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Quantification of Electrical Deactivation by Triply Negative Charged Ga Vacancies in Highly Doped Thin GaAs Layers

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We demonstrate for the first time a theoretical approach to electrical deactivation by triply negative charged Ga vacancies (V_{Ga}^{3-}) in n-GaAs thin layers grown by molecular beam epitaxy, and successfully quantify their deactivity under as-grown and annealed conditions. We also show that thinning n-GaAs epitaxial layers introduces low electrical deactivation. Furthermore, we successfully deduce from this study the thermal equilibrium concentration of V_{Ga}^{3-} in intrinsic GaAs. The resulting expression is $[V_{Ga}^{3-}(i)] = 1.73\times10^{32} \exp(-4.72\mathrm{eV}/k_BT)\ \mathrm{cm}^{-3}$.

1. Introduction

In highly n-type doped GaAs, electrical activity is known to be low, and it is generally accepted that Ga vacancies (V_{Ga}), which act as acceptors, are responsible for compensation in n-GaAs. For example, Uedono and Tanigawa concluded from their variable-energy positron beam study that Ga vacancies with a very high concentration are introduced in highly doped n-GaAs layers grown by molecular beam epitaxy (MBE) and that Ga vacancy acceptors act to reduce the concentration of free carriers in the highly doped GaAs.[1)] Uematsu and Maezawa also presented from laser Raman spectroscopy that Ga vacancy-related acceptors dominate the compensation mechanism.[2)] These experimental results strongly suggest that the generation of V_{Ga} is dependent on the Fermi energy in n-GaAs layers. This is consistent with theoretical studies of point defects in GaAs. Baraff and Schlüter claim that the formation energy of an ionized V_{Ga} decreases with an increase in the Fermi energy, meaning that the concentration of V_{Ga} increases with the Fermi energy.[3)] Using their theoretical results, Walukiewicz proposed the concept of amphoteric native defects and pointed out that in n-GaAs, triply negative charged Ga vacancy (V_{Ga}^{3-}) compensates intentionally introduced donors. Moreover, the author successfully presented electrical deactivation by V_{Ga}^{3-} in n-GaAs bulk.[4)] However, systematic study concerning the quantification of the electrical deactivation in n-GaAs thin epitaxial layers such as those popularly used for practical device structures has not been presented thus far, even though highly doped n-GaAs layers have become increasingly important in device applications such as heterojunction field effect transistors.[5)]

In this study we demonstrate for the first time a theoretical approach to electrical deactivation in n-GaAs thin layers grown by MBE, and successfully quantify their deactivity under not only as-grown conditions but also annealed conditions. Moreover, the thermal equilibrium concentration of V_{Ga}^{3-} in intrinsic GaAs is deduced from this study.

2. Theoretical analysis

The basic equations used here are Poisson's equation and an equation of the equilibrium concentration of V_{Ga}^{3-}. The one-dimensional Poisson's equation is

$$\frac{\partial^2}{\partial x^2}V(x) = -\frac{q}{\varepsilon}\left\{N_D^+(x) - N_A^-(x) + p(x) - n(x)\right\} \quad (1)$$

where ε is the dielectric constant; q is the modulus of the electron charge; $N_D^+(x)$ is the ionized donor concentration; $N_A^-(x)$ is the ionized acceptor concentration; $p(x)$ is the hole concentration; and $n(x)$ is the electron concentration. In our analysis, Poisson's equation was first solved to obtain the Fermi energy in an MBE-grown sample in the case of a 100% electrical activity condition, that is, in the case of no generation of compensating species. Then, the Fermi energy that provides concentration of the compensating species V_{Ga}^{3-} was calculated to equal the Fermi energy that provides carrier concentration under compensated conditions. This is expressed as the following equations;

$$n_a(x) = n(x) + 3\cdot V_{Ga}^{3-}(x) \quad (2)$$

$$n(x) = N_C \cdot F_{1/2}\left(\frac{E_F - E_C(x)}{k_BT}\right) \quad (3)$$

$$V_{Ga}^{3-}(x) = c\cdot\exp\left(\frac{3\cdot(E_F - E_C(x))}{k_BT}\right) \quad (4)$$

where $n_a(x)$ is the electron concentration in the case of a 100% electrical activity condition; N_C is the effective density of state; $F_{1/2}(\eta)$ is the Fermi-Dirac integral;

$E_C(x)$ is the energy of conduction band edge; and $V_{Ga}^{3-}(x)$ is the equilibrium concentration of V_{Ga}^{3-}. Here, N_C depends on both the temperature and degeneracy.[6)] In our calculation, the only unknown parameter is a coefficient c in Eq. (4), which is a temperature-dependent parameter. The coefficient c was determined by being varied to best fit the experimental data. This way we could get various physical quantities, such as the whole quantity of V_{Ga}^{3-} generated in GaAs. Then, electrical deactivity was defined by the ratio of carrier concentration of the noticing doped layer under compensated conditions to that under uncompensated conditions.

