Extended Abstracts of the 1992 International Conference on Solid State Devices and Materials, Tsukuba, 1992, pp. 653-655

Charge Balanced Heteroepitaxial Growth of GaAs on Si

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We propose the charge balanced heteroepitaxy, where GaAs/Si interface is neutralized by inserting the one monolayer of column II elements in place of the Ga atoms at GaAs/Si interface. We have constructed this structure using the Be atoms, and have investigated GaAs MBE initial growth stages on this charge balanced surface by high-energy electron diffraction (RHEED) and ultraviolet photoemission spectroscopy. The RHEED measurement reveals that GaAs growth mode proceeds in a Stranski-Krastanow mode.

1. Introduction

Epitaxial growth of compound semiconductor on Si substrate has been the subject of intense research in recent years in order to combine the optoelectronic devices with the Si very large scale integrated technology.[1] However, there exist several kinds of problems: one of them is three-dimensional growth at the initial stages.[2,3] The island growth in the initial stages affects not only the surface morphology, but also the quality of epitaxial layer on Si.[4,5] The origin of the island growth has not been clarified. One of causes is thought to be an accumulation of nuclear charge at the interface. An atomic abrupt polar-nonpolar interface is indicated to be energetically highly unfavorable.[6,7] We consider that GaAs is formed islands on Si in order to reduce the interface energy.

In order to eliminate the charge imbalance at the GaAs/Si(111) interface, we propose the charge balanced heteroepitaxy, where the GaAs/Si interface is neutralized by inserting the one monolayer of column II elements in place of the Ga atoms at GaAs/Si interface.

In this paper, we have constructed this structure using the Be atoms, which are the easiest to control in the column II elements, as shown in Fig.1, and have investigated the molecular beam epitaxial (MBE) initialgrowth stages of this structure using reflection high-energy electron diffraction (RHEED) and ultraviolet photoemission spectroscopy (UPS).

2. Experimental

The substrates were Si(111) surface aligned to within 1° of nominal direction. They were first degreased in organic solution, and then oxide film was removed in HF and was formed in hot HNO_3 several times. They were finally re-oxidized in boiled $HCl:H_2O_2:H_2O$ solution before loading into a

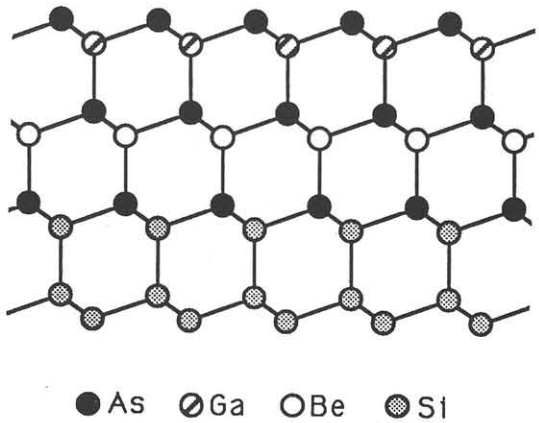

Fig.1 Schematic view of charge balanced structure.

combined MBE-surface analysis system under a base pressure of less than $1x10^{-8}$ Pa. After the sample was heated at 900°C, a sharp (7x7) RHEED pattern was obtained. For RHEED pattern a 13 KeV incident beam was used. The UPS observation was taken with a rotatable hemispherical electrostatic energy analyzer. A He I (21.22 eV) resonance lamp was used for valence-electronic structure measurements.

3. Results and Discussion

The Si(111)(1x1)-As structure was obtained by As exposure of Si(111)(7x7) clean surfaces at substrate temperature of 700°C. On this surface, both Be and As were deposited at the surface temperature of 450°C. The sharp (1x1) RHEED pattern changed into a streaked pattern. However, the spots from the BeAs islands were not observed at all, this pattern retained the Kikuchi bands and lines. This result indicates that BeAs grows two-dimensionally.

Figure 2 shows the evolution of the UPS spectra as a function of the coverage BeAs on Si(1x1)-As surface. The photon incident angle is 55° and electron emission angle is 0°, from the surface normal direction, that is, these spectra correspond to Γ point. The UPS spectrum for the Si(1x1)-As surface is shown in Fig.2(a). Bringans *et al.* have reported that As atoms are triply bonded to the underlying Si atoms, leaving only As lone-pair states.[8] The highly intensive peak arised from As lone-pair states is appeared at 1.5eV in the UPS spectrum. This peak gradually decreases as depositing both Be and As at substrate temperature of 450°C, as shown in Fig.2(b) and (c). After one monolayer deposition of BeAs, this peak completely disappears, as shown in Fig.2(c). These results indicate that BeAs completely covers the Si(1x1)-As surface and induce the change of surface electronic structures.

In order to study the effect of this interface structure, GaAs direct growth on Si(111) has been also investigated. After one monolayer GaAs deposition on Si(1x1)-As surface at 450°C, the peak arised from As lone-pair states is still observed from UPS spectrum, as shown in Fig.3(a). This band still existed even after several monolayers deposition of GaAs. Simultaneously, spotty RHEED pattern is obtained, as shown in Fig.4(a). These results indicate that the GaAs hardly cover the surface and forms islands at the very initial stages of GaAs MBE growth on Si(1x1)-As surfaces.

