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# Silicon doping into MBE-grown GaAs at high arsenic vapor pressures

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## Abstract

Properties of Si-doped, MBE-grown GaAs surfaces were studied. The doped lattice positions of Si depended on the As pressure and the state of surface reconstruction. The results show that the carrier density and Si incorporation depended on the intrinsic defects. Furthermore, Si-doped GaAs layers that were fabricated with periodic interruption of 2 s for each 5 ML had improved crystallinity as indicated by having sharper photoluminescence peaks and greater carrier densities over those samples grown without interruption. © 2002 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

Traditionally, III–V semiconductors such as GaAs are grown on (100)-oriented substrates because high-quality epitaxial layers can be grown on this surface under a wide range of growth conditions by molecular beam epitaxy (MBE). Although Si is widely used as an n-type dopant for GaAs(100), Si is found to be an amphoteric dopant on GaAs(*n*11)A with index  $n = 1–4$  [1–3]. Six elementary intrinsic point defect species are known in GaAs: vacancies in the Ga sublattice ( $V_{\text{Ga}}$ ), vacancies in the As sublattice ( $V_{\text{As}}$ ), Ga self-interstitials ( $I_{\text{Ga}}$ ), As self-interstitials ( $I_{\text{As}}$ ), and

antisite defects formed by either a Ga atom on an As site ( $\text{Ga}_{\text{As}}$ ) or an As atom on a Ga site ( $\text{As}_{\text{Ga}}$ ) [4]. Si atoms are included in Ga as donor point defects ( $\text{Si}_{\text{Ga}}$ ) and in As as acceptor point defects ( $\text{Si}_{\text{As}}$ ). These intrinsic point defects have different charge states depending on their energy-level position in the forbidden band. The native point defects affect many electrical and optical properties [1,3]. The type of doping depends on surface orientation, the temperature, and the As/Ga flux ratio [2,3]. Therefore, a lateral p–n junction can be formed using MBE by growing a Si-doped GaAs epilayer on a GaAs(*n*11)A-oriented substrate patterned to alternately expose slopes of different orientations. Compared with conventional vertical devices, lateral junction formation has the following possible advantages: device processing is simpler because the carriers can be injected directly

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into the active layer of the device by resonant tunneling. Also, device processing allows a successful combination of p–n junctions with other planar devices; for example, FETs and HEMTs in LSIs. The Si doping mechanism at high As pressures on high-index GaAs substrates is not fully understood; hence, further study is needed to fabricate high-quality films with high carrier concentrations for applications to lateral junction devices.

In this study, we determined the type of doping of Si on  $(n11)A$  with  $n = 1–4$  and  $(100)$  substrates for various MBE growth conditions.

## 2. Experimental procedure

Semi-insulating GaAs(100) and  $(n11)A$  ( $n = 1–4$ ) substrates were cleaned with Semico cleaning fluid, rinsed with distilled water, dried with  $N_2$  gas, mounted on an indium-free Mo holder, and then put into our VG Semicon V80H MBE machine. The substrates were then outgassed at  $450^\circ\text{C}$  for 1 h in the preparation chamber, then moved to the growth chamber where their oxide film was removed by heating at  $680^\circ\text{C}$  under an  $As_4$  flux for 5 min. For the growth of all samples, the Ga flux was constant at  $5.5 \times 10^{14}$  atoms/cm<sup>2</sup>s, which

produced a growth rate of 930 nm/h, and the substrate temperature was maintained constant at  $580^\circ\text{C}$ . The As flux was varied from  $4.3 \times 10^{-4}$  to  $7.1 \times 10^{-3}$  Pa. A GaAs buffer layer was first grown on the substrate. Then, a 930-nm thick, Si-doped, GaAs layer was grown. The Si K-cell temperature was set at  $1150^\circ\text{C}$ .

