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Atomic force microscopic study of surface morphology in Si-doped epi-GaAs on Ge substrates: effect of off-orientation

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Abstract

The Si-doped GaAs/Ge heterostructures have been grown under different growth conditions by low-pressure metal–organic vapor-phase epitaxial technique and investigated by atomic force microscopy (AFM). Our results indicate that the 6° offcut Ge substrate coupled with a growth temperature of ~675°C, growth rate of ~3 μm/h and a V/III ratio of ~88 are optimum set of growth conditions for the buffer layer growth of GaAs/Ge heterostructure solar cell. The surface morphology was found to be very good on 6° off-oriented Ge substrate and the root mean square (rms) roughness was approximately 3.8 nm over 3×3 μm^2 area scan compared to 2° and 9° off-oriented Ge substrates. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The nearly lattice matched GaAs/Ge (0.07%) heterostructures (HSs) have received a great deal of attention as starting materials for the space quality solar cell applications

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mainly because it can replace the conventional GaAs/GaAs solar cells, which suffer of their high cost and fragility [1–5]. Due to its high mechanical strength, Ge is an optimized substrate material in terms of its power-to-weight ratio for high efficiency GaAs/Ge solar cells, which are now replacing Si solar cells in some satellite applications [6]. As large area, minority carrier devices, III-V/Ge cells are extremely sensitive to defects. The elimination of antiphase domains (APDs) which are characteristic of the polar-on-nonpolar epitaxy, and suppression of large-scale interdiffusion across the GaAs/Ge heterointerface remains as key challenges for increased yield, reliability and performance.

Although the low lattice mismatch of the GaAs/Ge system suggests that it should be nearly dislocation free, polar-on-nonpolar heteroepitaxy poses several unique problems of its own, namely; the misfit dislocations (MDs) at the heterointerface due to the lattice and thermal expansion coefficient mismatch between the GaAs and Ge; the APDs bounded by antiphase boundary (APB) in the polar III-V epilayer due to the difference in lattice symmetry between GaAs and Ge and the interdiffusion of Ga, As and Ge across the heterointerface [7–15]. Suppression of APDs is the major obstacle to the realization of the device quality GaAs/Ge structures. These APDs separated by APBs are harmful for devices, which are based on the heterointerface properties, since the APBs act as nonradiative recombination surfaces [7,16]. Therefore, the careful control of the substrate surface structure and the initial growth conditions [7,10,17] are essential to grow device quality single-domain GaAs/Ge heterostructures.

It is essential to examine the surface roughening during the metal-organic vapor-phase epitaxial (MOVPE) growth of GaAs on Ge substrates in order to have structures with truly abrupt and planar interfaces formed during the growth. It is important to examine the surface morphology on an atomic scale, especially for MOVPE and correlate it to the growth mechanism. The morphology of the epitaxial film is influenced by deposition rate, which controls the adatom population on the surface, and substrate temperature, which affects the surface diffusion rate of the species [18]. An appropriate knowledge of the epitaxial growth mechanism will allow us to optimize the growth parameters for reproducibly grown APD-free GaAs on Ge substrates by MOVPE technique.

Atomic force microscopy (AFM) is a more recently developed technique and is capable of providing atomic scale images of surfaces [19–25]. A number of papers have recently appeared using the AFM to investigate the surface structure of GaAs layers grown by MOVPE. Nayak et al. [26] studied the surface morphology of MOVPE grown (001) GaAs with the influence of oxygen by using AFM. They showed that the concentration of impurity affects the periodicity and height of the features formed at the growth front. The surface morphology is controlled by a modification of the kinetic parameters by the impurity. Surface roughening due to high APD density of molecular beam epitaxial (MBE) grown GaAs on offcut Ge substrates has been studied by Xu et al. [27], using AFM measurement. The APDs can lead to surface root mean square (rms) roughness of the order of tens of nm, while Xu et al. observed the rms roughness of $\sim$1 nm averaged over 40 μm^2 areas for 2.5 μm thick GaAs films [12,27,28], which is similar to the roughness of homoepitaxial MBE-grown GaAs films [29]. In this investigation, we report the main results of surface morphology of Si-doped GaAs films on Ge substrates

