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**MBE Growth and In-Situ XPS Characterization of Silicon Interlayers
on (111)B Surfaces for Passivation of GaAs Quantum Wire Devices**

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Abstract

In nanostructures, the surface-to-volume ratio is increased, and surface state problems become more serious, making success of the future III-V nanoelectronics strongly dependent on surface passivation. To solve this problem, we have been investigating a passivation scheme using a Si interlayer called Si interface control layer (Si ICL) [1]. However, main efforts have been limited on (001) surfaces.

This paper investigates the applicability of the Si ICL approach to (111)B surfaces. An ultrathin (1nm) silicon layer was grown by MBE on GaAs and AlGaAs (111)B surfaces with (2×2) , $(\sqrt{19}\times\sqrt{19})$ and (1×1) surface reconstructions. Surfaces were characterized by *in-situ* X-ray photoelectron spectroscopy (XPS) technique. Si layers grew epitaxially with Si-Ga bonds at the Si/GaAs interface and Si-As termination on top, suggesting surfactant roles played by As atoms. On nitridation of Si layer by nitrogen radicals at room temperature, Si-As bonds were replaced by Si-N bonds leading to partial nitridation of the Si layer. Unlike the case of the As-stabilized GaAs (001)-(2x4) surface, large reduction of band bending by 250-420 meV took place on (111)B surfaces, indicating large reduction of surface states. The results indicate effectiveness of the Si ICL passivation on (111)B surface.

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1. Introduction

In nanostructures, the surface-to-volume ratio is increased, and surface state problems become more serious. Surface states deplete carriers, reduce gate control efficiency, cause field-induced current leakage, side-gating and charge-discharge related hysteresis effects, and reduce quantum efficiencies for optical transitions through surface recombination. Thus, success of future III-V nanoelectronics depends strongly on surface passivation.

For this issue, we proposed and have been investigating a Si interface control layer (Si ICL) -based passivation scheme [1]. The Si ICL is an ultra-thin Si interlayer grown by molecular beam epitaxy (MBE). Recently, we have shown that this scheme is very effective for nanostructures, increasing photoluminescence (PL) intensity from AlGaAs/GaAs quantum wires [2] and completely removing surface-state-induced side-gating in GaAs quantum wire transistors [3].

However, previous works were mainly on (001) surfaces, whereas III-V nanostructures possess many non-(001) surfaces. For example, we have recently proposed a hexagonal binary decision diagram (BDD) quantum circuit approach for ultra-high density quantum LSIs [4]. Here, BDD node devices are fabricated on a hexagonal nanowire network shown in **Fig. 1 (a)** grown on (111)B substrates by selective MBE [5]. Effectiveness of the Si ICL scheme for such non-(001) surfaces requires further investigation.

With this background, this paper presents the results of growing Si ICLs on GaAs and AlGaAs (111)B surfaces by MBE, and characterizing them by *in-situ* X-ray

photoelectron spectroscopy (XPS). The results indicate effectiveness of the Si ICL passivation on (111)B surfaces.

2. Experimental

The structure and fabrication sequence of the Si ICL passivation scheme are shown in **Fig. 1 (b)**. The basic idea is, firstly, to realize an ordered Si surface without Fermi level pinning by terminating III-V semiconductor surfaces with Si atoms, and then, to maintain this order by terminating the Si ICL with a Si-based ultra-thin insulator.

Experiments were carried out in an ultrahigh vacuum (UHV) multi-chamber system. At first, thick *n*-type GaAs or Al_{0.3}Ga_{0.7}As/GaAs layers were grown by MBE. Reflection high-energy electron diffraction (RHEED) patterns were well-defined Ga-stabilized ($\sqrt{19}\times\sqrt{19}$) patterns during and after growth at 670-700°C, and became As-stabilized (2x2) pattern after cooling the substrate below 500 °C, in agreement with previous works [6, 7]. A ($\sqrt{19}\times\sqrt{19}$) surface was obtained by annealing the sample at 500 °C with the As-beam flux off, while a (1x1) surface was prepared by monolayer deposition of Ga atoms onto it. Subsequently, the atmospheric As was evacuated, and a 1nm-thick Si ICL was grown by MBE at the growth temperature of 300 °C supplying Si atoms from the K-cell for 120 min.