We compared the carrier densities and photoluminescence (PL) spectra between samples that were continually grown (sample A) and samples with a periodic interruption of growth (sample B). Here interrupted growth means that the Si, Ga, and As K-cell shutters were closed for 2 s after each 5 ML of growth. This comparison was done for  $(111)A$  and  $(100)$  surfaces.

The carrier densities and conduction type were examined using measurements of the Hall-effect and PL at 13 K.

## 3. Results and discussion

The dependence of charge-carrier type on the As/Ga ratio for various substrates is plotted in Fig. 1. In general, the As/Ga boundary between n- and p-types decreased as the substrates angle increased away from  $(111)A$ . However, the  $(211)A$  surface has a change from p- to n-type

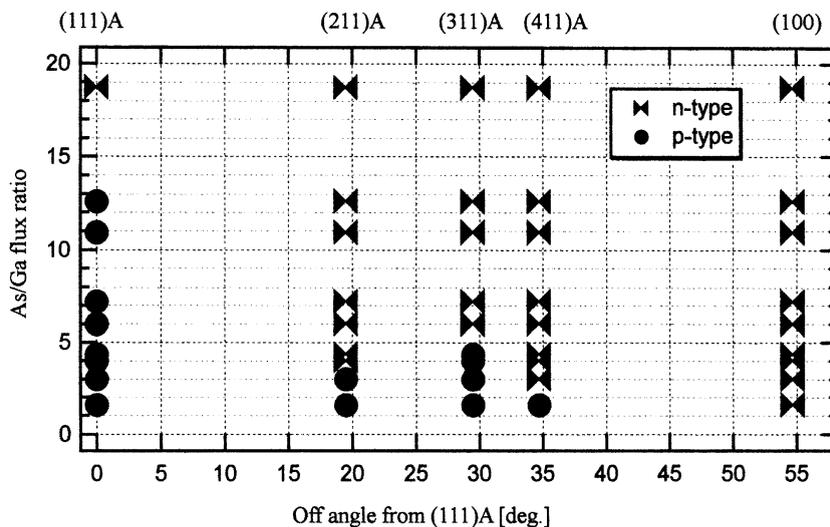


Fig. 1. Conduction type at various As/Ga flux ratios for several substrate orientations.

at lower As flux than the general trend. This might be related to the high density of pits (about  $1.5\text{-}\mu\text{m}$  sized pit per area of  $4.0\text{ }\mu\text{m}^2$ ) that we observed with the AFM. The (100) surface was n-type at all As/Ga flux ratios.

