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The Interaction between Si and Be in GaAs Grown by MBE

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In order to investigate the interaction between Si and Be, double doping of Si and Be has been carried out. The samples were characterized by secondary ion mass spectroscopy and Hall measurement. The results showed that the Si-Si pair formed in high Si-doped GaAs was prevented by the formation of the Si-Be pair and thus Si diffusion was suppressed.

I. Introduction

Recent observations of disordering in AlAs/GaAs superlattice (SL) induced by Si doping[1] or Si implantation[2] have been paid much attention for the device process applications and the physical interest. There have been a lot of experimental findings for the Si-induced disordering, but little was known about the disordering mechanism. Van Vechten[3] proposed some theoretical models of the disordering for Zn and Si, but the models have not been yet confirmed by experiments.

For the disordering of SL, it is necessary to diffuse impurity atoms around SL, but all kinds of the impurity atoms do not induce the disordering. Therefore, in order to understand the disordering mechanism, we will need to know a microscopic picture for the impurity diffusion.

It has been known that the Si-Si pair, which is formed by high doping of Si into GaAs, is main species for Si diffusion,[4] and thus Si-induced disordering occurs by the high doping of Si ($>10^{18}$ cm^{-3})[1]. Therefore, if the Si-Si pair formation can be prevented, the Si-induced disordering will be suppressed. This approach was carried out by Kawabe et al.[5] They observed that the Si-induced disordering was drastically suppressed by simultaneous doping of Be into Si-doped SL, when Be concentration was above the doping level of Si.

In this paper, we show that the diffusion of Si is significantly suppressed by Be doping and gives the explanation of the mechanism of this effect.

II. Experimental

Samples were grown by molecular beam epitaxy (MBE) on (100) oriented Cr-doped GaAs substrate at the growth temperature of 550°C under As-stabilized condition.

The growth rate of GaAs (0.5 μm/h) was determined by intensity oscillations in reflection high-energy electron diffraction (RHEED)[6] before the each growth run.

Two kinds of samples were grown for studying the interaction between Si and Be in GaAs. One, for the measurements of carrier concentration and mobility, consisted of a Si-doped GaAs layer of 0.5 - 0.75 μm thick with or without Be doping on an undoped GaAs buffer layer. Carrier concentration and mobility were measured by the van der Pauw method. The other was the sample for studying the incorporation and the diffusion of Si and Be in GaAs. In the sample, there were two Si-doped layers; in one layer, Be was doped simultaneously and in the other, there was no Be doping. The sample was annealed at 750°C for 70 minutes in a hydrogen ambient with face to face contact to another GaAs wafer. The depth profiles of Si and Be in the sample were measured by secondary ion mass spectroscopy (SIMS) using an O_2^+ as a primary ion. In this study, carrier concentration and mobility were mesured by the van der Pauw method.

III. Results and Discussion

Figure 1 shows the carrier concentration for Si-doped (closed circle) and double doped (Si and Be; open triangle) GaAs as a function of the Si cell temperature. Doping level of Be was kept constant in each sample (7×10^{18} cm^{-3}).

For Si-doped GaAs, the carrier concentration increases with a rise in the Si cell temperature,

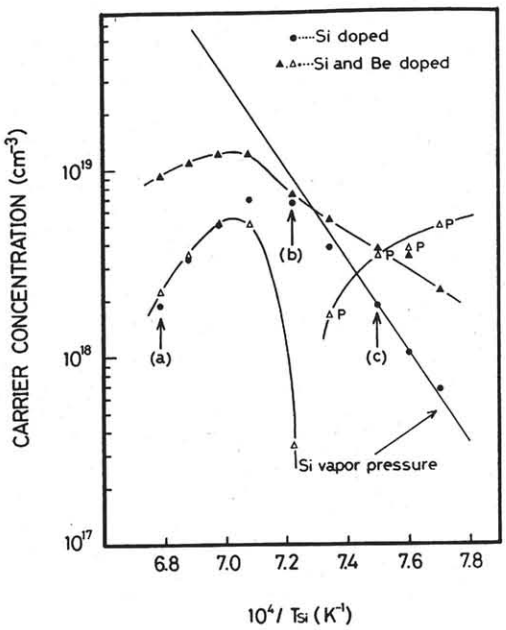

Fig.1 Carrier concentrations of Si-doped (closed circle) and double doped (open triangle) GaAs vs. Si cell temperature. Be doping level was kept constant ($7x10^{18}$ cm^{-3}). Closed triangle represents the value calculated by considering the compensation of Be. P denotes the p-type samples.

