

In-situ Characterization of the Initial Growth Stage of GaAs on Si by Coaxial Impact-Collision Ion Scattering Spectroscopy

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The initial growth stage of GaAs on Si has been in-situ characterized by coaxial impact-collision ion scattering spectroscopy (CAICISS). The behavior of As atoms on the Si surface and at the step sites are analyzed. The results of analysis on the initial growth stage strongly suggest that the three-dimensional island growth of GaAs on Si occurs even in 1 mono layer (ML) GaAs growth.

1. INTRODUCTION

The in-situ characterizations of semiconductor surface structures during crystal growth have been extensively studied in recent years along with the rapid increase of various nanoelectronics fabrication techniques. Coaxial impact-collision ion scattering spectroscopy (CAICISS) is one of the promising characterization techniques for in-situ or real-time studies of the surface structures of semiconductor materials.¹⁾ Some groups have already reported the surface structures of GaAs, InP and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ during MBE growth by the CAICISS.^{2,3)}

However, no report has been published on highly lattice mismatched epitaxial systems such as GaAs on Si by the CAICISS analysis. In lattice mismatched epitaxy, the controlling of dislocation formation and propagation in the epitaxial layers is the central problem which is strongly related to the growth mode and mechanism during the initial growth stage and the other factors such as differences in the thermal expansion coefficients. Therefore, it is urgently needed to deeply understand the initial growth stage using the new characterization method from the different aspects for improving the crystal quality, even though many pioneer studies using reflection high energy electron diffraction (RHEED), Auger electron spectroscopy (AES) and scanning tunneling microscopy (STM) have already been carried out.⁴⁻⁶⁾ In this report, we show the usefulness of in-situ CAICISS analysis in studying the initial growth stage of GaAs on a Si system.

2. EXPERIMENTAL

We used a newly designed CAICISS system, which has an off-axis arrangement of the ion source for analysis.²⁾ The CAICISS is connected to a III-V molecular beam epitaxy (MBE) chamber in a

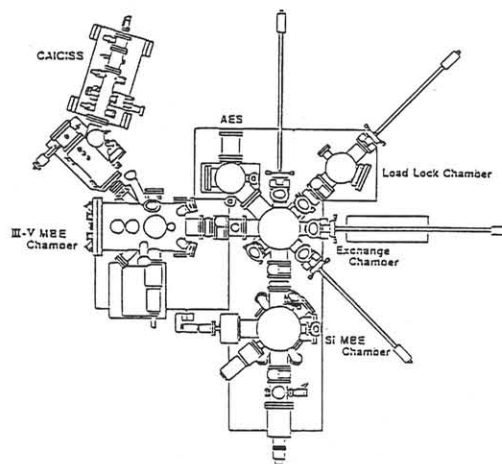


Fig.1 Multichamber MBE system.

multichamber MBE system, as shown in Fig. 1. (100) Si wafers inclined toward the $[0\bar{1}1]$ direction by 2° were used as substrates. They were transferred to the III-V MBE chamber from the Si MBE chamber via an exchange chamber just after the thermal cleaning of the Si surface and the buffer-layer epitaxy of Si with post growth thermal annealing in order to obtain clean (100) Si single-domain surfaces. The background pressure during the transfer was less than 3×10^{-10} Torr. In the CAICISS measurements, 2 keV He^+ ions were used for the probe beam; the azimuths of the incident beam were along the $[010]$, $[011]$ and the $[0\bar{1}\bar{1}]$ axes of the Si crystal and the pulse width of the incident beam was 100 nsec. The incident angle (α) of the He^+ ion beam was measured from the crystal surface along each azimuth. The energy loss of scattered particles was measured by a time-of-flight (TOF) method. Details regarding the CAICISS system have been already published.²⁾

3. RESULTS

3.1. Shadow cones of the GaAs and the Si

The shapes of the shadow cones of the GaAs and the Si targets under the present conditions were determined from the overall angular distribution of the normalized scattering intensity along the [011] and the [010] azimuths, as shown in Fig. 2. The open and closed circles represent the experimental values for GaAs and Si targets, respectively. The dashed and solid lines represent the calculated cone shapes for each target.⁷⁾ In the overall angular distribution, the peaks of the scattering intensity are due to focusing effects caused by the shadow cones of GaAs and Si targets. A good agreement between the experimental and the calculated values is obtained, as shown in Fig. 2.