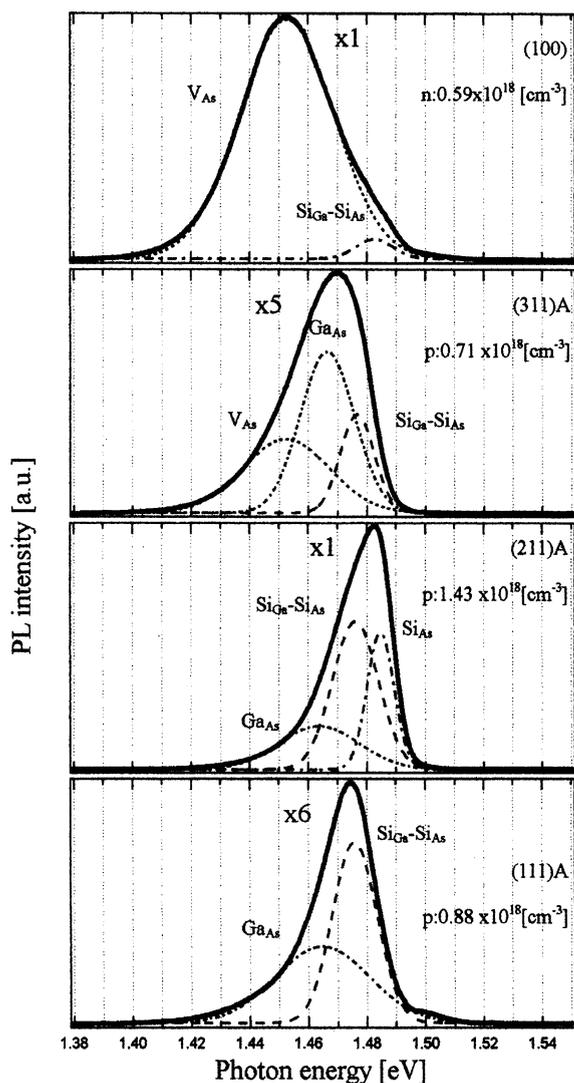


Fig. 2. PL spectra for samples grown at an As pressure of  $4.3 \times 10^{-4}$  Pa and As/Ga flux ratio of 1.5. The Si K-cell temperature was  $1150^\circ\text{C}$ . Solid curves are the measurements and the dashed curves are curves fitted to Gaussians. The substrate orientation and the charge carrier density are at the upper right of each plot. The symbols on the spectra indicate luminescence related to Si acceptor ( $\text{Si}_{\text{As}}$ ), Ga antisites ( $\text{Ga}_{\text{As}}$ ) and As vacancy ( $\text{V}_{\text{As}}$ ).

The PL spectrum of samples grown at low As pressure of  $4.3 \times 10^{-4}$  Pa shifted to lower energy as the substrate index increased as shown in Fig. 2. The peak for (211)A is an exception to this trend, as this surface has a higher-energy peak than that for (111)A, but this might be related to surface pits that were observed on the surface through AFM measurements. To identify peak positions, we fit the data to Gaussian curves as shown in Fig. 2. The (100) and ( $n11$ )A surface had two broad PL peaks as shown in Fig. 2. We assume that one peak is the luminescence for the As vacancy-to-conduction-band transition ( $\text{V}_{\text{As}}$ ) at about  $1.45\text{ eV}$  for (100) surface. For high-index surfaces, luminescence for the conduction-band-to-Si-acceptor transition ( $\text{Si}_{\text{As}}$ ) is at about  $1.48\text{ eV}$ , and the conduction-band-to-Ga-antisite-defect transition ( $\text{Ga}_{\text{As}}$ ) is at  $1.47\text{ eV}$ . ( $\text{V}_{\text{As}}$  is donor,  $\text{Ga}_{\text{As}}$  is acceptor.) The intrinsic point defects are As vacancies, Ga antisites, and Ga interstitials for As-poor conditions; whereas they are Ga vacancies, As antisites, and As interstitials for As-rich conditions [1–3]. However, the energy of the As vacancy is higher in our samples. Luminescence from a band gap was not seen. These energy values probably arise because the concentration of As vacancies is large for (100) surface and the concentration of Ga antisite defects is large for high index surfaces. Energies of As vacancies and Ga antisites are higher than the previous studies [1–3], probably because of differences in the growth conditions or defect concentrations [5–7]. Luminescence from As vacancy levels occurred on (311)A because the As dangling bond density on (311)A is larger than that on (111)A and (211)A. For (211)A, luminescence related to the Si acceptor occurred. This is probably the primary cause of the higher-energy peak position and the larger incorporation rate of Si atoms than other surfaces at the same low As pressure. Thus, the Si acceptor density is also the largest of all orientations at an As pressure of  $4.3 \times 10^{-4}$  Pa. The pits on (211)A might have influenced the incorporation of Si atoms and the change of conduction type to p-type at low As pressure (Fig. 1) in spite of the high density of dangling bonds at the surface [2,3].