and the slope of the Si vapor pressure curve agrees well with the experimental points. Above $4x10^{18}$ cm^{-3}, the carrier concentration deviates from the slope of the Si vapor pressure curve. After reaching the maximum point of about $8x10^{18}$ cm^{-3}, the carrier concentration begins to decrease with an increase in the Si cell temperature. Similar results were reported by several researchers.[7,8]

In order to investigate the origin of the decrease in the carrier concentration at high Si cell temperature, we measured the Si concentration of each sample by SIMS. The results show that the Si concentration increases up to $2x10^{20}$ cm^{-3}, having the same slope as the Si vapor pressure curve. Therefore, we conclude that Si arriving at the GaAs surface was incorporated at a constant rate, and the discrepancy between the carrier concentration and the Si concentration is attributed to the site change of Si from the Ga site to the As site.

If no interaction between Si and Be exists when both dopants are simultaneously doped into GaAs, measured carrier concentration will be the difference between electron concentration in Si-doped GaAs and hole concentration in Be-doped GaAs. However, as shown in Fig.1, there is no difference between closed circles and open triangles in high temperature region in spite of the doping of Be, which indicates that there is strong interaction between these dopants.

If we assume that all of Be doped into GaAs form the shallow acceptor level (exist at the Ga site), we can calculate the difference between the concentrations of Si at the Ga site N_D and Si at the As site N_A by taking into account the compensation by Be. Closed triangles in Fig.1 shows this case.

In high temperature region, there is no difference in carrier concentration btween the Si-doped (closed circle) and double doped (open triangle), that is, the Be doping effect is eliminated. The perfect compensation for Be incorporated in GaAs would be attributed to an increase in the incorporation of Si, the amount of which is almost equal to that of the incorporated Be. In low temperature region, an increase in the calculated value (closed triangle) is observed. Two possible explanations can be considered; one is the site change of Si and the other is the increase in the incorporation of Si. However, the SIMS measurement shows that Si concentration is almost equal to carrier concentration, that is, the amount of Si atoms at As sites is neglegible, and the amount of the increased Si by Be doping is not large enough to explain this increase. Therefore, both explanations can not well explain this effect. At this stage, we can not give the proper explanations of this effect.

Figure 2 shows the room-temperature Hall mobilities for Si-doped GaAs. Top scale is the Si concentration N_{Si} and bottom scale is the carrier concentration. The Hall mobility monotonously decreases with an increase in the Si concentration, and ranges from 2900 cm^2/Vs at $N_{Si}=6x10^{17}$ cm^{-3} to 680 cm^2/Vs at $N_{Si}=2x10^{20}$ cm^{-3}.

Chattopadhyay and Ghosal[9] theoretically calculated electron mobility using the data reported by Druminski et al.[10] They concluded that the consideration of dipoles (i.e. donor-acceptor pair) is essential in accounting for the electron transport in high Si-doped GaAs. For comparison, we draw the theoretical mobilities

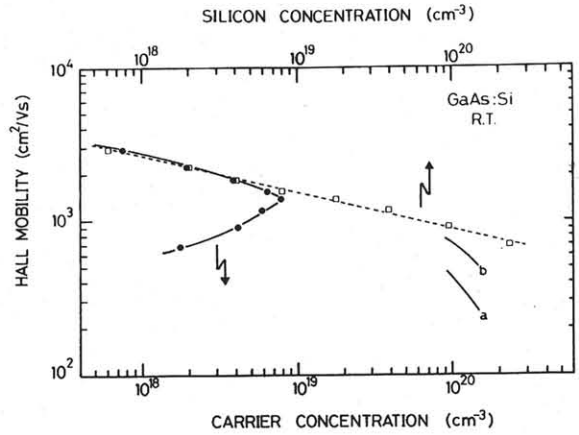

Fig.2 Si concentration (top scale) and carrier concentration (bottom scale) vs. room temperature Hall mobility in Si-doped GaAs. Curves a and b are the calculated lines;[9] curve b considers dipole scattering and curve a does not.

calculated by Chattopadhyay and Ghosal on the figure. Curves a and b represent the result obtained by completely neglecting the formation of dipoles and that obtained by considering the presence of dipoles, respectively.