To complete surface passivation, a passivation dielectric should be deposited on the Si ICL. However, our previous experiences [1] have shown that its direct deposition results in poor passivation due to process induced damage. For this reason, a part of the Si ICL was converted to SiN_x by direct nitridation by irradiating Si ICL with a nitrogen radical beam at room temperature. Finally, a thick Si-based passivation dielectric such

as SiO₂ and Si₃N₄ film was deposited by a standard thermal chemical vapour deposition (CVD) or plasma enhanced CVD process.

At each step of fabrication except the last one, the sample surfaces were characterized *in-situ* in the XPS chamber. The X-ray source was AlK α (1486.6 eV).

3. Results and discussion

3.1 MBE growth of Si ICL

The in-situ XPS technique was found to be highly powerful for characterization. An example is shown in **Fig. 2** for Ga3p and Si2p spectra obtained on (2x2)-reconstructed AlGaAs surface after various steps. Such spectra were taken on GaAs and AlGaAs surfaces for different exit angles of photoelectrons, and observed exit-angle dependence of the Ga3p spectra indicated that a uniform Si layer was formed on both GaAs and AlGaAs surfaces and that the thickness of the Si ICL was 1 nm in agreement with the value calculated from the Si flux intensity and time.

Additionally, being independent of the initial reconstruction pattern, the RHEED pattern changed to (1x1) pattern at the early stage of Si growth, and it was maintained during Si growth. It strongly indicates that the Si film grows epitaxially.

3.2 Band bending change and its interpretation

The changes of the Ga3d core level peak position before and after Si-ICL growth are summarized in **Fig. 3** for GaAs and AlGaAs (111)B surfaces with different surface reconstructions together with reference data for the standard As-stabilized GaAs (001)-(2x4) surface. Since As3d, Ga3d, and Ga3p core level peaks also showed the

same shifts, the observed shifts can be interpreted as changes of band bending. The scale for the position of the surface Fermi level, E_{FS} , for GaAs obtained using the relation of Ga3d peak = VBM - 18.80 eV by Kraut [8] is given on the right axis.

It is seen that E_{FS} is strongly pinned at 600-800 meV above VBM on all of the MBE grown clean GaAs surfaces in spite of the fact that these surfaces gave well-defined surface reconstruction patterns. On the other hand, large shifts of E_{FS} by 250-420 meV toward E_C took place after Si-ICL growth on all of the (111)B GaAs and AlGaAs surfaces, showing remarkable reduction of band bending. The best result was obtained on the GaAs (111)B-($\sqrt{19} \times \sqrt{19}$) surface, realizing an almost flat band condition. However, in the case of the standard As-stabilized (001)-(2x4) surface of GaAs, band bending stayed nearly the same or became even slightly worse by Si-ICL growth in agreement with our previous result [9] and also with a more detailed study by Chambers and Loebis [10].

3.3 XPS spectra analysis and growth mechanism

In order to get more detailed information on interface formation, deconvolution of Ga3d, As3d and Si2p core level spectra obtained at each process step was attempted by using Voigt fitting functions for spin split doublets with published values of spin-orbit splitting and branching ratio together with certain values of disorder induced broadening. Chemical shift values reported in the literature [11] were also used, when they were appropriate. Since the tedious description of the fitting procedure is beyond the scope of this paper, only the gross results are given in **Fig. 4 (a)** and **(b)** for the GaAs sample

with ($\sqrt{19} \times \sqrt{19}$) initial surface reconstruction. Similar results were obtained on other surfaces.

As shown in **Fig. 4 (a)**, a monolayer level broad peak appeared on the lower energy side in Ga3d spectra after Si growth, which we interpreted as a Ga-Si related peak with possible inclusion of Ga-Ga component. In the As 3d spectra, a larger As-Si component was detected at the sample surface together with an As-As component. These results seem to be consistent with the work by Huen et al [11], although the interpretation of the band bending change is different. In Si2p peak, only As-Si component could be separated, since Ga-Si peak, if it exists, has a peak very close to the Si-Si peak [12].

Our interpretation for the observed spectra is that the Si layer grows mostly on Ga atoms and is terminated by As atoms at the surface together with a thin elemental As layer on top. Since the As-terminated (111) Si surface is known to exhibit (1x1) RHEED pattern [12], such an interpretation is consistent with the observed (1x1) pattern. Since it has been reported that As atoms can take roles of surfactants for Si epitaxial growth [13], and that a highly stable As-terminated surface can be formed at 300°C [12], As atoms should have acted as surfactants in the present case, enhancing Si MBE growth at a low temperature.

