

## Formation and Thermal Stability of Au-GaAs(001) Interfaces Studied by Angle Resolved XPS and Rutherford Backscattering

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Formation of clean Au-GaAs(001) interfaces and their thermal stability were studied by in-situ XPS and RHEED observations using a combined MBE-surface analysis system. The samples were also examined by He<sup>+</sup> ion Rutherford backscattering, and SEM. The results indicate that Au deposition causes Ga-As bond breaking in the very early stage of the interface formation even at room temperature. The released As atoms segregate on the Au overlayer surface. Thermal stressing at 100°C results in detectable outdiffusion of Ga. The Ga and As out diffusions become faster with increasing stressing temperature. Two kinds of microstructure formation, and one dimensionally disordered solid phase epitaxy were found to take place by 240°, and 305°C stressing, respectively.

### I. Introduction

Gold and gold based alloys have been widely used in semiconductor devices due to their excellent electronic and metallurgical characteristics. In GaAs devices such as lasers and FETs, they are frequently used as materials for ohmic as well as Schottky contacts. However, it is well known that difficulties sometimes arise in device fabrication process due to unstable thermal characteristics of interfaces between GaAs and them. This instability also degrades reliability of the devices.

Here we report new phenomena observed during the formation and thermal stressing of the Au-GaAs(001) interfaces by means of angle resolved X-ray photoemission spectroscopy (XPS) and He<sup>+</sup> ion Rutherford backscattering (RBS).

### II. Experimentals

Sample preparation and XPS observation were done in a combined MBE-surface analysis system under basic pressure of less than  $1 \times 10^{-10}$  mb. Clean GaAs(001) surfaces with c(4x4) reconstruction were prepared by molecular beam epitaxial (MBE) growth of undoped GaAs layers of about 5000 Å on n-type substrates. These samples were

transferred to the analysis chamber, which is isolated from the MBE chamber by a gate valve. Gold films were deposited onto these clean surfaces in the analysis chamber, not in the MBE chamber, to avoid contamination by residual As vapor in the MBE chamber. The deposition rate was  $1 \times 10^{-1}$  Å/sec. The Ga, As, and Au XPS signals were observed with Al K<sub>α</sub> X-ray excitation. Surface structures of the samples were examined by RHEED. After these experiments the samples were taken out from the system and RBS measurements were done with MeV He<sup>+</sup> ions accelerated by PELETRON 5SDH electrostatic accelerator. Optical microscope and SEM observation of the sample surfaces were also performed.

### III. Au overlayer formation at room temperature

Figure 1 shows the XPS signal intensities as functions of the Au film thickness. The surface sensitive Ga 2p signal, whose probing depth is about 10 Å, decreases rapidly with increasing Au deposition. It diminishes at around 50 Å Au film thickness. Attenuation of As 2p signal by Au deposition, whose probing depth is somewhat smaller, is slightly weaker than that of Ga 2p. The As 2p signal intensity decreases to about 1/3 of the initial value at around 10 Å, and further deposition does not greatly vary the

intensity. These suggest that the As atoms are released from the substrate and segregate at the surface of the Au overlayer from the very early stage even at room temperature.

Figure 2 shows polar angle dependence of As 2p and Au 4f signal intensities of an  $\sim 11 \text{ \AA}$  Au deposited surface. The As 2p signal gradually changes with polar angle, whereas the angle dependence of Au 4f signal exhibits several fine structures. These fine structures are due to scattering of the Au 4f photoelectrons by ordered array of atoms near the surface. Thus the result indicates that at least a part of Au atoms forms ordered structure.

The surface As atoms were also observed by  $\text{He}^+$  RBS measurements as shown in Fig. 3. Figure 3 shows a channeling spectrum of  $43 \text{ \AA}$  Au deposited surface. Hatched peak corresponds to the surface As.