The Hall mobilities obtained in this work are much higher than curve a. The large discrepancy between the experimental and the theoretical is improved by considering the formation of dipoles (curve b). This result suggests that a fair amount of dipoles (Si-Si pairs) is formed in high Si-doped GaAs.

For the evaluation of the number of the paired Si, we used the theoretical calculation developed by Wiley.[11] The solid line in Fig.3 represents the ratio of the concentration of Si-Si pair N_P to the total Si concentration N_{Si}, which was calculated from the compensation ratio N_A/N_D (dot-dash line) determined experimentally. From Fig.3, about 60 % of N_{Si} are known to form pairs at around $N_{Si}=1\times10^{20}$ cm^{-3}.

In order to clarify the effect of Be on the incorporation and the diffusion of Si, three samples with different Si doping levels were made. Shown in Fig.4 are the depth profiles of Si and Be for these samples. Si doping conditions were indicated by the three arrows in Fig.1. They are about 3×10^{20} for (a), 2×10^{19} for (b) and 2×10^{18} cm^{-3} for (c). In the samples of (b) and (c), Si concentration is increased about 10 % with Be doping. Akimoto et al.[12] reported that a fair amount of Si was desorbed from GaAs surface at the substrate temperature of 540°C. Therefore, the increase in the Si concentration with Be doping is attributable to the reduction of the desorbed Si from the GaAs surface. The incorporation of Be is also affected with Si doping when Si doping level is high, as shown in (a). The peak and the dip in Be profile at the both edges of Si-doped region were clearly observed. This result indicates that the accumulated Be at the GaAs

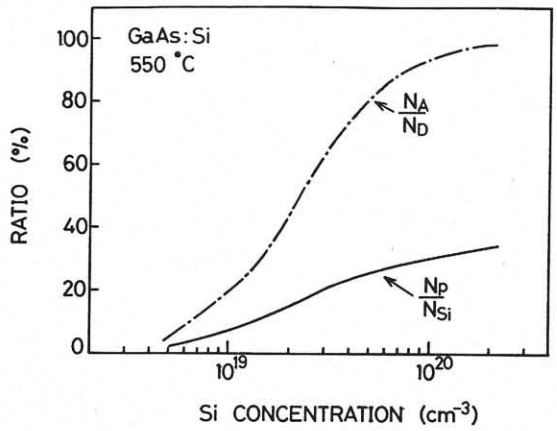

Fig.3 Solid line represents the ratio of the concentration of Si-Si pair (N_P) to the total Si concentration (N_{Si}). Dot-dash line represents compensation ratio (N_A/N_D).

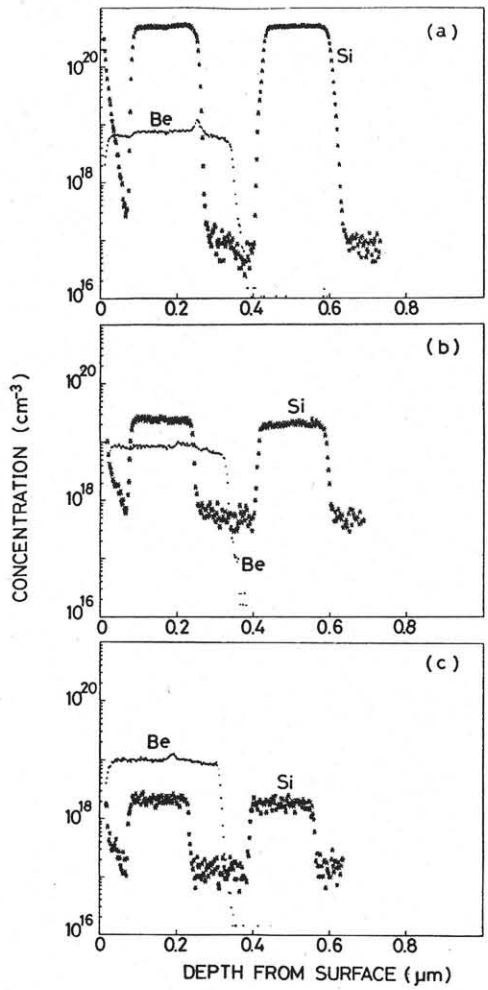

Fig.4 SIMS profiles of Si and Be for as-grown samples.

