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Initial stage and reconstruction of GaAs/Si heterostructures

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GaAs epitaxial layers on Si(1 0 0) substrates having a single or a double domain 2 × 1 have been grown by molecular beam epitaxy using the two-step growth mode and thermal regrowth techniques. The initial stage and the reconstruction of the GaAs/Si heterostructures have been investigated *in situ* by Auger electron spectroscopy and reflection high-energy electron diffraction. GaAs layers grown by both methods show the reconstruction of a single domain, and models for the process of GaAs growth have been presented to explain the self-annihilation of the antiphase boundary.

1. Introduction

In recent years, rapid developments and improvements in epitaxial film growth technology such as molecular beam epitaxy (MBE) and metallorganic chemical vapour deposition (MOCVD) have made possible the fabrication of high quality strained-layer heterostructures [1, 2]. The advances have allowed novel samples to be grown not only for basic physical investigation but also for many applications [3]. Although GaAs/Si heterostructures have inherent difficulties due to the large lattice mismatch ($\Delta a/a = 4.1\%$ at 25 °C) and thermal expansion coefficient difference ($\Delta\alpha/\alpha = 62\%$ at 25 °C), they are particularly interesting due to the number of possible electronic and optical applications [4–7] which result from utilizing the benefits of the high mobility capabilities of GaAs and the wafer cost of Si. Until now, several kinds of techniques such as two-step growth [8], rapid thermal annealing [9] and Si(1 0 0) 2° tilted [0 1 1] substrates [10] have been used to reduce the dislocation density of the GaAs epitaxial layers near the GaAs/Si hetero-interfaces. However, to our knowledge, a firm theory about the growth principle of the initial stage has not yet been established.

In this study, although Sakai *et al.* have suggested growth models of GaAs on Si [11], other models for the self-annihilation mechanism are proposed and experimental results are given. Because of the observation that the initial stage and reconstruction of the GaAs layer growth are useful to improve the quality of GaAs thin layers on Si substrates, the surface reconstruction at the initial stage has been investigated. Several types of surface rearrangements and crystal qualities with a variation of layer thicknesses were studied by Auger electron spectroscopy (AES) and reflection high energy electron diffraction (RHEED).

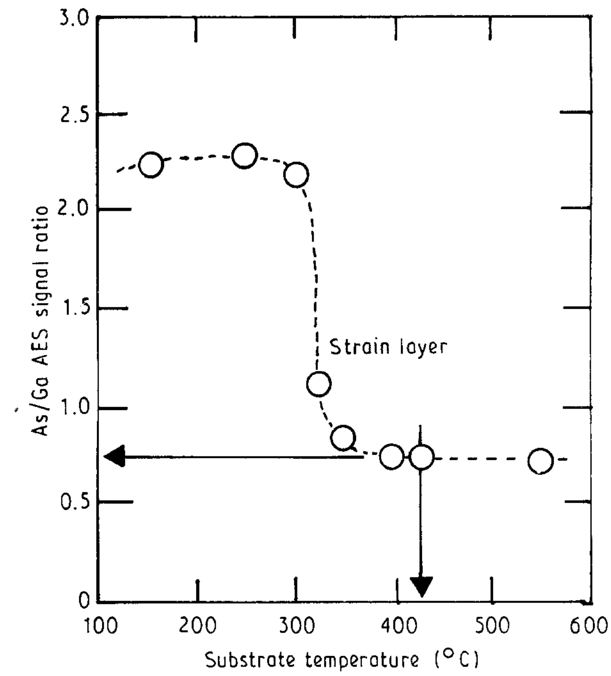

Figure 1 Variation of the Auger signal ratio for As/Ga deposited at 150 °C when the temperature is raised.