#### IV. Thermal stability of the Au-GaAs interface

Thermal stability of the Au-GaAs(001) interfaces were examined by observing XPS signal evolutions of approximately  $45 \text{ \AA}$  Au deposited samples during the thermal stressing. Both the Ga and As outdiffusion were observed to take place by heat treatment. Even at a low temperature of  $100^\circ \text{C}$ , Ga 2p signal becomes detectable several tens minutes after the start of the thermal stressing. The As 2p signal increases whereas Au 4f signal decreases slightly by this heat treatment.

At  $240^\circ \text{C}$ , the Ga signal variation is very similar to that of at  $100^\circ \text{C}$ . However, As signal change is peculiar. It increases in the first stage and shows a maximum at around 50 min after the start of stressing, and slowly decreases with further increase of stressing time. The Au signal intensity shows a weak minimum corresponding to the maximum of the As signal intensity. These intensity variations are reasonably understood by assuming competition of two processes, that is, outdiffusion of As and condensation into crystallites.

The SEM observation of this sample surface

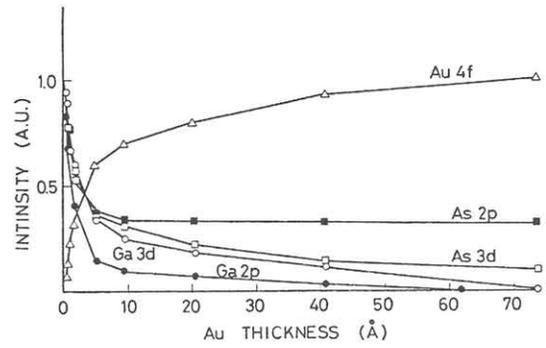


Fig. 1 XPS signal intensities as functions of Au film thickness. The Au film was deposited at room temperature.

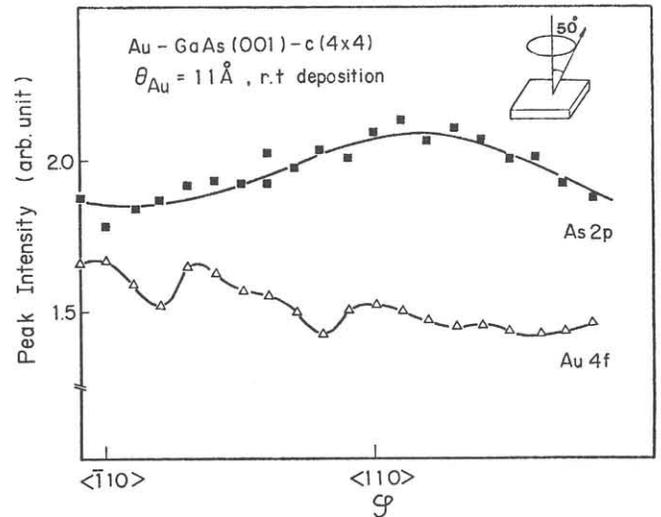


Fig. 2 Angular dependence of As 2p and Au 4f signal intensities for  $11 \text{ \AA}$  Au deposited surface.

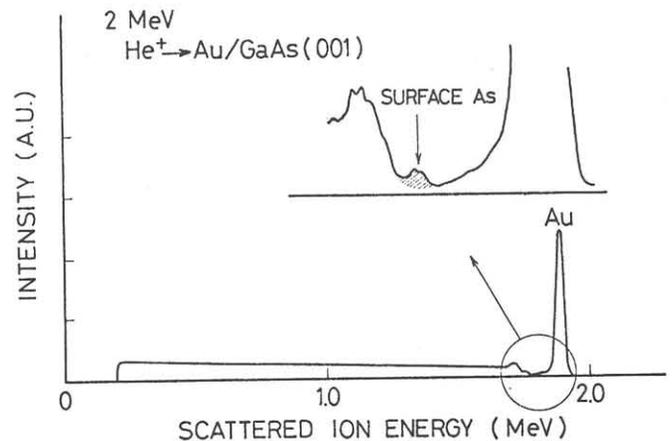


Fig. 3 An example of RBS spectrum for a Au-GaAs(001) surface. The Au film thickness is  $43 \text{ \AA}$ .

revealed the existence of crystallites. Small triangular particles, which are presumably As crystallites and rectangular structures, which are arranged along 110 direction, were observed as shown in Fig. 5(a). These triangular crystallites were also recognized on the surface of the sample stressed at 100 C.

