). The deviation from the conditions (6) led to pronounced island growth that resulted in the non-planar epitaxial layer surface (Fig. 3b).

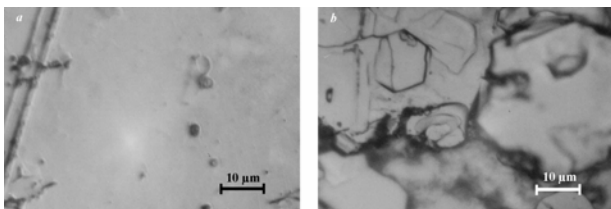


Fig. 3. Morphology of GaSb/InAs (111) epitaxial layers obtained: a) adhering the conditions (6); b) not adhering the latter (6).

4. Conclusions

Thus, influence of strains during the initial growth stages of GaSb/InAs heterostructure on epitaxial layer planarity was considered. The availability of strains increases the chemical potential in the solid phase. To compensate this increase, it is necessary to provide the supercooling temperature higher than 7.8°C for [111] and 5.8°C for [100] growth directions. Also, the elastic strains can cause distortion of epitaxial layer surface. To suppress all distortion modes the minimal growth rate must be 22 nm/s.

Such growth conditions must be provided until the epitaxial layer thickness reaches the critical thickness value for misfit dislocation formation when elastic strains considerably relax. The calculated critical thicknesses are 50 nm for [100] and 54 nm for [111] growth directions, respectively.

Experiment shows that adherence of calculated growth conditions causes obtaining the unbroken GaSb heteroepitaxial layer on the InAs substrate with a small roughness. Using the insufficient supercooling leads to an island growth mode.

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