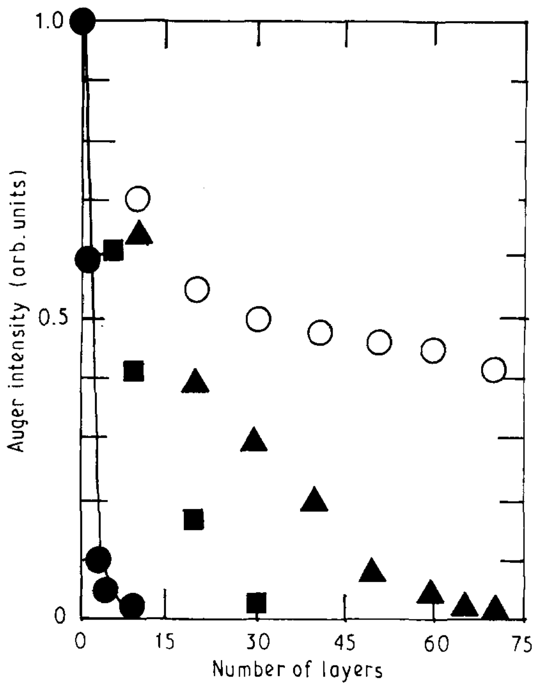

Figure 2 Variation of the Auger signal for Si as a function of the number of deposited GaAs layers for various substrate temperatures; the solid line is a theoretically fitted curve. (●) 150 °C; (■) 350 °C; (▲) 430 °C; (○) 550 °C.

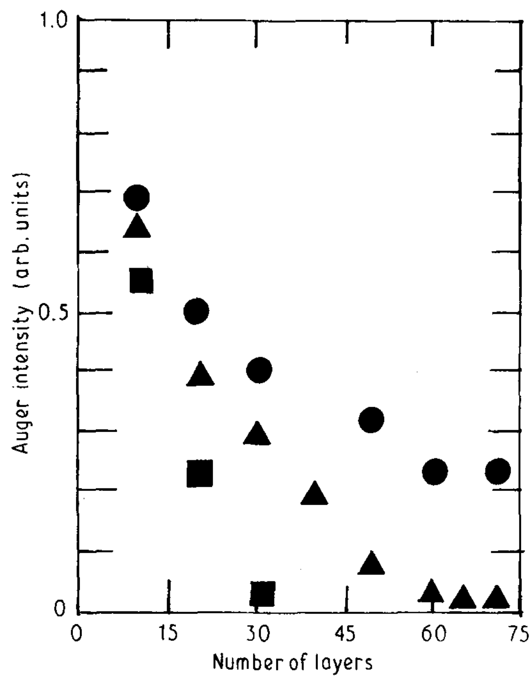

Figure 3 Variation of the Auger signal for Si as a function of the number of deposited GaAs layer for various growth rates at a substrate temperature of 430 °C. (■) 15 nm s^{-1}; (▲) 10 nm s^{-1}; (●) 5 nm s^{-1}.