At 305 C, both the Ga and As signals increase to about 70 % of the clean surface values, and Au signal decreases to about 45 % of the value at the start of the stressing. The Ga outdiffusion is as fast as that of As, and surface Ga/As concentration ratio is approximately unity at this temperature.

The SEM observation of the sample stressed at 305 C reveals elongated rectangular patched surface as shown in Fig. 5(b). The RHEED patterns of this surface with several different azimuth angles are shown in Fig. 6. These RHEED patterns suggest that the surface structure is one dimensionally disordered. In order to clarify the microscopic structure of this surface, channeling measurements of the He<sup>+</sup> ions were performed. Figure 7 shows the results. The Au signal shows channeling effect as strongly as that of substrate GaAs in 111 direction, but not in 111 direction. Both the RHEED and channeling results indicates that occurrence of one dimensionally disordered solid phase epitaxy.

#### V. Summary

The Au deposition onto clean GaAs(001) surface causes Ga-As bond breaking even at room temperature. Released As atoms outdiffuses and segregate on the surface of the Au layer. Both the Ga and As outdiffusions are detectable by surface sensitive XPS measurements after few tens minutes thermal stressing at 100 C. Concentrations of surface Ga and As atoms increase with increasing the stressing temperature. The Ga/As concentration ratio at the surface estimated by XPS is approximately unity after 305 C stressing. Occurrence of one dimensionally disordered solid phase epitaxy was

confirmed by RHEED and He<sup>+</sup> channeling observation.

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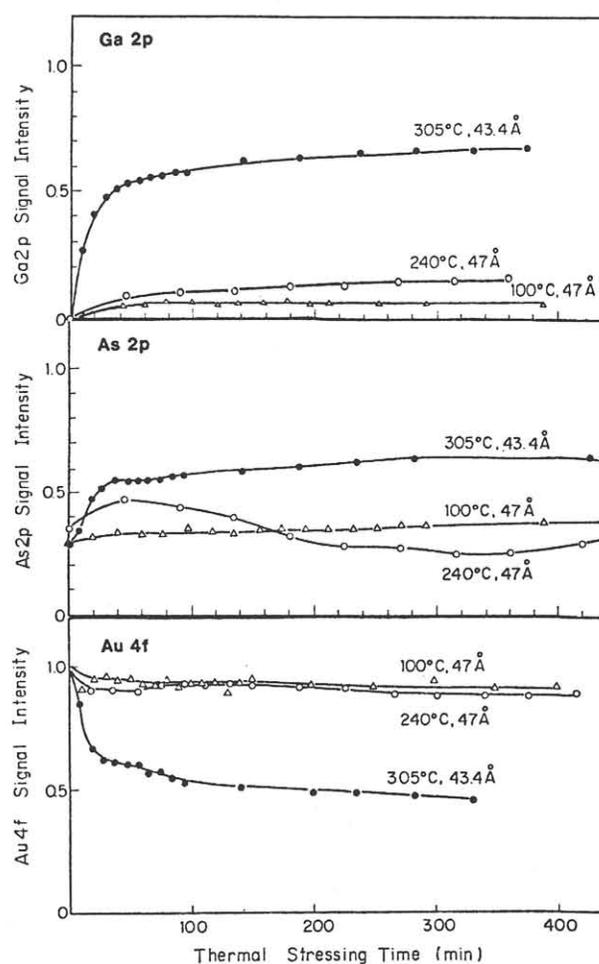


Fig. 4 XPS signal intensity changes during thermal stressing at 100, 240, and 305°C. The Ga and As signal intensities are normalized by those of the clean surface, whereas the Au signal intensity is normalized by that at the start of the stressing.

