Al Growth on Si(111)(√3x√3)-Ga Surfaces at Room Temperature

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The initial stages of Al growth on Si(111)(√3x√3)-Ga surfaces at room temperature (RT) have been studied by reflection high-energy electron diffraction and X-ray photoemission spectroscopy. The exchange reaction takes place, that is, Al-Si bonds are formed at the interface. Al films contain both (111)- and (100)- oriented structures. The Ga atoms segregate at surfaces of Al overlayer from the very initial stage even at RT.

1. Introduction

The formations and electronic properties of metal/semiconductor interfaces are of importance in semiconductor physics and their applications, in particular, Al is widely used in metallization of Si devices and integrated circuits. Lander and Morrison[1] reported that almost perfectly oriented epitaxial Al(111) layers with a few monolayers' coverage have grown on the Si(111)(√3x√3)-Al surfaces at room temperature (RT), however relatively disorder layers on other surfaces in thin film.

Previously, we reported Al epitaxial growth on Si(111)(√3x√3)-Al surfaces at RT using with low-energy electron diffraction (LEED), electron-energy-loss spectroscopy (EELS) and low-energy electron transmission spectroscopy (LEETS).[2,3] The LEED and EELS observations indicated that the Al overlayers grow in layer-by-layer fashion surfaces without severe atomic rearrangement at the interface. The LEETS measurements revealed that the Al/Si interface is very abrupt and the (√3x√3) structure still remains at Al/Si interface. We suggest that the initial (√3x√3) structure is essentially important for excellent epitaxial growth.

Si(111)(√3x√3)-Ga surfaces are well defined, well understood, and the stablest surface phase among the Ga adsorbed Si(111) surfaces.[4,5] Moreover, the electronic and atomic structures of Si(111)(√3x√3)-Ga surfaces are quite similar to those of Si(111)(√3x√3)-Al surfaces.[6,7]

In this paper, we have investigated Al molecular beam epitaxial (MBE) growth on Si(√3x√3)-Ga surfaces at RT by reflection high-energy electron diffraction (RHEED) and X-ray photoemission spectroscopy (XPS).

2. Experimental

Experiments were performed with a combined MBE-analysis system under a base pressure of less than 1×10^{-8} Pa. RHEED patterns were observed with 13 keV electron beam. XPS spectra were measured with Mg Kα and Al Kα lines.

The Si(111) substrates used were first degreased in organic solution, and then etched in HF and oxided in boiled $HCl:H_2O_2:H_2O$ solution. Finally, they were treated under UV light. The samples were heated at 900°C for 10 min, the sharp (7x7) RHEED pattern was obtained. It was also confirmed by the absence of C $1s$ and O $1s$ XPS peaks. The Si(111)(√3x√3)-Ga surfaces were obtained by deposition of 1/3 ML_{Si} onto Si(111)(7x7) surfaces at 500°C, where 1 ML_{Si} is defined as the number of sites on ideal Si(111) (1 ML_{Si}=7.83 x 10^{14} cm^{-2}). We also define 1 ML_{Al} as being equal to the surface site density of Al(111) of 1.41 x 10^{15} cm^{-2}, so that 1 ML_{Al}=1.8 ML_{Si}.