On the other hand, after one monolayer GaAs growth on the charge balanced surface, a UPS spectrum is obtained, as shown in Fig.3(b), which has a new shoulder at about

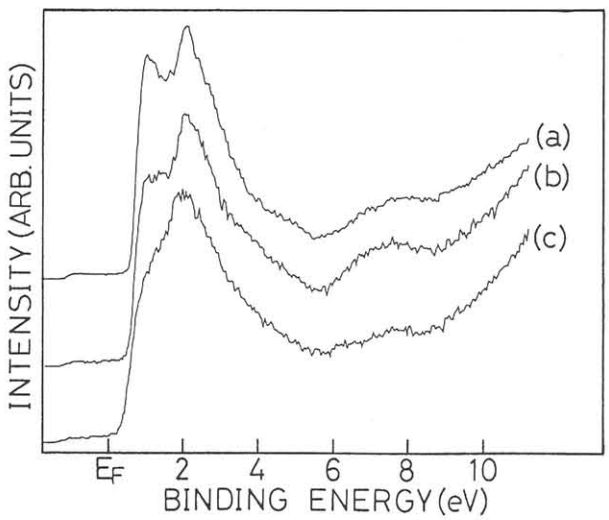

Fig.2 UPS spectra for (a) Si(111)(1x1)-As surface, (b) 1/3 monolayer of BeAs on Si(1x1)-As surface and (c) one monolayer of BeAs on Si(1x1)-As surface.

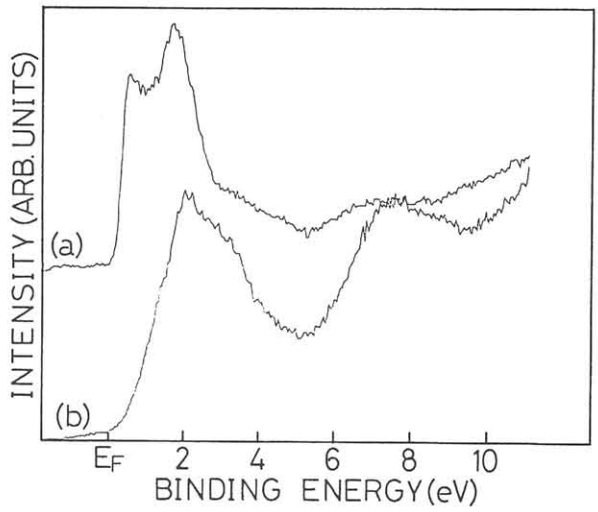

Fig.3 UPS spectra for one monolayer of GaAs (a) on Si(1x1)-As surface and (b) on charge balanced surface.

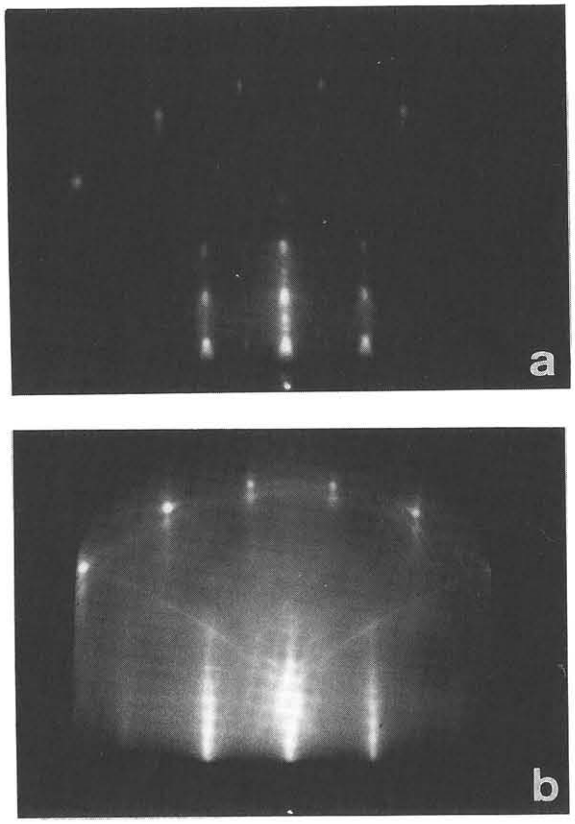

Fig.4 RHEED patterns for one monolayer of GaAs (a) on Si(1x1)-As surface and (b) on charge balanced surface. These RHEED patterns are taken from <211> direction.

3.5 eV. This is the characteristic peak from GaAs film.[9] The electronic structure like GaAs surface is considered to be obtained. Furthermore, broad streaked (1x1) RHEED pattern remained till 2 monolayer GaAs deposition on this surface at 450°C, as shown in Fig.4(b). These results indicate that accumulation of nuclear charge at the interface is extinguished and GaAs growth mode proceeds in a Stranski-Krastanow mode.

Further deposition of GaAs resulted in the formation of GaAs islands from RHEED pattern, which, we think, is due to the large lattice mismatch between GaAs and Si. This is very consistent with the results of Ge growth on Si, which exhibits the transition from 2D to 3D growth at three monolayer growth.[10]

4. Conclusions

We propose the charge balanced heteroepitaxy, where GaAs/Si interface is neutralized by inserting the monolayer of column II elements in place of the Ga atoms at GaAs/Si interface. We have constructed this structure using the Be atoms, and have investigated GaAs MBE initial growth stages on this surface by RHEED and UPS. The RHEED measurement reveals that GaAs growth mode proceeds in a Stranski-Krastanow mode. GaAs growth on the charge balanced Ge surfaces will be needed in order to study this lattice mismatch effect.

Acknowledgment

This work was supported in part by the Grant-in-Aid for Encouragement of Young Scientists from the Ministry of Education, Science and Culture of Japan.

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