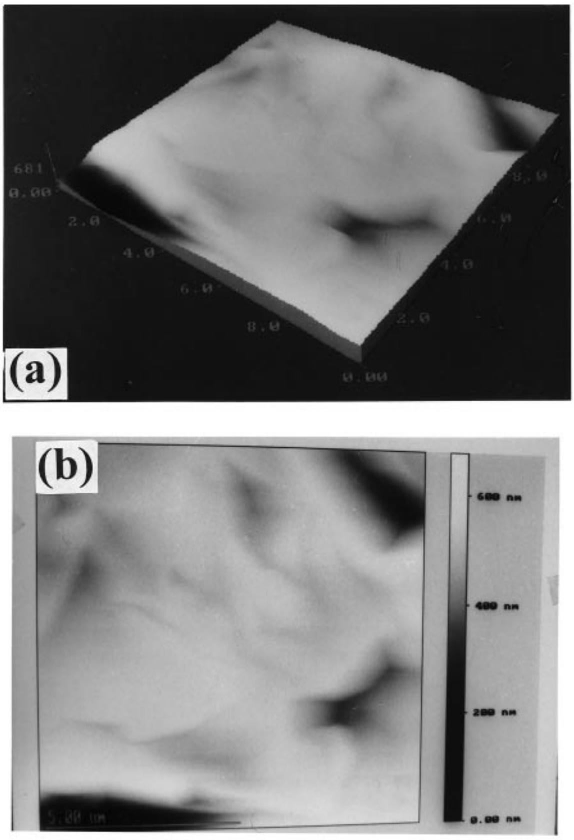

Fig. 1. Topographical image of the 1.5 μm thick Si-doped GaAs epitaxial layer grown on a 6° off-oriented Ge substrate with a growth rate of 3 μm/h, V/III ratio of 88.20 and growth temperature of 650°C. The different scan sizes are (a) 3 D, 10 μm × 10 μm and (b) 2 D, 10 μm × 10 μm.

grown by MOVPE technique with the effect of off-orientation and growth temperature by using AFM.

2. Experimental

The GaAs/Ge heterostructures were grown by low-pressure metal–organic vapor-phase epitaxial (LP-MOVPE) technique. High quality Sb-doped n^+-Ge substrates 2°, 6° and 9° off (100) towards [110] direction were used as substrates in each MOVPE growth run. The source materials were trimethylgallium (TMGa), 100% arsine (AsH_3), and palladium-purified H_2 as carrier gas. During the growth, the pressure inside the reactor was kept at 100 Torr and the growth temperature was varied from 600 to 700°C. The TMGa and AsH_3 fluxes were adjusted in such a way that a growth rate ranging from 3 to 12 μm/h was obtained. The total flow rate was 2 SLPM. The thickness of the epitaxial layers investigated ranged from about 1.5 to 6.5 μm. The details of the growth procedure can be found elsewhere [30–33]. The surface morphology was investigated by AFM in a constant-force mode.