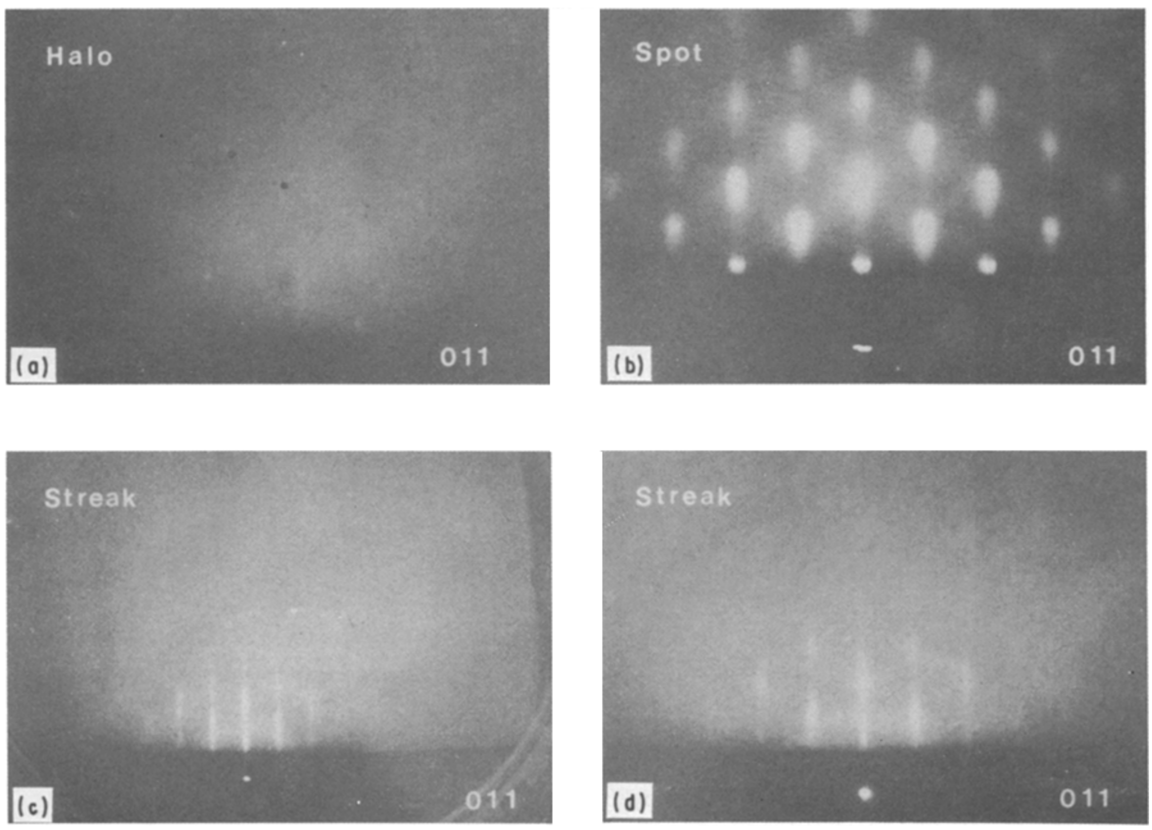

Figure 4 RHEED patterns of (a) a deposited GaAs layer at 150 °C; (b) after 590 °C heating; (c) after a growth of 1×10^4 nm at 590 °C; and (d) after a growth of 1 μm at 590 °C.

2. Experimental procedure, results and discussion

To obtain a single domain GaAs epitaxial layer on Si(1 0 0) substrates, the conditions for surface cleaning by heat and chemical treatment and the initial deposition temperature are very important. The bulk Si(1 0 0) substrates were chemically etched and cleaned in a MBE growth chamber by Ga-beam bombardment at 830 °C. In this process, a GaAs layer of 5×10^3 nm thickness was deposited between 150 °C

