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Characterization of Interface Roughness in Ge/SiGe Heterostructures Using Photoreflectance Spectroscopy

Hiroyuki YAGUCHI, Kaori TAI,* Keizo TAKEMASA, Kentaro ONABE, Yasuhiro SHIRAKI[1] and Ryoichi ITO

Department of Applied Physics. The University of Tokyo

7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

[1] *Research Center for Advanced Science and Technology (RCAST), The University of Tokyo*

4-6-1 Komaba, Meguro-ku, Tokyo 153, Japan

We have investigated Ge/SiGe strained-barrier quantum well (SBQW) structures using photoreflectance (PR) spectroscopy. On the basis of transition energies related to the quantum well formed at the Γ point, band offsets at the Ge/SiGe heterojunction was found to vary linearly with germanium composition in the SiGe layer. Conduction band offset ratio $Q_c (= \Delta E_c/(\Delta E_c + \Delta E_{vh}))$ at the Γ point was evaluated to be 0.68 ± 0.08. From the intrinsic linewidth of the optical transitions, interface roughness at the Ge/SiGe heterointerface was characterized for the first time and estimated to be one monolayer (ML). In addition, the splittings in PR spectra were observed in some samples at low temperatures. These splittings were due to the difference in the well width and corresponded to the height (or depth) of about 10 ML.

1. INTRODUCTION

In the SiGe system, the Ge/SiGe heterostructure is expected to be one of the most promising candidates for modulation-doped field-effect transistors (MODFETs),[1,2] because the use of a Ge layer as a channel layer is superior to that of a SiGe alloy layer owing to its lighter effective mass and no alloy scattering. Although band offsets and roughness at the heterointerface are of crucial importance in realizing the Ge/SiGe MODFET, they have not been fully clarified yet and there exists some confusion.

In the present study, we have employed photoreflectance (PR) technique to investigate the band offsets and roughness at the Ge/SiGe heterointerface. From quantum-number dependence of the intrinsic linewidth, the interface roughness was found to be ±1 monolayer (ML) at the Ge/SiGe heterointerface. In addition, the splittings in PR spectra were observed at low temperatures in some samples. This is considered to be due to the difference in the well width. The comparison between the calculation of QW levels and experimental data indicates the step with a height of about 10 ML exists.

2. EXPERIMENT

The samples used in this study were Ge/SiGe single strained-barrier quantum well (SBQW) structures grown on Ge(100) substrates in a solid source Si molecular beam epitaxy (MBE) system. The PR experimental setup used in this study was a conventional one. To modulate the surface electric field in the sample, the 488 nm emission from an Ar ion laser was used as a pump beam chopped at 800 Hz. PR measurements were carried out at temperatures between 4.2 and 300 K.

3. RESULTS AND DISCUSSION

We have measured PR signals due to interband transitions at the Γ point in Ge/SiGe SBQW structures. Since the SiGe barrier layers are under biaxial tensile strain, electron–light hole band gap becomes smaller than electron–heavy hole band gap. Conduction, heavy-hole valence and light-hole valence band offsets are defined as ΔE_c, ΔE_{vh}, and ΔE_{vl}, respectively.

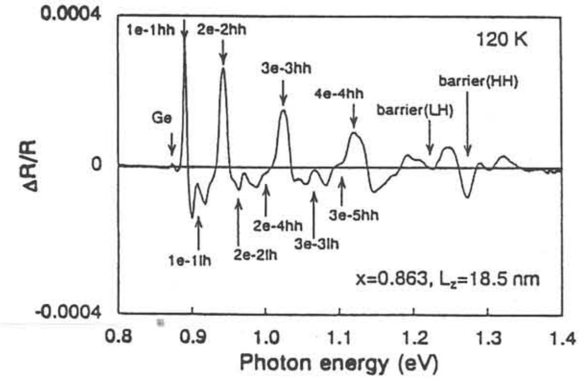

Fig. 1 PR spectrum of Ge/SiGe SBQW structure.

Figure 1 shows a PR spectrum of the Ge/SiGe SBQW structure. The QW-related transitions are distinctly observed, as well as the transitions corresponding to the splitting band gap energies of the strained SiGe barrier layer. From the comparison between experimental and theoretical transition energies, we could determine the band offsets at the heterojunction and their dependence on the germanium composition. The results are shown in Fig. 2. It is found that the band offsets are almost linearly dependent on the Ge composition. If Ge composition in the barrier layer is extrapolated to $x = 0$ (i.e., Si), the light-hole valence band offset becomes $\Delta E_{vl} = 0.52 \pm 0.22$ eV.

Next we would like to compare our results with other studies concerning the band offsets in the Ge/SiGe heterostructures. Schwartz *et al.*[3] reported $\Delta E_{vl} = 0.17 \pm 0.13$ eV based on photoemission spectroscopy of core levels. On the other hand, from the PR measurements of Ge/SiGe strained-layer superlattices, Rodrigues *et al.*[4] reported $Q = 0.73 \pm 0.03$ which corresponded to $\Delta E_{vl} = 0.32 \pm 0.08$ eV at the Si/Ge(001) interface.