surface is incorporated by Si doping. The similar effect was obserbed by Miller and Asbeck[13]. Although they considered that the shift in Fermi level upon Si doping was the dominant driving force toward increased incorporation of Be, we consider that the appearance of the peak and the dip in Be profile is the strong suggestion of the existence of the direct interaction between Si and Be like Si(donor)-Be(acceptor) pair. It is also to be noted that the incorporation of Be is increased about 15% with Si doping. This also results from the reduction of the desorption of Be from the GaAs surface with existence of Si.

Figures 5(a),(b) and (c) correspond to the post-annealed depth profiles of Si and Be of the samples shown in Figs.4(a),(b) and (c), respectively. Significant suppression of the diffusion of Be is observed. The effect of Si doping on the suppression of the Be diffusion becomes stronger with an increase in the Si doping level. It is to be noted that the Be diffusion toward the substrate is abruptly stopped by the presence of Si as shown in (b) and (c). For Si, the diffusion of Si is also suppressed by Be

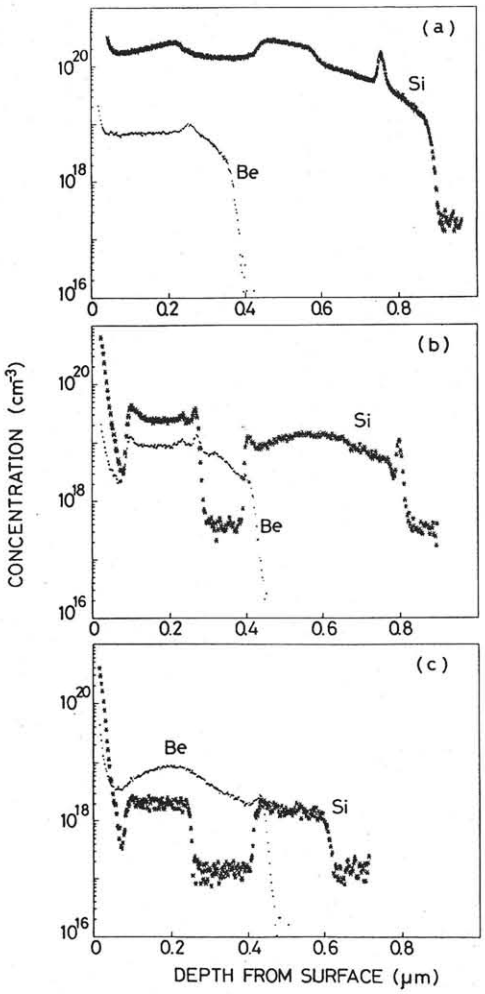

Fig.5 SIMS profiles of Si and Be for after annealing at 750°C for 70 min.

doping except for the case in (a). The degree of the suppression of the Si diffusion depends strongly on the relative concentration of Si and Be. In the region without Be doping, the diffusion constants of Si for (a), (b) and (c) were about 1×10^{-13}, 5×10^{-14} and 5×10^{-16} cm^{-3}, respectively. For the sample (b), the diffusion constant of Si in the region without Be doping is about 100 times larger than that in the double doped region. In Fig.5, the most interesting point is that the depth profiles of Si and Be in (b) show the similar shape in the double doped region. This result indicates that Si and Be diffuse in the form of the Si-Be pair. It is known that the main diffusion species of Si in GaAs is the paired Si in the high doping condition.[4] Therefore, we conclude that the suppression of the diffusion of Si in the double doped region is due to the decrease in the concentration of the Si-Si pair resulting from the formation of the Si-Be pair.

IV. Conclusion

In this paper, we demonstrated that the diffusion constant of Si was significantly suppressed by Be doping, and the degree of the suppression depends strongly on the relative concentration of Si and Be. We attributed this effect to the formation of the Si-Be pair.

From our results, the suppression of the Si-induced disordering of SL with Be doping was due to the decrease in the diffusion constant of Si with Be doping.

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