After surface nitridation, the As-Si component disappeared completely. Comparing with Si2p spectra shown in Fig. 4(b), this indicates that As-Si bonds were replaced with N-Si bonds. The Si2p spectra also show that the Si layer still remains, indicating the successful partial nitridation. The residual Si-ICL thickness was estimated to be around 0.5nm. On the other hand, the peak corresponding to As-As bonds became more intense

after nitridation. Since this peak disappeared completely by thermal annealing, it most likely corresponds to physisorbed As atoms on the SiN_x layer. Furthermore, Ga3d spectra in **Fig. 4 (a)** show that Ga-Si component exists after surface nitridation in consistent with the interpretation that the Ga-Si bonds exist at the Si/GaAs interface. Based on the above results, the most likely bonding configurations in the vicinity of the Si ICL during Si growth and after surface nitridation are summarized in **Fig. 5** for the GaAs sample.

As for the observed band bending change, it was previously argued [10,11] that it is not due to surface state removal, but due to compensation of negative surface state charge by positive charge of As donors incorporated in the Si layer. However, such a simplistic view does not seem to be valid, firstly because the amount of As atoms incorporated into Si is at most in the range of 10^{11}cm^{-2} , and not large enough to compensate 10^{13}cm^{-2} level interface state charge, and secondly, and more importantly, because of difficulty of donor ionization in the present structure. Namely, the band gap of the Si layer is very much reduced by tensile stress. Furthermore, Si forms a surface quantum well where the first confined electron state lies high above the lowered Si conduction band edge. These two facts make the ionization of shallow donors difficult.

On the other hand, we have recently directly shown [14] by scanning tunnelling microscopy and spectroscopy study of the Si ICL formed on a Ga-rich (001)-(4x6) surface of GaAs that the Si ICL grows epitaxially, and the surface becomes completely free of surface states and Fermi level pinning. Furthermore, the results showed strong correlation with macroscopic band bending measurements by XPS [15]. Thus, considering the achievement of a nearly flat band in the present study, it is highly likely that the ultrathin epitaxial Si ICL removes surface states from (111)B surfaces. A recent

PL study [2] on quantum wires grown on (111)B substrates also supports such an interpretation.

4. Conclusions

MBE growth of Si on GaAs and AlGaAs (111)B surfaces with various surface reconstructions have been investigated by XPS. Si layers grow epitaxially with Si-Ga bonds at the Si/GaAs interface and Si-As termination on top, suggesting surfactant roles by As atoms. On nitridation by nitrogen radicals at room temperature, Si-As bonds are replaced by Si-N bonds leading to partial nitridation of the Si layer. Unlike the case of an As-stabilized GaAs (001)-(2x4) surface, large reduction of band bending of 250-420 meV is observed on (111)B surfaces, indicating large reduction of surface states, and thus effectiveness of the Si ICL passivation.

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Figure captions

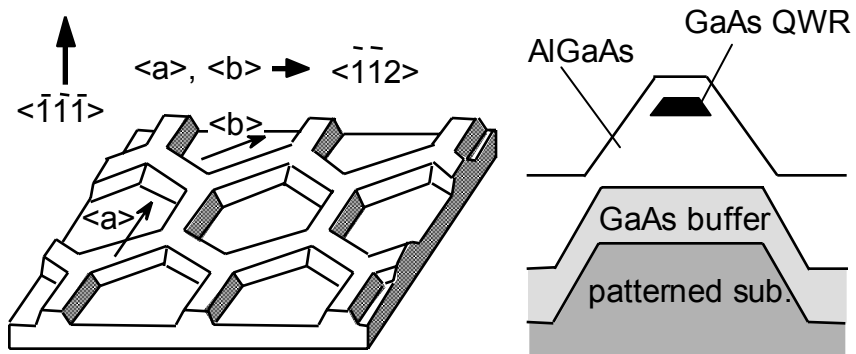
Fig. 1 (a) Hexagonal BDD quantum circuits formed on (111)B surface. (b) Structure and fabrication sequence of the Si ICL based passivation.

Fig. 2 Ga3p and Si2p spectra from AlGaAs surface after each fabrication step.