The PL spectrum at high As pressure shifted to higher energy as the substrate index increased as

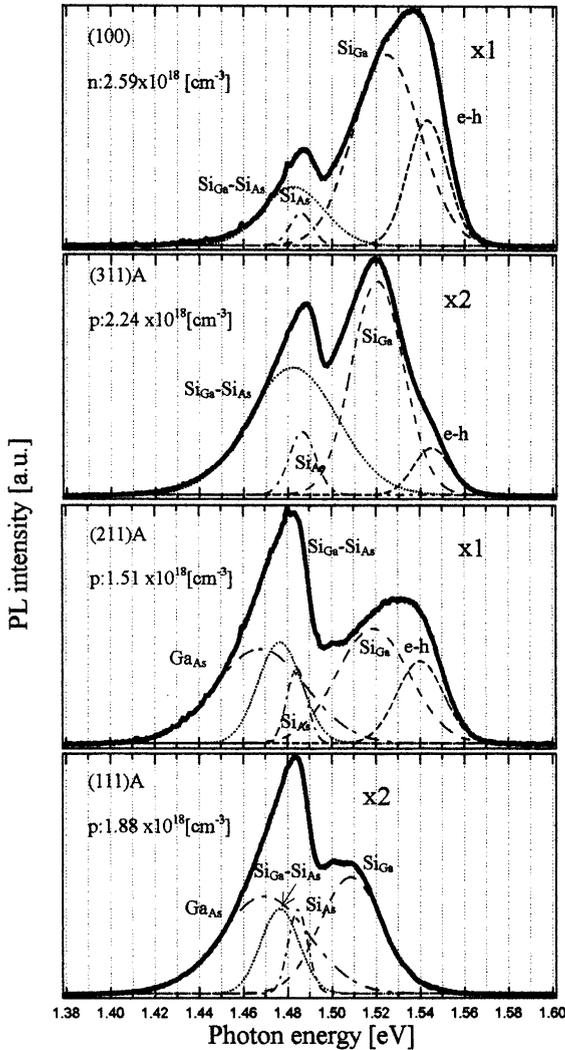


Fig. 3. PL spectra for samples grown at higher As pressure than that for the data in Fig. 2. The As pressure was  $7.1 \times 10^{-3}$  Pa, the As/Ga flux ratio was 18.7, and the Si K-cell temperature was  $1150^\circ\text{C}$ . Solid curves are the measurements and the dashed curves are the Gaussian fits. The orientation of substrate and carrier density are at the upper right. The symbols on the spectra indicate luminescence related to the band gap (e-h), Si donor ( $\text{Si}_{\text{Ga}}$ ), Si acceptor ( $\text{Si}_{\text{As}}$ ) and Ga antisite ( $\text{Ga}_{\text{As}}$ ).

shown in Fig. 3. The peak positions were determined using Gaussian fitting. The results in Fig. 3 show the peak energies of four or five separate peaks: luminescence related to the band gap (e-h), the Si-donor-to-valence-band transition ( $\text{Si}_{\text{Ga}}$ ), the Si-donor-to-Si-acceptor transition ( $\text{Si}_{\text{Ga}}\text{-Si}_{\text{As}}$ ), the

conduction-band-to-Si-acceptor transition ( $\text{Si}_{\text{As}}$ ), and the conduction-band-to-Ga-antisites transition ( $\text{Ga}_{\text{As}}$ ). At this high As pressure level, the spectra indicate that Si primarily incorporates as a donor on all surfaces, and secondarily incorporates as an acceptor. On (100), (411)A, and (211)A, the luminescence spectrum related to the Si donor is broader and the energy of peak shifts higher compared with that on (311)A and (111)A. The value of the peak is larger than 1.519 eV and the intensity is weak. (The energy gap is 1.519 eV at about 2 K [4].) Ga antisite defect peaks were measured only on (111)A and (211)A.