3. Results and Discussion

Firstly, the initial stages of Al growth have been investigated by RHEED. Figures 1(a)-(c) show the evolution of the RHEED pattern as a function of Al coverage on the Si(111)(√3x√3)-Ga surfaces at RT. These RHEED patterns are taken from <110> direction. Figure 1(a) shows Si(√3x√3)-Ga surface obtained by 1/3 ML_{Si} deposition of Ga on Si(7x7) surface at 500°C. As Al is deposited on Si(√3x√3)-Ga surfaces at RT, the RHEED intensities from Si(√3x√3)-Ga surfaces gradually decreases. After the deposition of 1ML_{Al}, (√3x√3) structure is scarcely observed, and new streaks are appeared at the outside of Si(1x1) struc-
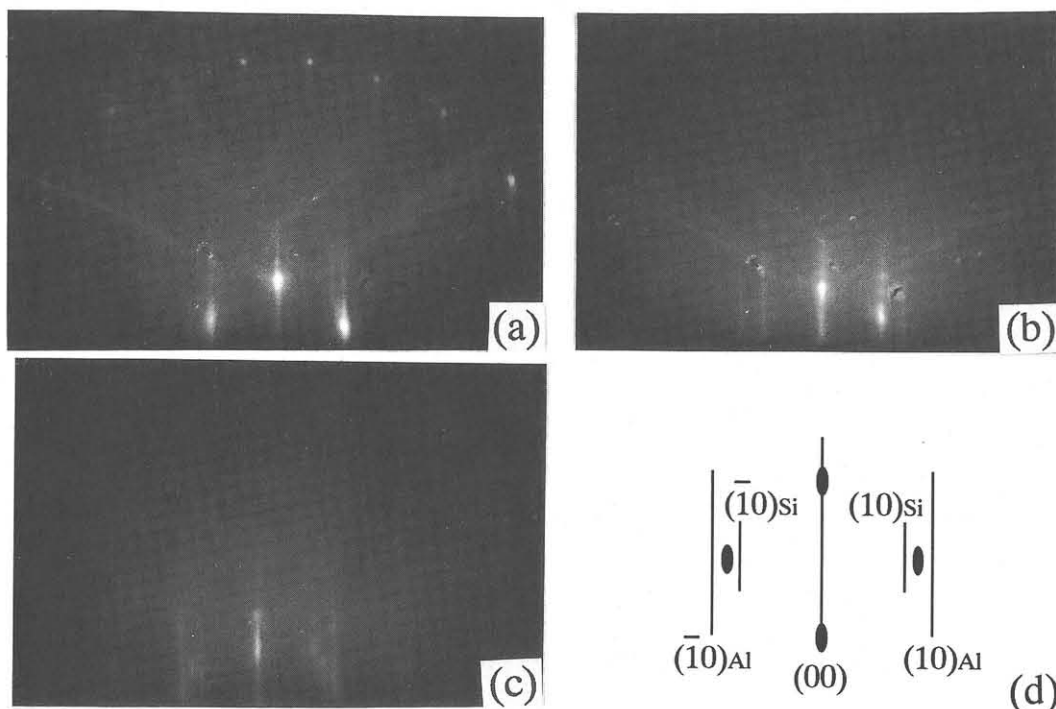
Fig.1 Evolution of the RHEED pattern as a function of Al coverage on Si(111)(√3x√3)–Ga surfaces at RT : (a)Si(√3x√3)–Ga pattern, (b)1ML$_{Al}$ deposition, (c)3ML$_{Al}$ deposition and (d)schematic illustration corresponding to Fig.1(c).

ture, as shown in Fig.1(b). Taking account of the lattice constant of Si(5.43 Å) and Al(4.05 Å), this result indicates that atomically flat Al(111)(1x1) surface is obtained with <110>$_{Al}$ parallel to <110>$_{Si}$. After the deposition of 3ML$_{Al}$, a spotty pattern is appeared in addition to Al(111)(1x1) pattern, as shown in Fig.1(c). Figure 1(d) shows schematic illustration corresponding to Fig.1(c). If the reflections from both Si(111) and Al(111) surfaces are taken off, this spotty pattern appeared at every 30° rotation of the azimuthal angle. This result indicates that Al islands grow, which epitaxial relation is (100)$_{Al}$//(111)$_{Si}$, <110>$_{Al}$//<110>$_{Si}$ with three equivalent domains. The Al films on Si(√3x√3)–Ga surfaces contain both (111)- and (100)–oriented structure.

Figures 2 and 3 show XPS signal intensity and binding energy for Ga 2p and Al 2p core levels as a function of Al thickness on Si(111)(√3x√3)–Ga surfaces at RT, respectively. 0 ML$_{Al}$ means XPS signals from Si(√3x√3)–Ga surfaces and no Al signals are obtained. The Ga 2p signal intensities are normalized to Si(√3x√3)–Ga surface value, and the Al 2p signal intensities to that of 4 ML$_{Al}$ thickness.

When Al is deposited on Si(√3x√3)–Ga

surfaces at RT, Ga 2p and Al 2p core levels shift toward lower binding energies, then becomes constant values. The binding energy of Si 2p core level which is not shown did not change. Therefore, the changes in binding energy of Ga 2p and Al 2p core levels are caused by chemical shifts. The value of Ga 2p binding energy at Si(√3x√3)–Ga surface shows Ga–Si bonding. Considering the Si and Ga electronegatively, electron charge density is considered to localize at the Si side. Therefore, the observed Ga 2p core level shift toward the lower binding energy side is thought to be caused by the metallic Ga formation. Moreover, from similar consideration, the Al 2p core level shift toward the lower binding energy side results from the metallic Al formation. Therefore, the shifts in the binding energy of Ga 2p and Al 2p indicate that by Al deposition on Si(√3x√3)–Ga surfaces at RT, the Ga–Si bonds are broken and the Al–Si bonds are formed.