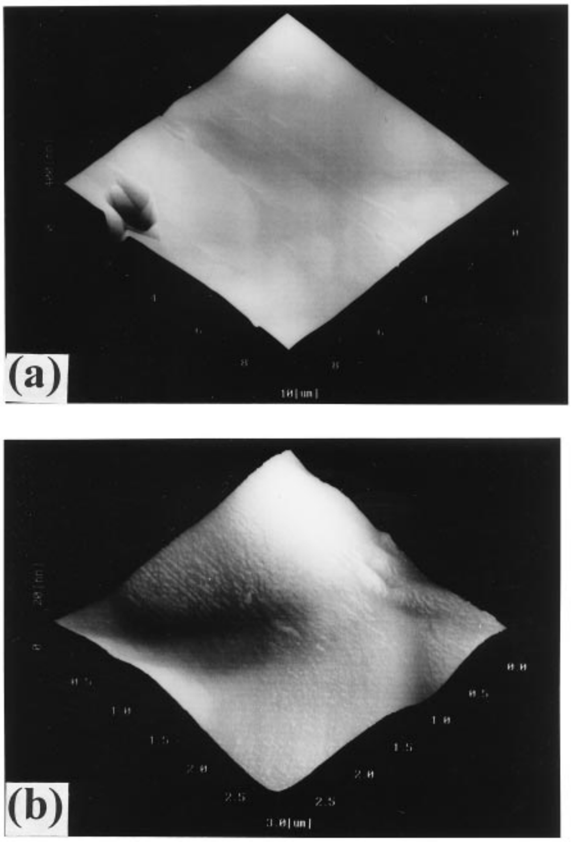

Fig. 2. Topographical image of the 1.5 μm thick Si-doped GaAs epitaxial layer grown on a 6° off-oriented Ge substrate with a growth rate of 3 μm/h, V/III ratio of 88.20 and growth temperature of 675°C. The different scan sizes are (a) 3 D, 10 μm × 10 μm and (b) 3 D, 3 μm × 3 μm.

3. Results and discussion

3.1. Effect of growth temperature on 6° off-oriented Ge substrate

The epitaxial films were investigated by AFM to reveal the surface roughening and other defects, probably the APBs. In general, the surface roughening in GaAs films on Ge substrates by MOVPE growth process is mainly due to APDs. Careful control of the substrate surface structure is essential to realization of APD-free GaAs on different off-oriented Ge substrates by MOVPE technique. AFM images on different length scales were taken to observe the top surface morphology of the epitaxial Si-doped GaAs films on 6° off-oriented Ge substrates. Three such AFM images of a small area scan are shown in Figs. 1–3 as a function of growth temperature in the range of 650 to 700°C, with a V/III ratio of 88.20 and a low growth rate of ~3 μm/h. The root means square (rms) roughness (σ), with

$$\sigma = \sqrt{\langle[\mathrm{h(r)} - \bar{\mathrm{h}}]^2\rangle}$$

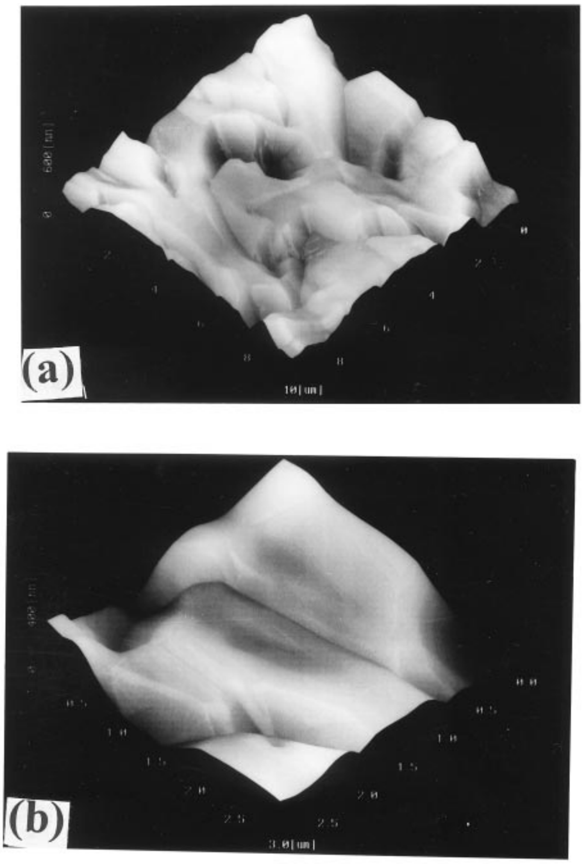

Fig. 3. Topographical image of the 1.5 μm thick Si-doped GaAs epitaxial layer grown on a 6° off-oriented Ge substrate with a growth rate of 3 μm/h, V/III ratio of 88.20 and growth temperature of 700°C. The different scan sizes are (a) 3 D, 10 μm × 10 μm, and (b) 3 D, 3 μm × 3 μm.

