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LEED Analysis on Initial Stages of Ge Growth on Si(111)(1x1)-As and As-Desorbed Si(111)(1x1) Surfaces

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We have investigated the initial stages of Ge growth on the Si(1x1)-As and the As-desorbed (1x1) surfaces using spot profile analysis of low-energy electron diffraction and Auger electron spectroscopy. It is found that at 500°C 2 dimensional islands are formed on either the Si(1x1)-As or the As-desorbed (1x1) surfaces. In contrast, at 300°C, on the As-desorbed (1x1) surfaces, much smaller islands are formed, while Ge growth on the Si(1x1)-As surfaces initially proceeds in the step flow mode. The effect of As surfactant in surface diffusion is deeply related to the growth temperatures, and As atoms enhance migration of Ge atoms at low growth temperatures.

1.Introduction

The initial stages of heterostructure formation are important both for theoretical and practical reasons. Since the Si-Ge system is one of the simplest semiconductor heterostructures and is utilized in fabrication of strained superlattices, the growth of Ge on Si has been intensively investigated for several years. However, for the large lattice mismatch of 4.2%, Ge growth on the Si(111)(7x7) clean surfaces proceeds in the Stranski-Krastanov mode (SK-mode); the layer-by-layer growth followed by islanding. Recently, it has been reported that when the growth front is terminated by a specific third species (surfactant), the growth mode of Ge/Si or Si/Ge system can be changed from the SK-mode to the layer-by-layer mode.[1)] The effect of surfactant on growth kinetics have been investigated, and two models of the surfactant mediated epitaxial growth; enhanced diffusion model[2,3)] and hindered diffusion model,[4)] has been proposed.

This paper presents a study of the initial stages of Ge growth on As covered Si(1111)(1x1) surfaces using Low-energy electron diffraction (LEED), spot profile analysis of LEED (SPA-LEED) and Auger electron spectroscopy (AES). It is found that the effect of As surfactant in surface diffusion is deeply related to the growth temperatures, and As atoms enhance migration of Ge atoms at low growth temperatures.

2.Experimental

The experiments were performed in an UHV apparatus(base pressure: $1x10^{-10}$ Torr) equipped with LEED-AES optics and an angle-resolved electron energy spectrometer composed of an electron gun and a rotatable hemispherical electrostatic energy analyzer. Precise SPA-LEED measurements were carried out using the spectrometer interfaced to a computer. The scattering angle 2θ was held fixed while the sample was tilted so that all the beams in a given azimuth passed through the aperture of the analyzer.

The samples used in this study were cut from n-type Si(111) wafer with resistivity of 100 Ωcm. The samples were thermally cleaned at 1200°C for several minutes. After the thermal cleaning, the surface exhibited a well-developed (7x7) LEED pattern.

As was evaporated from GaAs wafer heated by running direct current. Ge was evaporated from a PBN crucible in a Knudsen cell. Here 1ML is defined as the number of sites on an ideal Si(111) (1ML = $7.83x10^{14}$ cm^{-2}). In this experiment Ge deposition were carried out without As exposure.

3. Results and Discussion

3.1. As-desorbed Si(1x1) structure

Adsorption of As on the Si(111)(7x7) at 700°C leads to a well-ordered (1x1) structure (indicated (1x1)-As), as can be seen from the sharp (1x1) LEED spot profiles with low background shown in Fig. 1. By annealing the (1x1)-As at temperatures above 780°C in vacuum, desorption of As occurred. It is derived from AES (not shown) and SPA-LEED (Fig. 2) that the surface annealed at 850°C (indicated As-desorbed (1x1)) still exhibits a (1x1) structure, although it has 90% less As atoms than the Si(1x1)-As. The detailed LEED spot profile measurements along <110> azimuth revealed diffuse scattering structures near √3 Bragg spot positions, indicating that Si adatoms are distributed to hollow sites of the truncated Si(1x1) surface without sharing dangling bonds of the substrate, in order to decrease Si dangling bonds produced by desorption of As.[5] Therefore, it is thought that the As-desorbed (1x1) still has a lot of Si dangling bonds as compared with the Si(1x1)-As having As lone-pairs instead.[1,6,7]