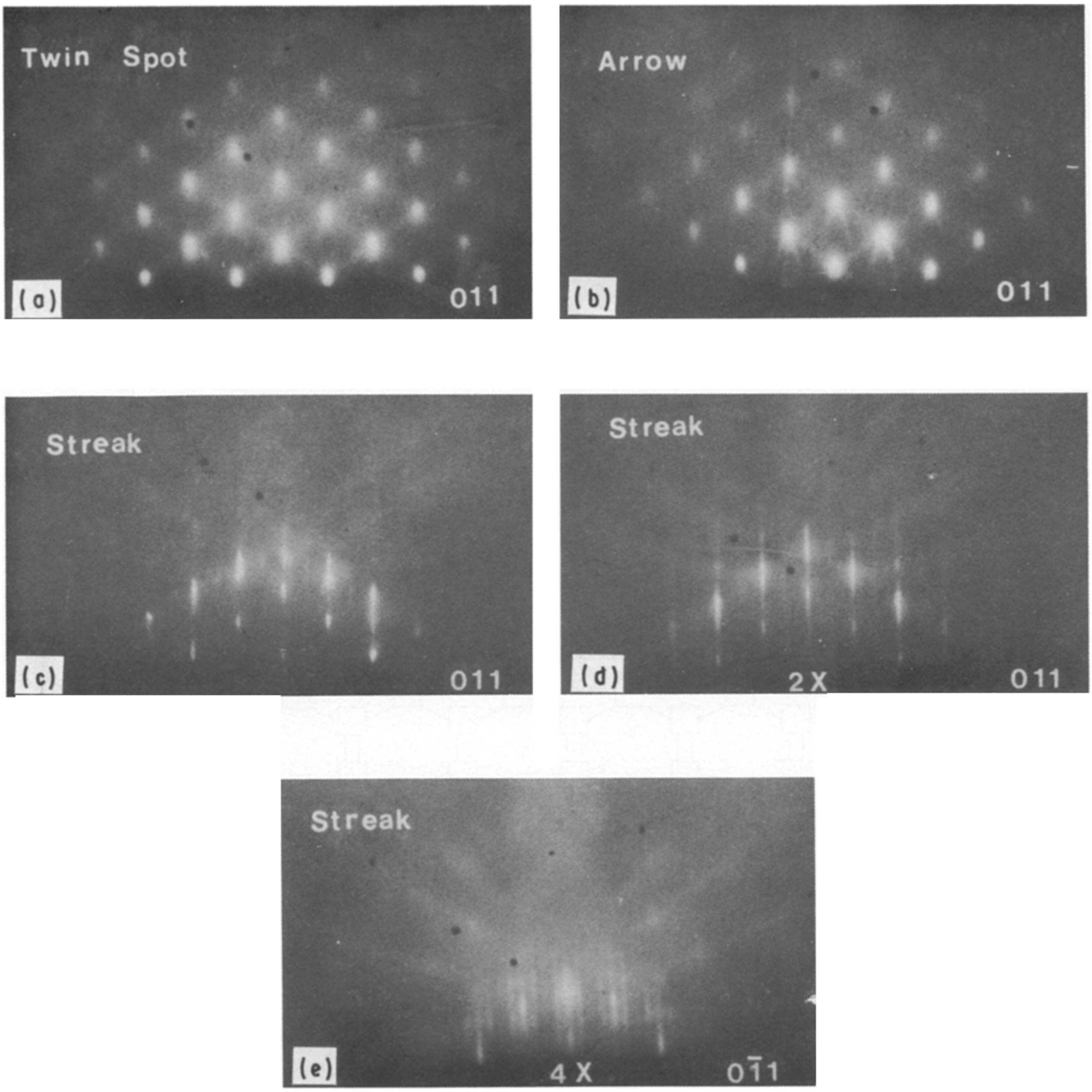

Figure 5 RHEED patterns of the GaAs epitaxial layer grown on double domain Si(1 0 0): (a) after a growth of 2×10^3 nm at 430 °C; (b) after 590 °C heating; (c) after a growth of 1×10^4 nm; (d) after a growth of 1 μm with [0 1 1]; and (e) after a growth of 1 μm with [0 $\bar{1}$ 1].

and 500 °C as shown in Fig. 1. The AES ratio for As/Ga is about 2.2 below 300 °C and rapidly decreases between 300 °C and 350°C reaching proper stoichiometry above 350 °C. As the growth temperature becomes lower and the epitaxial layer comes closer to a layer-by-layer growth mode, a single-storey growth of the GaAs epilayer is in good agreement with a theoretically fitted line at 150 °C [11] as shown in Fig. 2. At higher growth rates, the GaAs layer approaches a two-dimensional nucleation instead of a three-dimensional one as shown in Fig. 3.

Three kinds of GaAs epitaxial growth methods were used in the present experiment: thermal regrowth, two-step growth and Si(1 0 0) 3° tilted toward the [0 1 1] substrate. In the case of thermal regrowth, a residual oxide was removed by raising the substrate temperature to 950 °C; then, the substrate temperature was cooled to 150 °C, and a thin GaAs amorphous layer was deposited as the buffer layer. Subsequently, a GaAs epitaxial film was grown on the GaAs buffer layer which had been recrystallized at 590 °C while the RHEED pattern was being observed. The experimental procedure and growth conditions are shown in Table I. When a GaAs layer of thickness 5×10^3 nm was grown at 150 °C, it was seen to be an amorphous layer which was observed by RHEED as shown in Fig. 4a. While a GaAs epilayer 1×10^4 nm thick was being deposited as shown in Fig. 4c, the RHEED pattern was changing gradually to a streaky figure, and with the growth of an additional 1 μm of GaAs, a clear 2×4 reconstructed GaAs layer with a single domain was observed as shown in Fig. 4d.