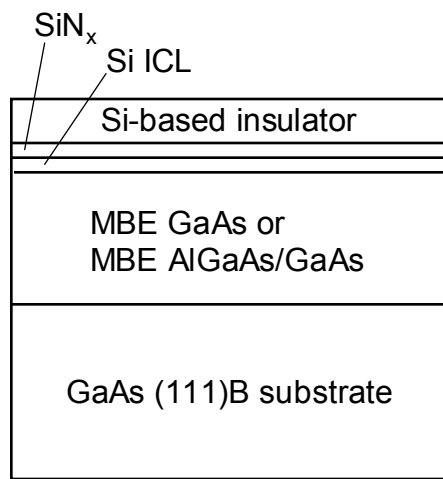
Fig. 3 Changes of Ga3d peak positions and surface Fermi level positions caused by Si growth.

Fig. 4 Changes of (a) Ga3d and As3d spectra and (b) Si2p spectra taken on GaAs surface at each process step.

Fig. 5 The most likely bonding configurations in the vicinity of the Si ICL on GaAs during Si growth and after surface nitridation.



(a)



(b)

fabrication sequence

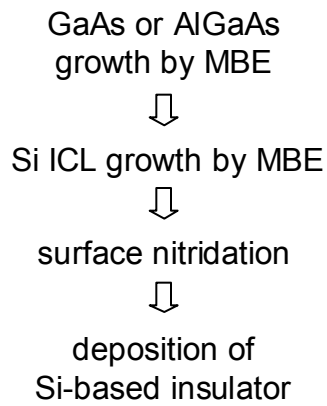


Fig. 1 Akazawa and Hasegawa

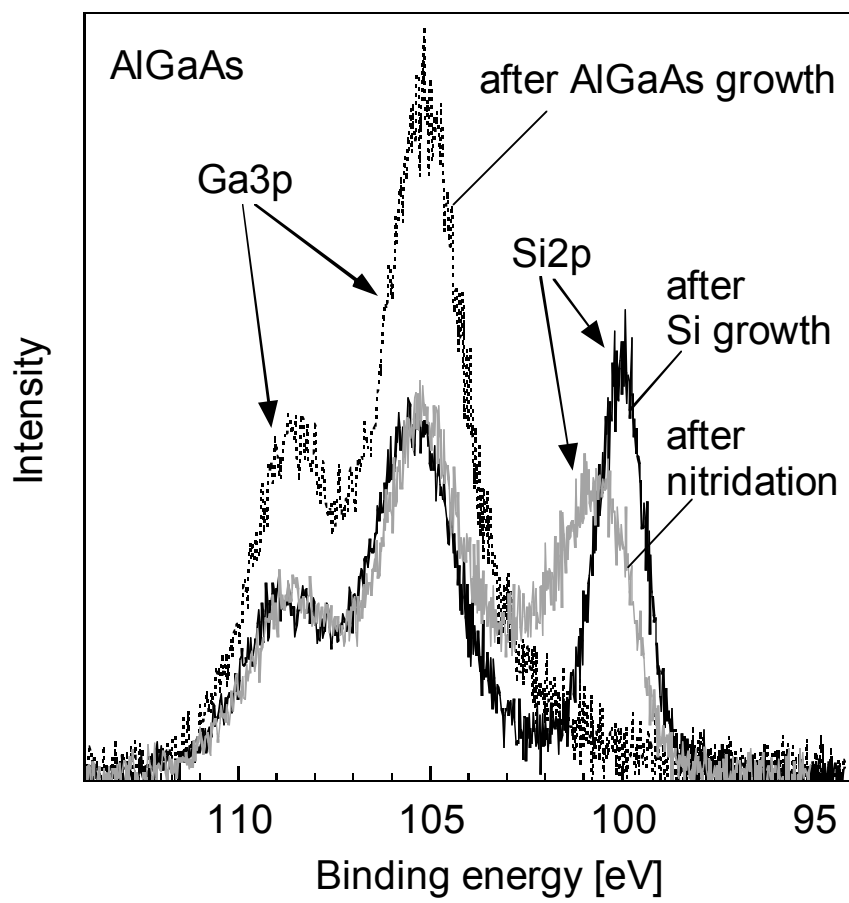