3.2 Ge growth at 500°C

Figures 1 and 2 show evolution of LEED spot profiles between (00) and (02) spots for the (1x1)-As and the As-desorbed (1x1) as a function of Ge coverage, respectively. Primary electron energy is 55eV and scattering angle is 130°, which corresponds to the out-of-phase condition for bi-layer (BL) height steps (about 3.2Å). Up to 3ML deposition on the Si(1x1)-As, the surfaces exhibit well-ordered (1x1) structures without any diffuse scattering structures, while even at 1.5 ML deposition on the As-desorbed (1x1), fractional order spots appear, reflecting a (7x7) reconstruction. This indicates that growth temperature of 500°C is high enough for As atoms to float to the growing film surfaces during Ge deposition. For both surfaces, it is apparent that up to 1 ML, full width at half maximum (FWHM) of (00) peaks gradually decrease with increasing a coverage of Ge. In contrast, when taking the corresponding spot profiles under the in-phase condition (Ep=40eV and θ=120°), such coverage dependence of FWHM of (00) peaks was not observed. Therefore, it is considered that 1 ML (half bi-layer) Ge deposition results in surface roughness due to nucleation of small two-dimensional (2D) islands on the terraces. This surface roughness decreases at around 2 ML (1 BL) because of completion of the first bi-layer. However, it seems that the second bi-layer already grows before completion of the first bi-layer since the 3 ML deposited surfaces have broader (00) peaks than the (1x1)-As.

3.3 Ge growth at 300°C

Figures 3 and 4 show evolution of LEED spot profiles for Ge growth on the (1x1)-As and the As-desorbed (1x1), respectively. These are taken under the out-of-phase condition as mentioned above. For the (1x1)-As, (1x1) LEED structures are observed without any significant changes of FWHM of the peaks. Surprisingly, precise spot profile measurements for the 3 ML deposited surface revealed almost the same diffuse scattering structures as observed on the As-desorbed (1x1), suggesting that growth temperature of 300°C is too low for As atoms to float to the growing film surfaces. Therefore, it is presumably expected that Ge atoms can readily move around on the inert (1x1)-As surface, until they reach step edges. As a result, initially, Ge layers grow in step flow mode, which is consistent with the result of FWHM of the (00) peaks. In contrast, for the As-desorbed (1x1), FWHM of the peaks show drastical changes between 0.5 ML and 1ML of Ge deposition. When taking the corresponding spot profiles under the in-phase condition, such coverage dependence of FWHM was not observed. This indicates that Ge deposition on the As-desorbed (1x1) results in surface roughness due to nucleation of small 2D islands with about 20Å in diameter, The formation of small 2D nucleus is interpreted as the decrease of surface diffusion due to the capture of Ge adatoms by dangling bonds of the substrate.

4. Summary

We have investigated the initial stages of Ge growth on the Si(1x1)-As and the As-desorbed (1x1) surfaces using SPA-LEED and AES. It is found that at 500°C, 2D islands are formed on either the Si(1x1)-As or the As-desorbed (1x1) surfaces. In contrast, at 300°C, on the As-desorbed (1x1) surfaces, much smaller islands are formed, while Ge growth on the Si(1x1)-As surfaces initially proceeds in the step flow mode. In conclusion, the effect of surfactant (As atoms) in surface diffusion is deeply related to the growth temperatures, and As atoms enhance migration of Ge atoms at low growth temperatures. Preliminary LEED observation of Ge growth at 400°C suggest that Ge growth on the Si(1x1)-As surfaces proceeds in the step flow mode and As atoms adequately float up the growth front.

Acknowledgments

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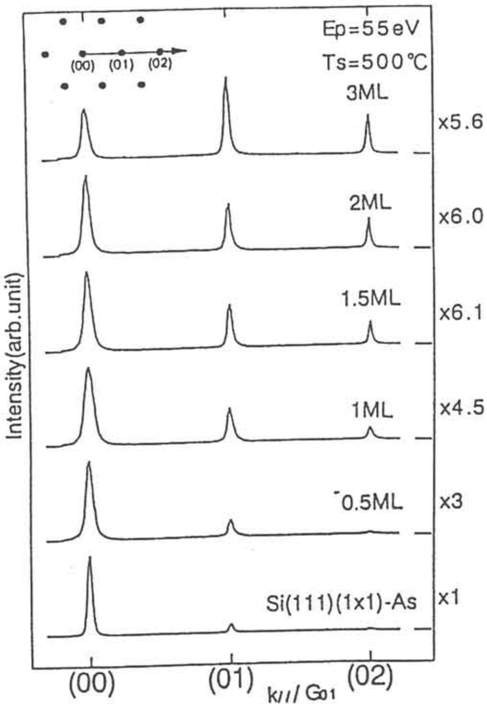

Fig.1 LEED spot profiles of Ge growth on Si(1x1)-As surface at 500°C.