For the case of two-step growth, the procedure is shown in Table II and the RHEED patterns from each step are shown in Fig. 5. After the double domain 2×1 surface structure of the Si(1 0 0) substrate was obtained by Ga-self-cleaning at 850 °C, the substrate was cooled to 430 °C, and a 2×10^3 nm GaAs layer was

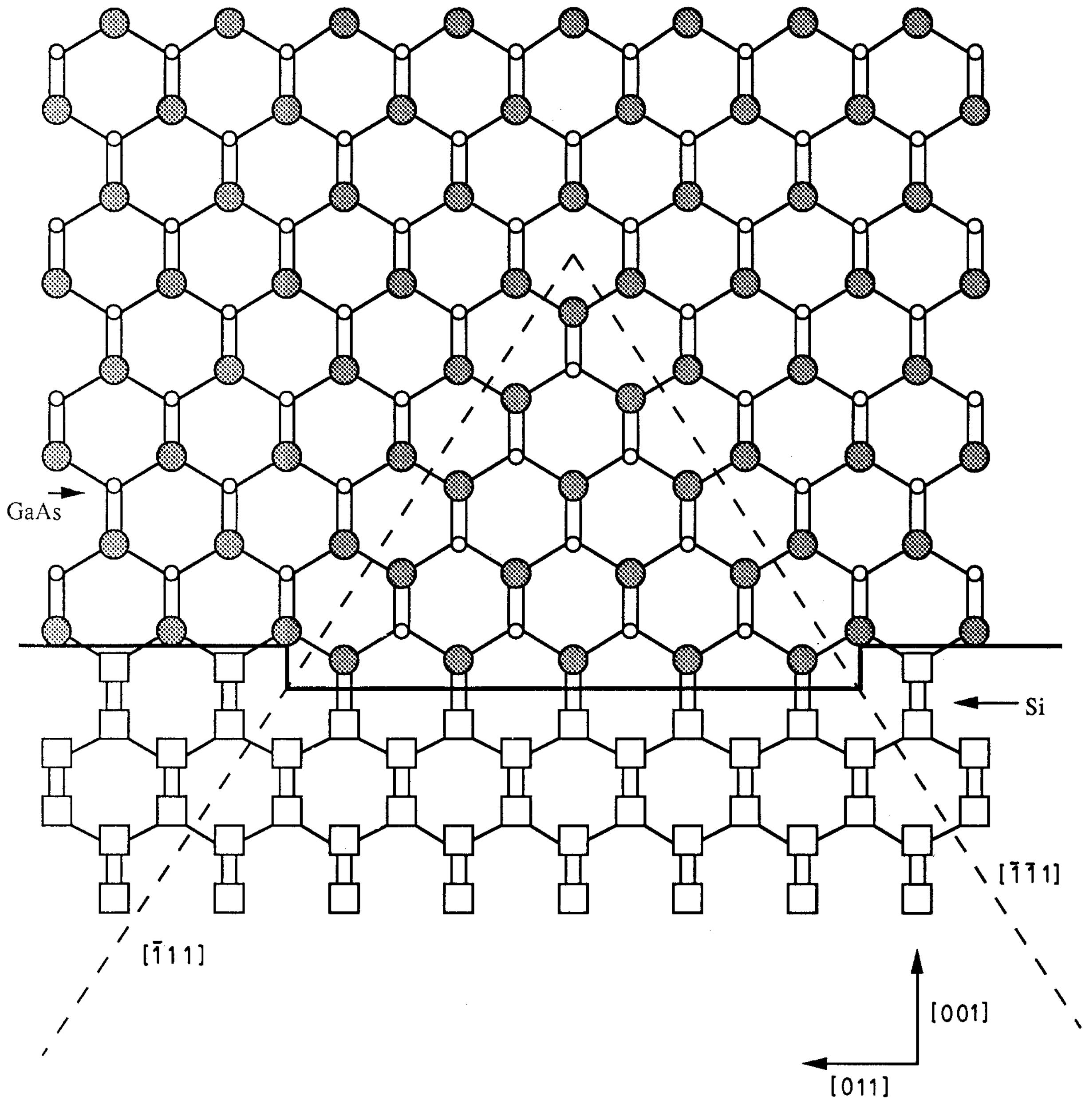

Figure 6 A model for self-annihilation of the antiphase boundary at ($\bar{1}$ 1 1) and ($\bar{1}$ $\bar{1}$ 1). (□) Si; (○) Ga; (◎) As.