where $\bar{h}$ is the mean height of the surface and h(r) is the height of the surface at a distance r on the surface, was calculated from the AFM images. Table 1 summarizes the values off-orientation of Ge substrate, growth temperature, average roughness, rms roughness, and peak-to-valley value for all the present investigated films.

The main observations from Figs. 1–3 are (1) the average, the rms roughness, and peak-to valley value increases with increasing growth temperature in 6° off-oriented Ge substrate except at growth temperature of 675°C; (2) the films grown at 700°C shows APBs; and (3) the film grown at 675°C shows reasonably low average and rms roughness and has better surface morphology. The average roughness was determined from scans over the top of the films for different areas. The surface morphology of a film grown at 700°C or higher temperature on a Ge substrate off-oriented by 6°, shown in Fig. 3, gives a higher average and rms roughness, compared with the films grown at 675°C. Hence, a 6° offcut of Ge substrate coupled with a growth temperature of ~675°C may be the appropriate choice for the buffer layer growth of the GaAs/Ge heterostructure solar cell.

Table 1
The values of off-orientation of Ge substrate, growth temperature, averge roughness (R_a), rms roughness (R_{rms}), and peak-to-valley (P-V) value for all the present investigated films

Off-orientation	V/III ratio	Growth temperature (°C)	Growth rate (μm/h)	Scan size (μm × μm)	R_a (nm)	R_{rms} (nm)	P-V (nm)
6°	88.20	650	3	10 × 10	40.12	70.35	521.32
6°	88.20	675	3	10 × 10	16.23	30.82	431.4
6°	88.20	675	3	3 × 3	2.860	3.791	22.10
6°	88.20	700	3	10 × 10	74.21	93.92	658.7
6°	88.20	700	3	3 × 3	54.18	69.65	429.97
2°	44.10	700	6	10 × 10	90.53	112.13	353.19
6°	44.10	700	6	10 × 10	22.94	28.96	163.2
6°	44.10	700	6	3 × 3	5.437	6.814	39.51
9°	44.10	700	6	10 × 10	9.711	12.47	162.4
9°	44.10	700	6	3 × 3	2.78	3.531	22.85