3.2 As atoms on Si

Figures 3 (a) and (b) show, respectively, typical CAICISS spectra at $\alpha=14^\circ$ along the [011] azimuth from a Si substrate annealed at 750 °C after the low-temperature deposition of As at -30 °C, and from the Si substrate at 550 °C under a background pressure in the chamber. In spite of a closed As_4 beam shutter under a background pressure of 5×10^{-9} Torr in the chamber, the scattering intensity at 6780 nsec from As atoms dramatically increased at 550 °C compared to that at 750 °C. For the Si lattice parameter, an incident angle of 14° is near to the critical angle (α_c) which is the lowest value found for an enhancement in the scattering intensity by a focusing effect due to the nearest-neighbor surface As atoms. The enhancement of the scattering intensity at $\alpha=14^\circ$ indicates a partial As covering of the Si surface at 550 °C. On the other hand, the dramatically decreased As signal at 750 °C indicates that almost all As atoms on the Si surface are desorbed at this temperature. Figures 4 (a) and (b) show the low-angular distribution of scattering intensity under the same conditions given in Figs. 3. Peak at $\alpha=6^\circ$ is observed in the both cases, and a shoulder at $\alpha \sim 13^\circ$ is also observed in the case of 550 °C. The origin of the shoulder at 550 °C is due to a partial covering of Si surface by the As atoms, as stated above, and the origin of the peak at $\alpha=6^\circ$ is

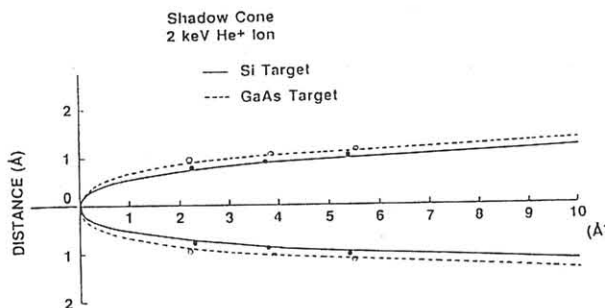


Fig.2 The shapes of the shadow cones of the GaAs and the Si targets.

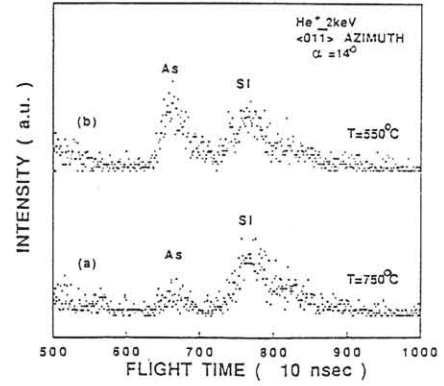


Fig.3 Typical CAICISS spectra at $\alpha=14^\circ$ along [011] azimuth (a) from a Si substrate annealed at 750 °C after the low-temperature deposition of As and (b) from the Si substrate at 550 °C.

discussed in section 4.

3.3 Initial growth stages of GaAs on Si

Figure 5 shows the low-angular distribution of GaAs and Si signals after 1 mono layer (ML) of GaAs growth on Si. The shoulder intensity at $\alpha \sim 13^\circ$ of the GaAs signal clearly increased after this 1 ML GaAs growth compared with that shown in Fig. 4 (b); this is in contrast with the slight decrease in the Si peak intensity at $\alpha=13^\circ$. The peak at $\alpha=30^\circ$ of the GaAs signal shows a focusing effect due to atomic ordering of 1 ML GaAs on Si, since the peak at $\alpha=30^\circ$ is due to a focusing effect by the As and/or Ga

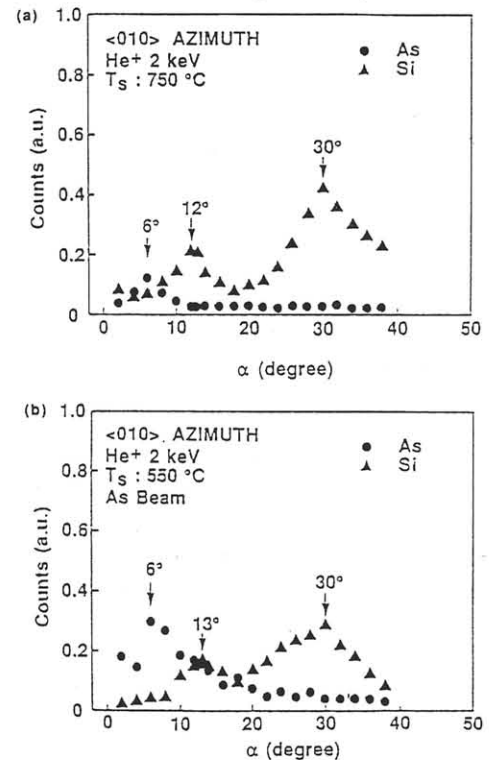


Fig.4 Low-angular distribution of scattering intensity from the As covered Si substrate (a) at 750 °C and (b) at 550 °C.