Fig. 2 Akazawa and Hasegawa

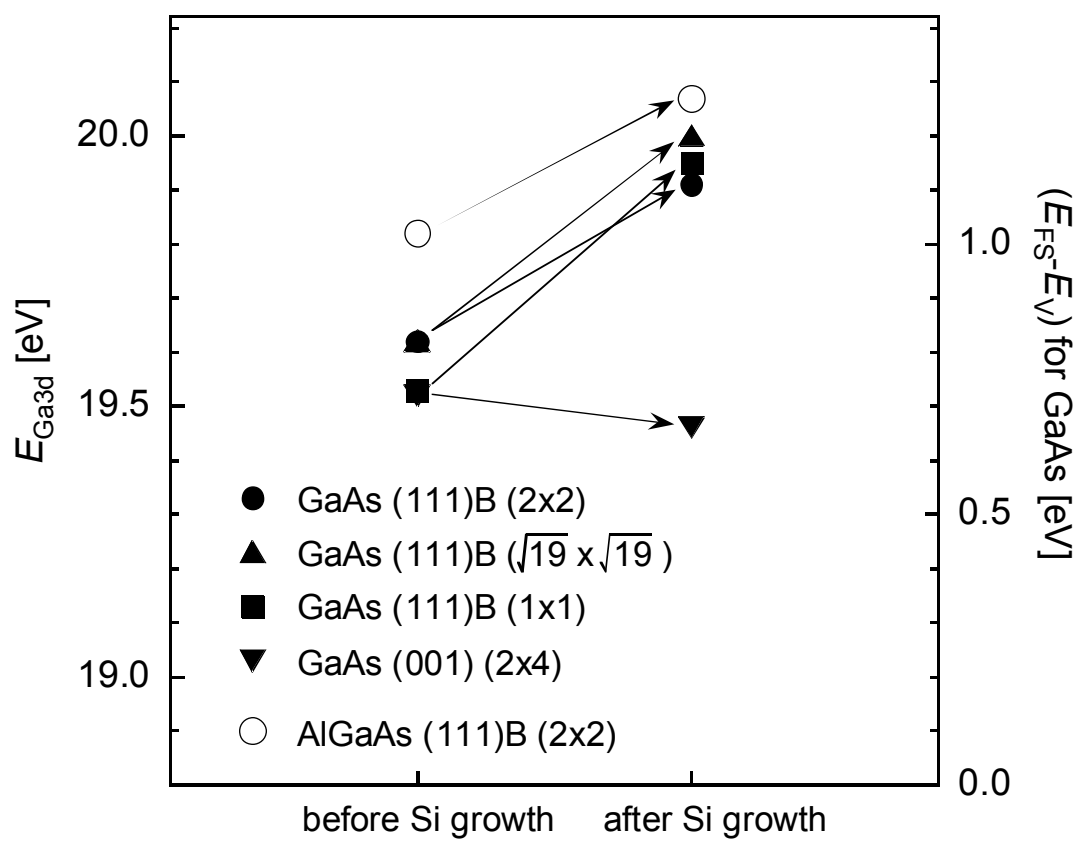


Fig. 3 Akazawa and Hasegawa

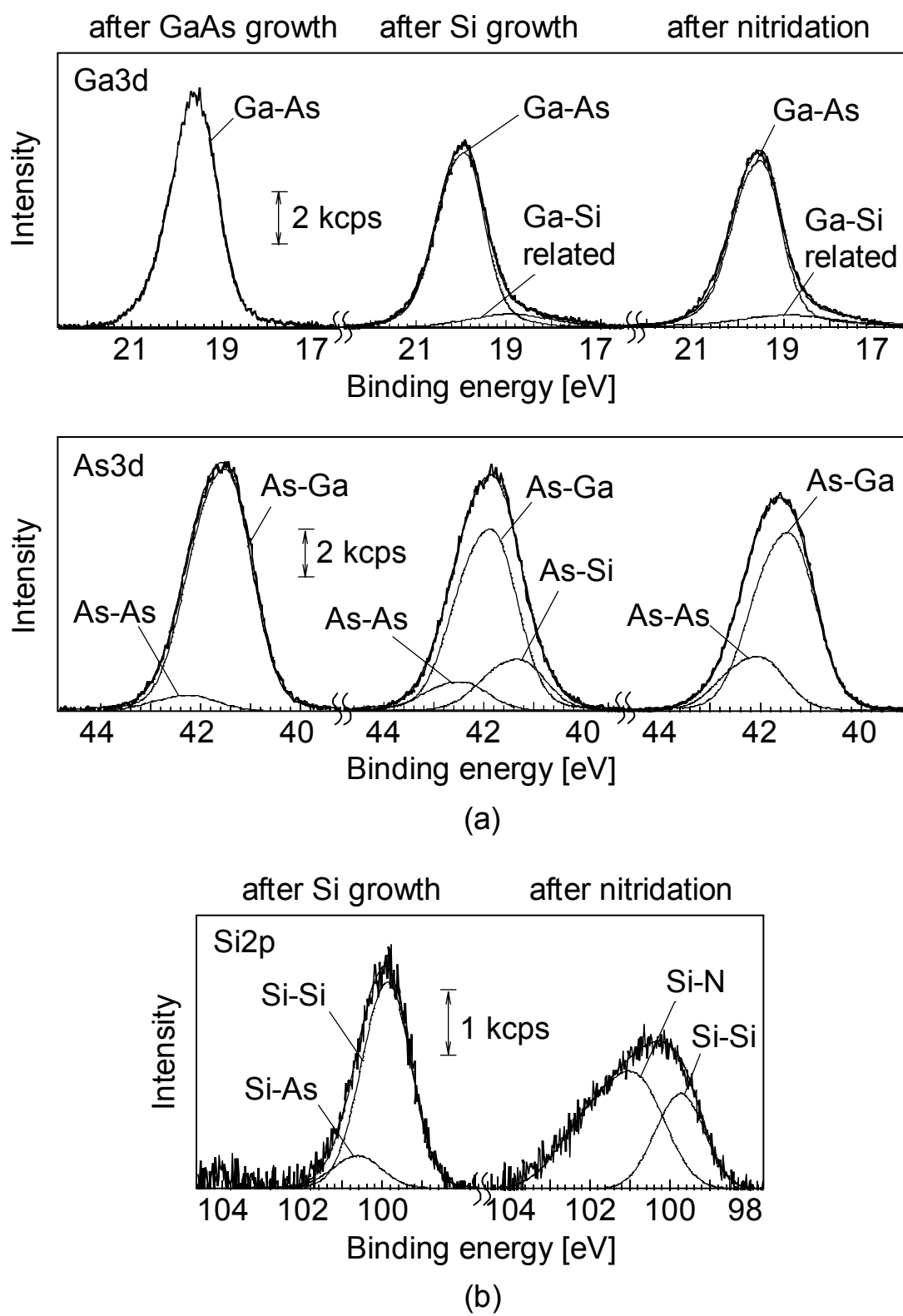


Fig. 4 Akazawa and Hasegawa

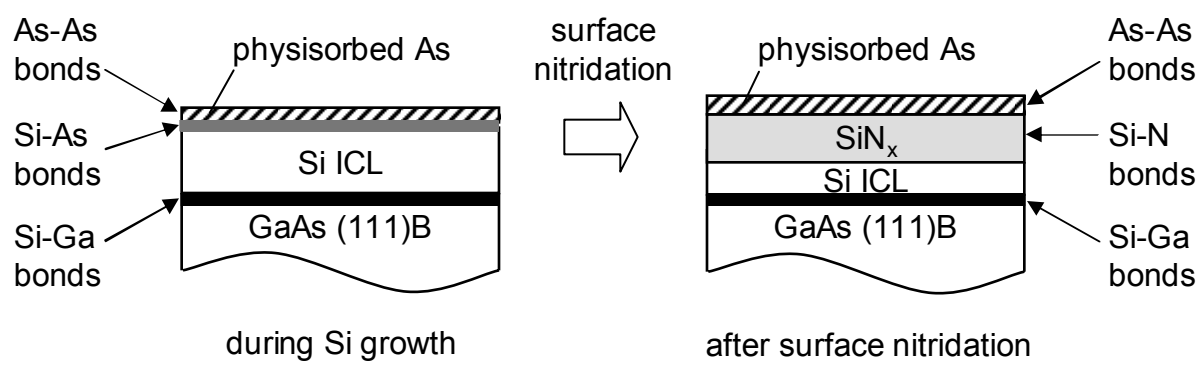


Fig. 5 Akazawa and Hasegawa