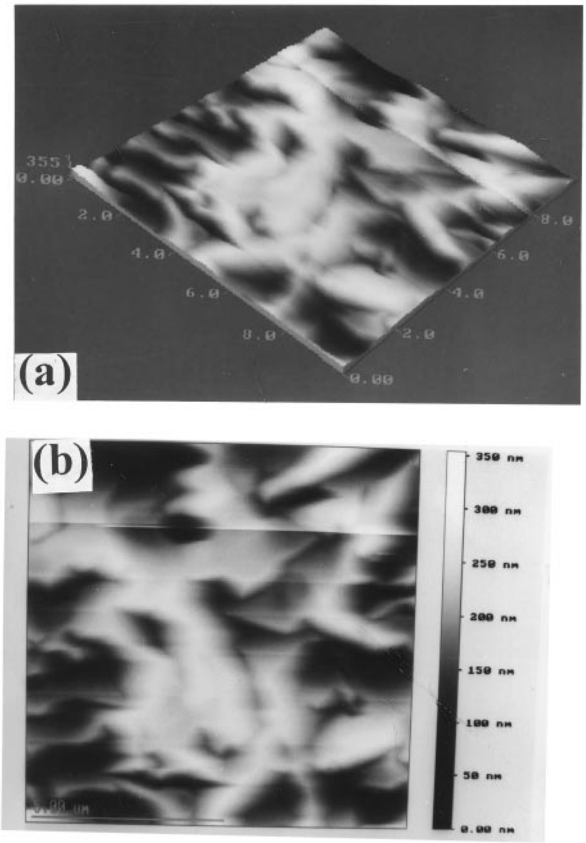

Fig. 4. Topographical image of the 3 μm thick Si-doped GaAs epitaxial layer grown at 700°C and a growth rate of 6 μm/h with a V/III ratio of 44.10 on 2° off-oriented Ge substrate. The different scan sizes are (a) 3 D, 10 μm × 10 μm, and (b) 2 D, 10 μm × 10 μm.

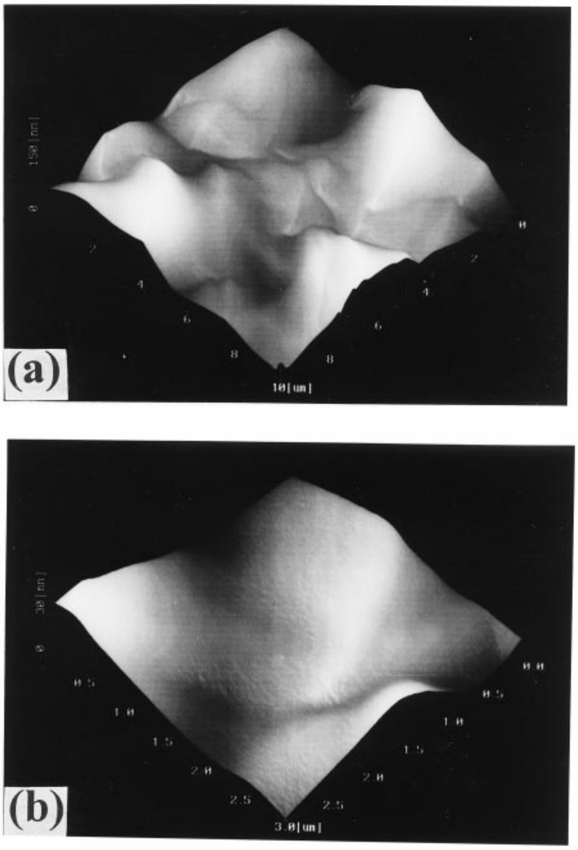

Fig. 5. Topographical image of the 3 μm thick Si-doped GaAs epitaxial layer grown at 700°C and a growth rate of 6 μm/h with a V/III ratio of 44.10 on 6° off-oriented Ge substrate. The different scan sizes are (a) 3 D, 10 μm × 10 μm, and (b) 3 D, 3 μm × 3 μm.

3.2. Effect of off-oriented Ge substrates

The effect of off-orientation on the surface morphology of Si-doped GaAs on Ge substrates was studied, keeping all growth parameters the same. The films were grown at the growth rate of ~6 μm/h, growth temperature of 700°C, and V/III ratio of 44.10. The average and rms roughness over the film on 9° show better surface morphology compared with 2° and 6° off-oriented Ge substrates. The average and rms roughness over these films are tabulated in Table 1. Figs. 4–6 show AFM images of the surface morphology of Si-doped GaAs on different off-oriented Ge substrates. From these observations, one can find that 9° off-oriented Ge substrate would be the proper choice for growing a buffer layer. Unfortunately, the Si incorporation into GaAs films on 9° off-oriented Ge substrate is not uniform along the depth, although the film/substrate interface was found to be abrupt [17] and, thus, rules out the possibility of using this orientation. On the other hand, the film on 2°off-oriented Ge substrate has APBs (Fig. 4), which was not observed on 6° and 9° Ge substrates. In order to confirm this, we have grown a film at 600°C, growth rate of ~3 μm/h, and V/III ratio of 88:1