TABLE I Growth conditions of the GaAs epilayers—thermal regrowth

Parameters	I	II	III	IV	V	VI
Substrate temperature (°C)	0–950	950	950–150	150	150–590	590
As pressure (Pascal)	–	–	–	1.066×10^{-6}	1.066×10^{-3}	1.066×10^{-3}
Ga cell temperature (°C)	–	–	–	960	–	980
Thickness (nm)	–	–	–	5×10^3	–	1×10^4
Time (min)	30	20	20	9	20	120

TABLE II Growth conditions of the GaAs epilayers—two-step growth

Parameters	I	II	III	IV	V	VI
Substrate temperature (°C)	0–850	850	850–430	430	430–590	590
As pressure (Pascal)	–	–	–	1.066×10^{-3}	1.066×10^{-3}	1.066×10^{-3}
Ga cell temperature (°C)	–	960	–	960	–	980
Thickness (nm)	–	–	–	2×10^3	–	1×10^4
Time (min)	30	4	20	3.43	10	120

grown as the first layer. The RHEED pattern is shown in Fig. 5a. Subsequently, the substrate was heated to the growth temperature of 590 °C, and a second layer of 1×10^4 nm was grown. After this buffer layer was grown, the RHEED pattern showed a twin-spot and was milky and arrow-like, indicative of the formation of GaAs islands with a small grain as shown in Fig. 5c; however, when the substrate temperature was raised to 590 °C, arrowhead-like configurations were dominant in the RHEED pattern as shown in Fig. 5b. While 1×10^4 nm of GaAs was deposited at 590 °C, the spot patterns altered piecemeal to streaky patterns and Kikuchi lines, and they became clearer at a thickness of 1 μm as shown in Figs 5d and 5e. Thus, in spite of using a double domain surface substrate, a single domain GaAs epitaxial layer was also obtained.

In addition to thermal regrowth and two-step growth of Si(1 0 0) substrates, GaAs buffer and epitaxial layers were also grown on Si(1 0 0) substrates tilted 3° towards the [1 1 0] surface using the same methods as mentioned above for two-step growth. Soon after the onset of layer growth, the RHEED pattern becomes streaky. As time goes on, the streaky patterns, which show the 2×4 structures, are more clearly visible. This implies either that the surface stages have single-atomic-layer heights or that the directions of the stages with two-atomic-layer heights are [0 1 1] and [0 $\bar{1}$ 1] [12].

In view of the above-mentioned experimental results, the following annihilation process of the anti-phase domain (APD) boundary is suggested. Fig. 6 shows a lattice diagram of GaAs epitaxial layers on untilted Si substrate surfaces. For simplicity, the lattice mismatch between GaAs and Si is ignored, and the surface steps presumably consist of a single atomic height. Kawabe and Ueda [12] suggested that the APD can be made to disappear by tilting the direction of misorientation from (1 0 0) to [0 $\bar{1}$ 1] at an initial stage. However, in this study, our experimental results show that single domain GaAs with a single atomic height can be grown on Si(1 0 0) substrates irrespective of the tilting of the substrates; that is, the APD boundary vanishes. In such a case, the APD boundary evanesces along the [0 1 1] planes. In contrast to this, although Ga–Ga binding is dominant at the corners as shown in Fig. 6, the APD boundary disappears along the {1 1 1} planes.

In addition to this model, Sakai *et al.* [11] proposed that the APD boundary lines of the (1 1 2) or (1 1 0) planes are generated easily in comparison with those of the (1 1 1) or (1 0 0) planes, as was determined from an excess energy calculation using Petroff's theory