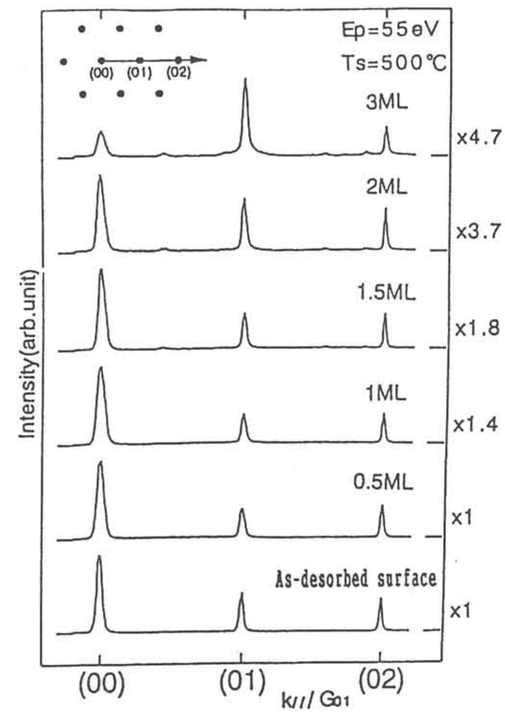

Fig.2 LEED spot profiles of Ge growth on As desorbed (1x1) surface at 500°C.

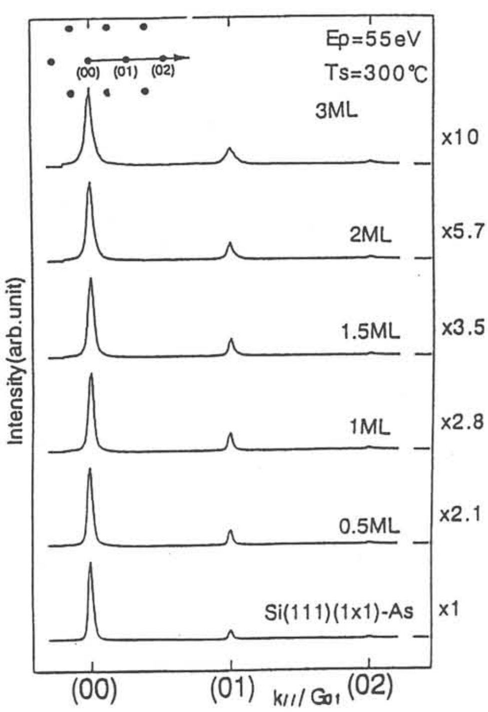

Fig.3 LEED spot profiles of Ge growth on Si(1x1)-As surface at 300°C.

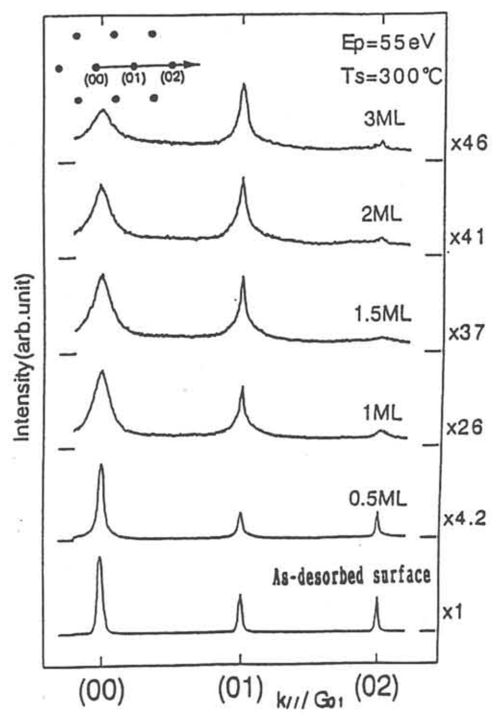

Fig.4 LEED spot profiles of Ge growth on As desorbed (1x1) surface at 300°C.