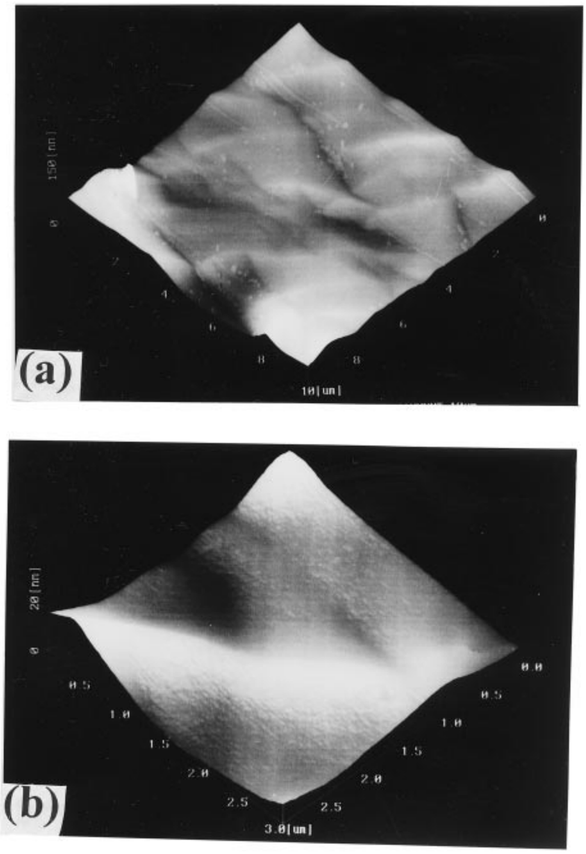

Fig. 6. Topographical image of the 3 μm thick Si-doped GaAs epitaxial layer grown at 700°C and a growth rate of 6 μm/h with a V/III ratio of 44.10 on 9° off-oriented Ge substrate. The different scan sizes are (a) 3 D, 10 μm × 10 μm, and (b) 3 D, 3 μm × 3 μm.

on 2° off-oriented Ge substrate. Fig. 7 shows the AFM images of the surface morphology of this film. From this figure, one can find that the film is clearly showing the mounds structure. One can also observe that there is no APB formation on 2° Ge substrate at a growth temperature of 600°C. One can rule out the possibility of growing GaAs on 2° off-oriented Ge substrate under the growth conditions specified in Fig. 4.

From Figs. 4 and 7, one can observe that the surface topography is different even though the films were grown on the same off-oriented Ge substrates. It is apparent that either the growth temperature or the growth rate plays a major role in surface morphology. The transition of APD-free → APDs → APD-free film with increasing growth temperature has already been found experimentally by Fischer et al. [34], in MBE-grown GaAs on Si. Li et al. [35] pointed out that in the MOVPE growth of GaAs on Ge substrates, such a transition temperature will depend on other parameters as well, such as the substrate misorientation angle and the growth rate. These APDs tend to make the film very rough. Nucleation of GaAs directly on the Ge surface (without any epitaxial Ge growth) typically results in high defect densities due to the uncontrolled initial surface. Ringel et al. [29] found that a Ge epitaxial