We interpret this data as supporting the following. On (100) at all As pressures and on (*n*11)A at high As pressures, Si atoms preferentially attach to Ga sites to become donors, whereas at low As pressures on the (*n*11)A surfaces, the Si atoms preferentially attach to As sites to become acceptors. The PL characteristics are governed by As vacancy and Ga antisites defects at low pressure, whereas luminescence related to these defects is not seen at high pressure on (100) and (311)A. The (100) surfaces had low quality at high pressure, which might have made it difficult to detect such defects. Intrinsic defects, for example the Ga vacancy, are thought to produce a PL peak below 1.38 eV, which is the lowest energy in our experiments. Also, Ohachi et al. [3] reported that luminescence from the  $\text{Si}_{\text{Ga}}\text{-V}_{\text{Ga}}$  complex occurs at about 1.26 eV [1].

The PL spectrum from (100) shifted to higher energy and had more structure at high As pressure as shown in Fig. 4. According to the reflection high-energy electron diffraction (RHEED) pattern, the growing surface at low As pressures of  $< 1.3 \times 10^{-3}$  Pa had the  $(2 \times 4)$  reconstruction. Peaks at As pressures of more than  $10^{-3}$  Pa, which separated into four components as in Fig. 3, were produced when the growth surface was  $c(4 \times 4)$ . The PL from the As vacancy at 1.45 eV is strong at the lowest pressures, and the PL signal from the Ga antisite defect appeared at higher As pressure. The PL signal from the Si donor to acceptor near 1.49 eV became strong at  $1.2 \times 10^{-3}$  Pa, and the Si donor to valence band at about 1.5 eV appeared. Above  $2.5 \times 10^{-3}$  Pa, the PL for the acceptor and donors decreased and increased, respectively. PL

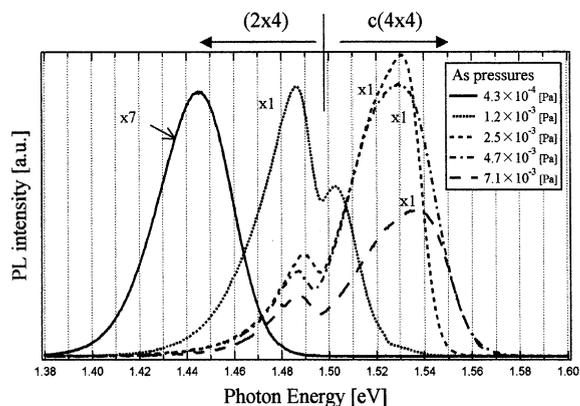


Fig. 4. PL spectra for (100) at various As pressures. The Si K-cell temperature was 1150°C. The surface reconstructions of these surfaces were (2 × 4) for the two leftmost spectra and c(4 × 4) for the three rightmost spectra. The carrier density is  $0.93 \times 10^{18} \text{ cm}^{-3}$  for  $4.3 \times 10^{-4} \text{ Pa}$ ,  $0.93 \times 10^{18} \text{ cm}^{-3}$  for  $4.3 \times 10^{-4} \text{ Pa}$ ,  $3.9 \times 10^{18} \text{ cm}^{-3}$  for  $1.2 \times 10^{-3} \text{ Pa}$ ,  $1.7 \times 10^{18} \text{ cm}^{-3}$  for  $2.5 \times 10^{-3} \text{ Pa}$ ,  $3.0 \times 10^{18} \text{ cm}^{-3}$  for  $4.7 \times 10^{-3} \text{ Pa}$  and  $2.6 \times 10^{18} \text{ cm}^{-3}$  for  $7.1 \times 10^{-3} \text{ Pa}$ .

characteristics show that the intrinsic defects clearly affected the incorporation of Si atoms. The surface reconstruction becomes (2 × 4) below  $1.3 \times 10^{-3} \text{ Pa}$ , which corresponds to the presence of As vacancies and Ga antisite defects at low As pressure. This suggests that the type of reconstruction affects the incorporation of Si atoms.