atoms in the GaAs layer. These results indicate that the coverage of the GaAs layer on the Si surface slightly increased than the As covering case, since the peak intensity of Si signal at $\alpha=13^\circ$ is due to surface scattering by the focussing effect at the critical angle of Si surface, $\alpha_c=13^\circ$. However, the coverage of GaAs may be not complete at this stage, because the Si signal at $\alpha_c=13^\circ$ can be still observed more than background noise. The fact that the peak of the GaAs signal at $\alpha=6^\circ\sim 8^\circ$ was still observed in spite of the increase in the GaAs coverage on the Si surface, may reflect an independent origin of the peak at $\alpha=6^\circ$ to the surface coverage.

4. DISCUSSION

In this section the origin of the peak at $\alpha=6^\circ$ below the critical angle ($\alpha_c=13^\circ$) as well as the growth mode of GaAs on Si during the initial stage are discussed. The peaks at $\alpha=6^\circ$ in Figs. 4 and 5 may be due to the As atoms at the step sites of Si surface, because little scattering intensity should be expected below the critical angle by the shadowing effect from the nearest-neighbor atoms of the top surface. Kubo et al have reported an enhancement of the scattering intensity below the critical angle in an off-angle substrate for the GaAs, and calculated the step density using the CAICISS data.⁸⁾ Moreover, in the present experiment, the peak intensity at $\alpha=6^\circ$ depended on the substrate temperature, as shown in Figs. 4 (a) and (b); the shoulder at the critical angle in Fig. 4 (a) disappeared at 750°C , as shown in Fig. 4 (b). That is, as stated in section 3.2, almost all As atoms on the Si surface are considered to be evaporated at 750°C , although the considerable amount of As atoms remain at the step sites. This speculation seems to be reasonable, if we take into consideration the bond difference of As atoms on the Si surface and at the step sites. That is, As atoms on the Si surface may make the 2-fold covalent bonds to the Si atoms and they may form As-As dimers on the Si surface. In contrast, As atoms at the step sites

make the 3-fold covalent bonds to Si atoms. Therefore, As atoms at the step sites are more energetically stable and can remain at the step sites of Si up to a rather high substrate temperature. From these considerations, the origin of the peak at $\alpha=6^\circ$ will be ascribed to the As atoms at the step sites.

The peak of the Si signal at a critical angle of 13° in Fig. 5 indicates that the Si surface was not completely covered with a GaAs layer after 1 ML of GaAs growth, because a considerable decrease in the Si signal intensity at $\alpha_c=13^\circ$ is expected if a complete coverage by the GaAs layer is achieved, as stated in section 3.3. This may be due to a 3-dimensional island growth of GaAs on Si, even in 1 ML GaAs growth. This result is resonable from STM observations.⁶⁾

5. CONCLUSIONS

We observed the initial growth stage of GaAs on Si by the CAICISS. The analysis suggested that As atoms at the step sites of the Si substrate remained there even at a substrate temperature of 750°C , although As atoms on the Si surface were considered to be almost evaporated at that temperature. Also the 3-dimensional island growth of GaAs on Si, even in 1 ML GaAs growth, was anticipated from the analysis.

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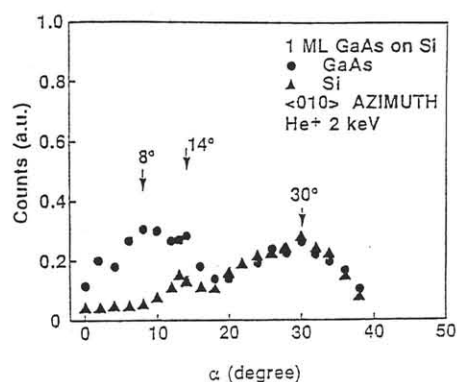


Fig.5 Low-angular distribution of GaAs and Si signals after 1 ML of GaAs growth on Si.