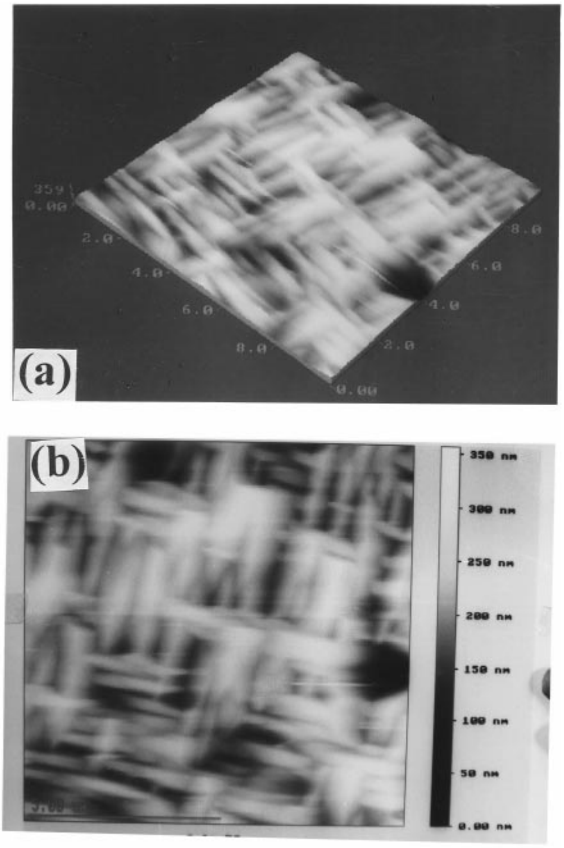

Fig. 7. Topographical image of the 1.5 μm thick Si-doped GaAs epitaxial layer grown at 600°C and a growth rate of 3 μm/h with a V/III ratio of 88.20 on a 2° off-oriented Ge substrate. The scan areas are (a) 3 D, 10 μm × 10 μm, and (b) 2 D, 10 μm × 10 μm.

film annealed above 640°C for ~20 min, coupled with a large 6° offcut, results in double-stepped Ge surfaces, which greatly suppress APD formation [36]. They also pointed out that growth on Ge surfaces that were not sufficiently annealed typically shows high APD density. The substrate temperature during the initial 100 nm GaAs growth is critical. The APDs may annihilate each other during growth, but they may propagate on the top of the film during the MOVPE growth process, as found by Li et al. [9,10,35], by etching the films from the top surface, through an optical microscope.

We have studied the optical properties of undoped and Si-doped GaAs epitaxial films on Ge substrates by photoluminescence (PL) spectroscopy. PL spectrum (exposed area 3 mm^2) of the top surface of the films was taken after etching the GaAs epitaxial layer. An electrochemical capacitance voltage (ECV) profiler was used to etch each portion (etch area $\approx$ 10 mm^2) of about 1.3 μm for undoped film and 0.8 μm for doped film, from the top surface of the layer. The PL spectrum from the depth below (either 1.3 μm for undoped or 0.8 μm for doped layer) shows a higher noise level, compared with that of the top surface spectrum [33]. This analysis tells us that very few nm thick GaAs films were rough, compared with the top surface. This may be due to the fact that there are many APDs within the few nm epilayer and they annihilate each other after thick GaAs layer growth.

Growth at too low a temperature, such as 550°C, results in excess of As point defects, which nucleate dislocation loops. These loops expand during the subsequent high-temperature GaAs growth, to generate high threading dislocation density in the thick GaAs film [12]. On the other hand, the growth at higher temperature and low growth rate may result in the formation of unwanted p-n junction due to simultaneous indiffusion of Ga and As inside the Ge substrate, which, in turn, reduces solar-cell efficiency [3]. If the temperature of the substrate during the growth is increased, the APD formation is increased. If the off-orientation is decreased, then a different kind of surface morphology is observed. Thus, the surface morphology can be controlled, by changing either the deposition rate or the growth temperature on the off-oriented Ge substrates.

4. Conclusions

The Si-doped GaAs/Ge heterostructures were grown by low-pressure metal-organic vapor-phase epitaxy and investigated by atomic force microscopy. We have identified MOVPE growth parameters to minimize antiphase domains during the growth of Si-doped GaAs films on different off-oriented Ge substrates. Our results indicate that 6° off-oriented Ge substrate coupled with a growth temperature of 675°C, a V/III ratio of $\sim$88, and a growth rate of $\sim$3μm/h comprise the optimum set of growth conditions for the buffer layer growth of Si-doped GaAs film on Ge substrate. This is an encouraging step towards the development of space-quality solar cells by LP-MOVPE technique.

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