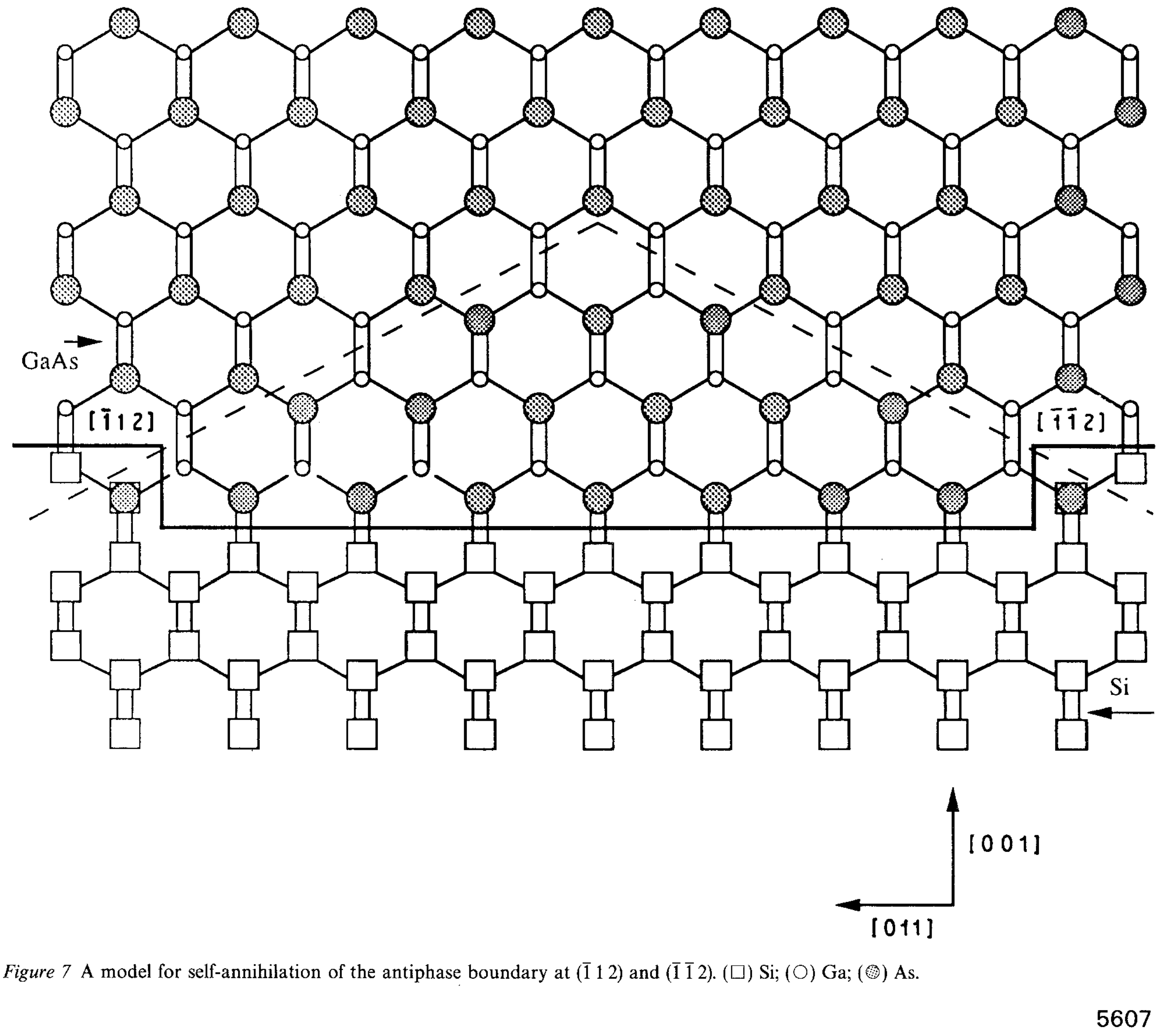

Figure 7 A model for self-annihilation of the antiphase boundary at ($\bar{1}$ 1 2) and ($\bar{1}$ $\bar{1}$ 2). (□) Si; (○) Ga; (◍) As.

[13]. Accordingly, another model can be suggested as shown in Fig. 7. Since As–As and Ga–Ga binding exist together at the APD boundary, this model is reasonably well satisfied under the condition of charge neutralization. Therefore, single domain GaAs epitaxial layers are grown continuously on the surface because of self-annihilation of the APD boundary. The initial growth stages of GaAs layers with pyramidal shapes on Ge substrates, as shown in Fig. 7, were also confirmed by transmission electron microscopy [14].

3. Conclusions

The present results demonstrate that GaAs epitaxial layers grown by MBE using two-step growth and thermal regrowth on Si(1 0 0) substrates with a single or a double domain 2×1 at the initial stage have a single domain. This confirms that single domain GaAs epitaxial layers can be grown on both single domain only and double domain only Si(1 0 0) substrates, and models for the self-annihilation structure of the APD boundary have been introduced.

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