The Ga 2p signal intensity decreases by Al deposition on Si(√3x√3)–Ga surfaces at RT. Beyond a thickness of 2 ML$_{Al}$, this intensity scarcely decreases. At 4 ML$_{Al}$ the Al 2p signal intensity is about 0.85 of the initial value. Considering that probing depth of Ga 2p signal is about 7 Å, this result indicate that Ga atoms are released
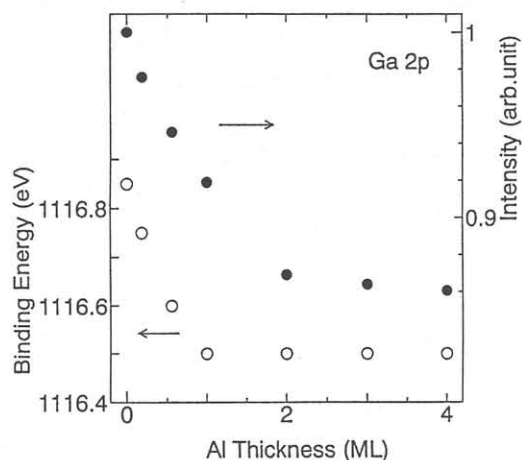
Fig.2 Ga *2p* XPS signal intensity and binding energy as a function of Al thickness on Si(111)($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT.
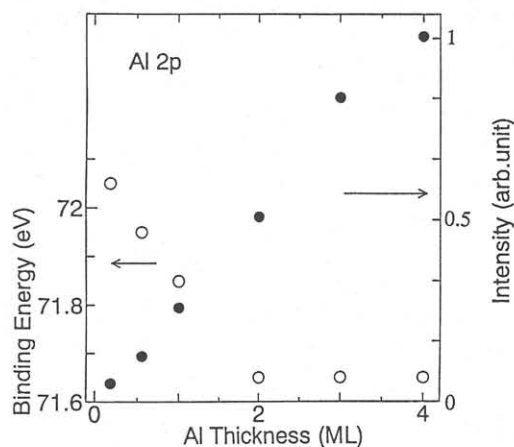

Fig.3 Al *2p* XPS signal intensity and binding energy as a function of Al thickness on Si(111)($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT.

from the substrate and segregate at the surface of the Al overlayer from the very initial stages even at RT.

These XPS measurements indicate that by Al deposition on Si($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT, Ga atoms are released from the surfaces, being isolated on Al films, and at interface Si–Al bonds are formed.

Based on these results, we have constructed a model for Al growth on Si(111)($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT as follows. By Al deposition on Si($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT, Si–Ga bonds are broken and Al–Si bonds are formed, and then the atomically flat Al(111)(1×1) surfaces are observed. The behavior that Al(111) surfaces are obtained at the initial stages, is very similar to that of Al deposition on Si(111)($\sqrt{3}\times\sqrt{3}$)–Al surfaces at RT.[1-3] It was reported that on only Si($\sqrt{3}\times\sqrt{3}$)–Al surfaces, excellent epitaxial Al(111) film grew,[1] and at Al/Si(111) interface ($\sqrt{3}\times\sqrt{3}$)–Al structure still remained.[3] As above mention, we suggest that in Al/Si($\sqrt{3}\times\sqrt{3}$)–Ga system, the ($\sqrt{3}\times\sqrt{3}$)–Al structure also exist at the Al(111)/Si(111) interface. However, as further deposition proceeds on Si($\sqrt{3}\times\sqrt{3}$)–Ga surfaces, Al(100) islands are formed. This phenomena was not observed during Al deposition on Si($\sqrt{3}\times\sqrt{3}$)–Al surfaces.[3] Yamada *et al.* investigated the initial stages of Al growth on Si(111)(7×7) surfaces at RT.[8] In this report, reflection electron diffraction measurement revealed that Al(100) islands nucleated at the initial stages. Therefore, at Al(100)/Si(111) interface, the ($\sqrt{3}\times\sqrt{3}$)–Al structure is considered not to be formed. By Al deposition on Si($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT, exchange reactions take place, that is,

($\sqrt{3}\times\sqrt{3}$)–Al structure is formed. On this structure, atomically flat Al(111) surfaces are obtained. However, at some regions ($\sqrt{3}\times\sqrt{3}$)–Al structure is not formed, and then on this regions Al(100) islands are formed.

4. Conclusions

We have investigated that the initial stages of Al growth on Si(111)($\sqrt{3}\times\sqrt{3}$)–Ga surfaces at RT by RHEED and XPS. The exchange reaction takes place, that is, Al–Si bonds are formed at the interface, and the Ga atoms segregate at surfaces of Al overlayer from the very initial stage even at RT. RHEED observations indicate that Al films contain both atomically flat (111) surfaces and (100) islands with three equivalent domains.

References

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