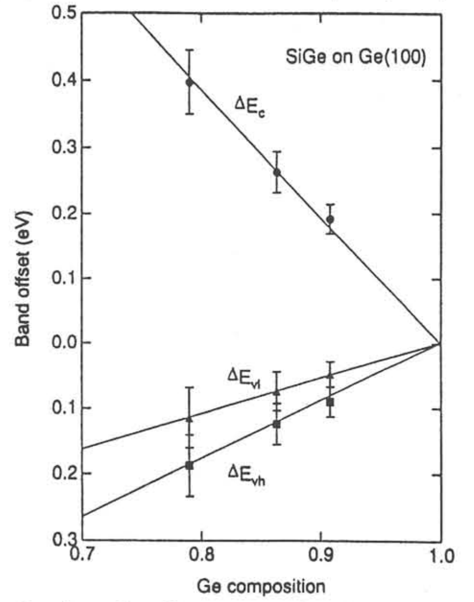

Fig. 2 Band offsets at the heterointerface in Ge/SiGe SBQW structures.

In our study, the light-hole valence band offset is somewhat larger than that obtained by other studies. In particular, the values obtained from photoemission measurements are rather smaller than our result. This discrepancy is probably due to the influence of the surface segregation of Ge atoms which smears the interfacial abruptness. Namely, there is possibility that the valence band offset not for the Si/Ge heterointerface but for the SiGe/Ge heterointerface was measured. The result of Rodrigues *et al.*[4] is relatively close to our result. The difference in conduction band offset ratio may be due to the difference in the sample structure and/or the nonparabolicity parameter of conduction band used in the calculation.

In order to consider the interface roughness at the heterojunction, we have focused our attention on the linewidth of optical transitions. From the temperature dependence of the linewidth of the QW-related transitions, the intrinsic linewidth could be estimated. The intrinsic linewidth is considered to originate mainly from interface roughness and alloy disorder in SiGe barrier layers. The results of the calculation shows that the contribution of the interface roughness is much larger than that of alloy disorder. Therefore, it is found to be appropriate for the characterization of the interface roughness to use the intrinsic linewidth.

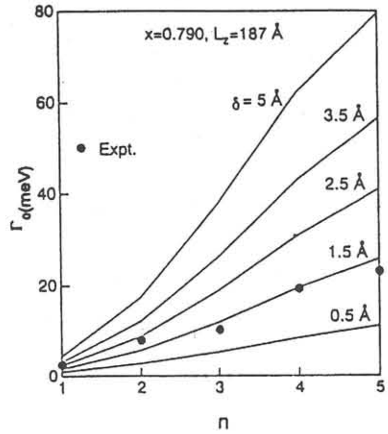

Fig. 3 Dependence of intrinsic broadening parameter on quantum number. Solid lines are calculated for various fluctuation in the well width.

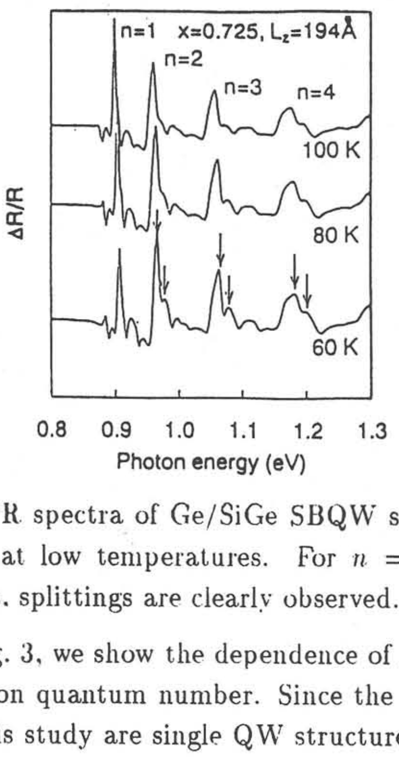

Fig. 4 PR spectra of Ge/SiGe SBQW structure measured at low temperatures. For $n = 2 \sim 4$ transitions, splittings are clearly observed.

In Fig. 3, we show the dependence of intrinsic linewidth on quantum number. Since the samples used in this study are single QW structures, there is no possibility of inter-well fluctuation and only intra-well fluctuation causes the linewidth broadening. It is seen in this figure, the quantum number dependence agrees well with the calculation and the height is found to be ± 1.5 Å. Thus, the interface roughness can be estimated to be ± 1 ML. In the estimation of the interface roughness, it should be noted that the size of the islands is assumed to be comparable to the exciton Bohr radius (~ 200 Å).

In some samples, we observed the splittings in PR spectra at low temperatures, as shown in Fig. 4. Since the splitting becomes larger as the quantum number increases, it is considered to correspond to the difference in the well width. Assuming that $\Delta L_z = 15$ Å as the difference in the well width, the energy difference between the splitting two peaks can be well explained. This indicates that rather large islands with the height of about 10 ML happens to be formed at the heterointerface between Ge and SiGe in some occasions.

4. CONCLUSIONS

We have investigated Ge/SiGe SBQW structures using PR spectroscopy. On the basis of the QW-related transition energy, band offsets at the Γ point could be estimated. Conduction band offset ratio was found to be 0.68 ± 0.08. From the intrinsic linewidth, interface roughness at Ge/SiGe heterointerface was characterized. It was revealed the height of island was 1 ML. In addition, the splittings in PR spectra were observed at low temperatures in some samples. This is due to the difference in the well width and corresponds to the height of about 10 ML.

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*Present address: Oki Electric Industry Co., Ltd., 550-1 Higashiasakawa, Hachioji, Tokyo 193, Japan

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