We now describe how growth interruption improved the electronic properties. Irrespective of the substrate index, the carrier density in interrupted samples was higher than that for continuous growth. Thus, interruption increased the Si incorporation rate. The method of growth also affected the PL spectra. The luminescence of the interrupted sample and the continuously grown sample is similar for (100) (Fig. 5, bottom), but luminescence for (111)A drastically sharpened when the growth was interrupted (Fig. 5, top). For luminescence with an interrupted (111)A surface, the Si acceptor peak is not only stronger but also sharper, whereas the Ga antisite defect peak is weaker than that with normal growth. Hence, with interrupted growth, the quality is better and more Si atoms became acceptors on (111)A. This agrees with the carrier densities inferred from the Hall-effect measurements. Therefore, the absorption of

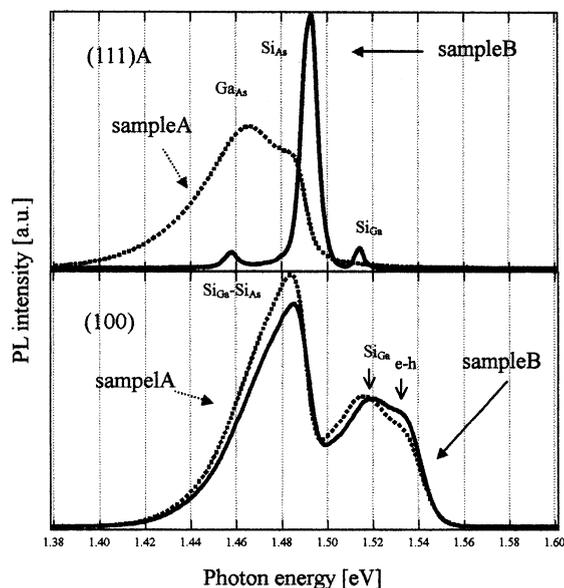


Fig. 5. PL spectra for (111)A and (100) surfaces grown with interruption (sample B) and without interruption (sample A). The Si K-cell temperature was 1150°C. For (100), the As pressure was  $1.32 \times 10^{-3} \text{ Pa}$  and the As/Ga flux ratio was 5.5. For (111)A, the As pressure was  $5.0 \times 10^{-4} \text{ Pa}$ , and the As/Ga flux ratio was 2.0. Solid curves are for interrupted growth and the dashed curves are for normal growth. The (111)A is p-type with carrier density of  $3.09 \times 10^{18} \text{ cm}^{-3}$  for interruption growth and  $2.06 \times 10^{18} \text{ cm}^{-3}$  for normal growth. The (100) is n-type with carrier density of  $2.45 \times 10^{18} \text{ cm}^{-3}$  for interruption (sample B) and  $2.03 \times 10^{18} \text{ cm}^{-3}$  for normal growth (sample A).

Si atoms is related to the state of the surface and the carrier density is probably influenced by the intrinsic defects, for example, the Ga antisite defects. This study indicates that interrupted growth decreased the intrinsic defect density and made the carrier density higher, especially on (111)A.

#### 4. Conclusions

We found that the incorporation of Si into GaAs substrates depended on orientation and growth conditions. The cause of the PL energy peak shifts depended on the substrate orientation and the presence of intrinsic defects. The (211)A surface had a higher-energy peak than other high-index surfaces at the same low As pressure, which

was caused by the higher incorporation rate of Si in As sites. By varying the As pressure on (100) substrates, we found that luminescence on  $(2 \times 4)$  surfaces differed from that on  $c(4 \times 4)$ . Luminescence from acceptor levels was strong for the  $(2 \times 4)$  reconstruction, which indicates that Si atoms tend to go into As sites. Whereas, in the  $c(4 \times 4)$  structure, luminescence from donor levels was strong, which indicates that Si atoms tend to go into Ga sites. Furthermore, higher levels of doping and a narrower range of band gap energies were obtained by periodically interrupting the Ga and As supplies during growth, thus showing that the absorption of Si atoms is related to the state of the surface.

The quality of Si-doped GaAs films was better when the supplies of Ga, As, and Si was shut off (interrupted) for 2 s every 5 ML. With interruption, the intrinsic defect density decreased and the carrier density increased.

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