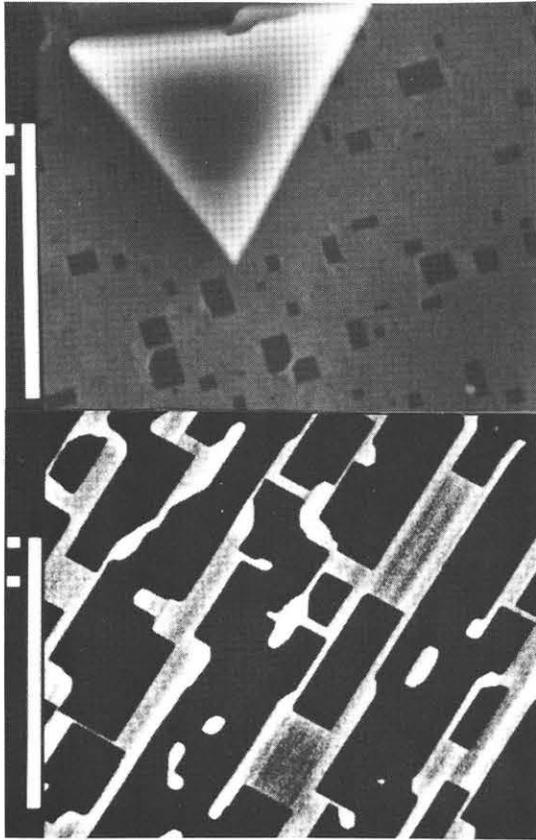


Fig. 5

SEM photographs of thermal stressed samples at (a) 240°C, and (b) at 305°C for about 15 hr.

(a)

(b)

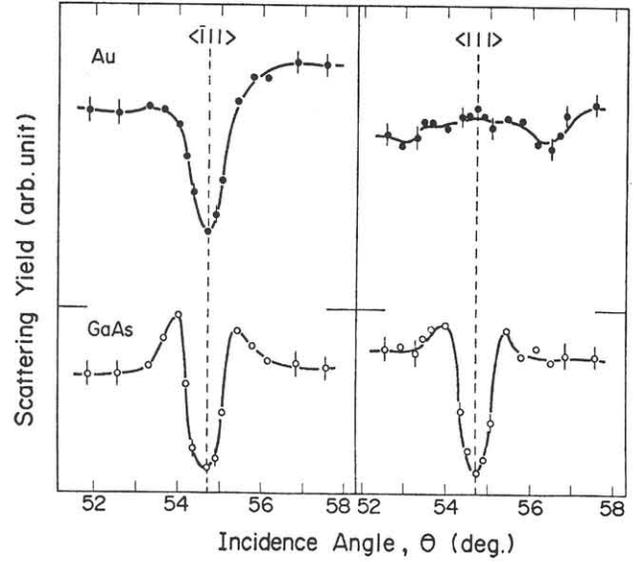
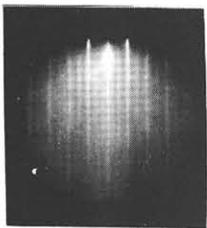


Fig. 7

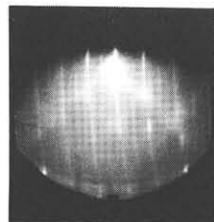
He<sup>+</sup> Channeling profiles of Au and surface GaAs signal. for the same sample whose RHEED patterns are shown in Fig. 6.

Fig. 6

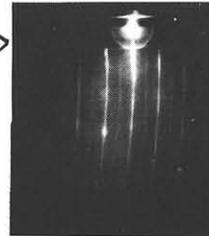
RHEED patterns of the sample after 15 hr stressing at 305°C.



$\langle 110 \rangle$  ← →  $\langle \bar{1}\bar{1}0 \rangle$



$\langle 010 \rangle$        $\langle \bar{1}00 \rangle$



$\langle \bar{1}\bar{1}0 \rangle$