3. Results and discussion

The epitaxial GaAs samples shown in Fig. 1 were used for quantification of electrical deactivation. Each layer was grown by MBE on an undoped (100) GaAs substrate. The substrate temperature during growth was 500℃. The residual background of the MBE-grown undoped GaAs layer was p-type of the order of 10^{15} cm^{-3}. The layer sequence is shown in Fig. 1 and consists of an undoped GaAs layer (800 nm), a highly Si-doped layer and a Si-doped top layer with a doping level of $2x10^{17}$ cm^{-3} (150 nm). The doping levels of the highly doped layers were $5.5x10^{18}$ cm^{-3} and $1x10^{19}$ cm^{-3}, and the thickness was varied in the ranges of 10-50 nm. The top layer was introduced to avoid the influence of surface depletion on the highly-doped layer. Figure 2 shows the experimental and theoretical results for electrical deactivation in the MBE-grown GaAs samples under as-grown conditions as a function of the doped layer thickness. In the figure, open squares and circles represent experimental data at doping levels of $5.5x10^{18}$ cm^{-3} and $1x10^{19}$ cm^{-3}, respectively, while the solid line represents our calculated results. As seen in the figure, the theoretical results agree well with the experimental results. It is worth noting that thinning the GaAs epitaxial layers introduces low electrical deactivation even at the extremely high doping level of $1x10^{19}$ cm^{-3}. Namely, the deactivity can be reduced from 25% to 5% by thinning the doped layers from 50 nm to 10 nm. This is because thinning the doped layer lowers the Fermi energy in the doped layer, thereby alleviating the generation of V_{Ga} acceptors as represented by Eq. (4).

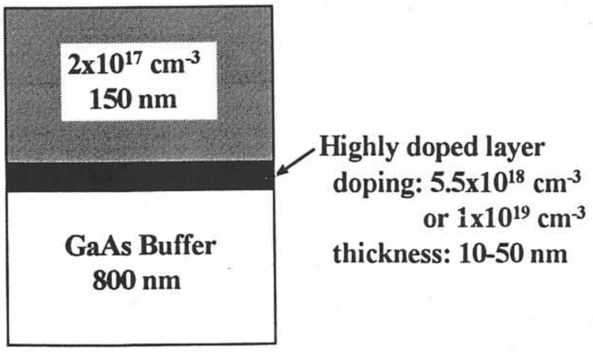

Fig.1 Schematic layer sequence of highly doped thin GaAs samples grown by MBE.

Our calculation was also performed for δ-doping in GaAs. Experimental data of Si δ-doped GaAs were quoted from Ref. 7. Figure 3 shows sheet carrier concentration in the δ-doping in GaAs layers as a function of the nominal 2-dimensional Si concentration. The deactivity of the δ-doped GaAs was calculated as the growth temperature of 550℃. The calculated result was represented by the solid line. It is clear that the theoretical results are quantitatively fitted to the experimental data. Therefore, our theoretical method is useful for all types of doping profiles in GaAs.

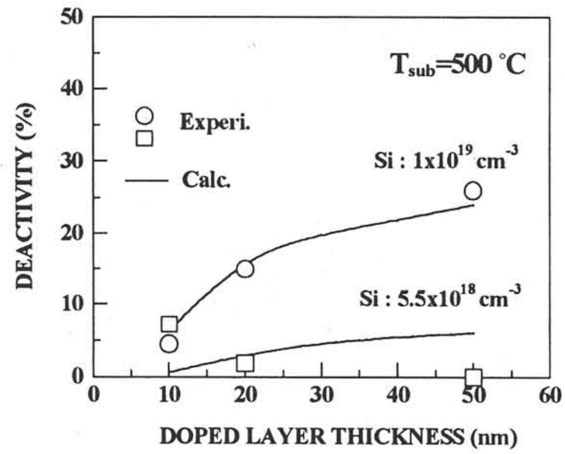

Fig.2 The experimental and theoretical results for the electrical deactivation in MBE-grown GaAs samples as a function of the doped layer thickness.

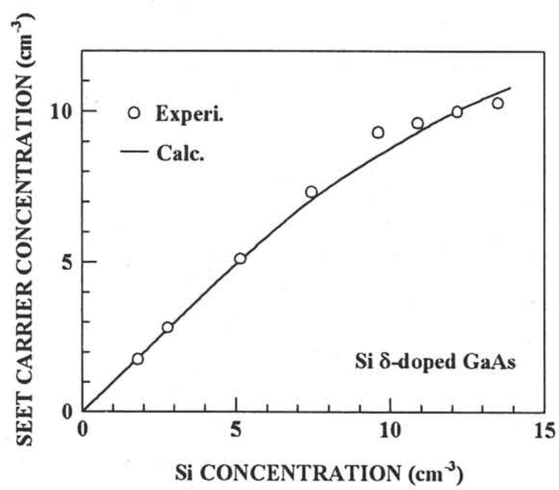

Fig. 3 The experimental and theoretical results for the sheet carrier concentration in Si δ-doped GaAs samples as a function of Si concentration.

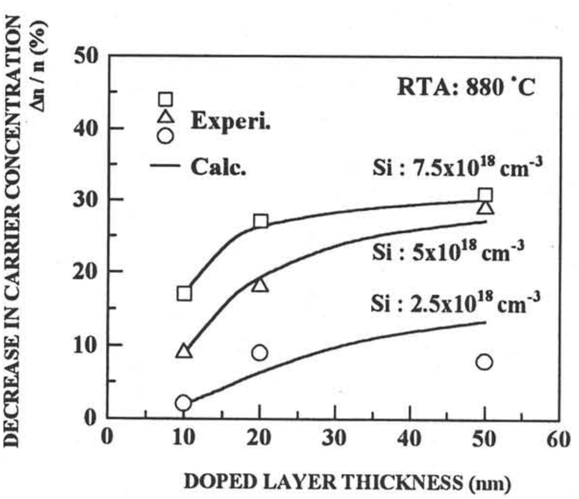

Fig. 4 The experimental and theoretical results for decrease in carrier concentration of the doped layers by annealing as a function of the doped layer thickness.

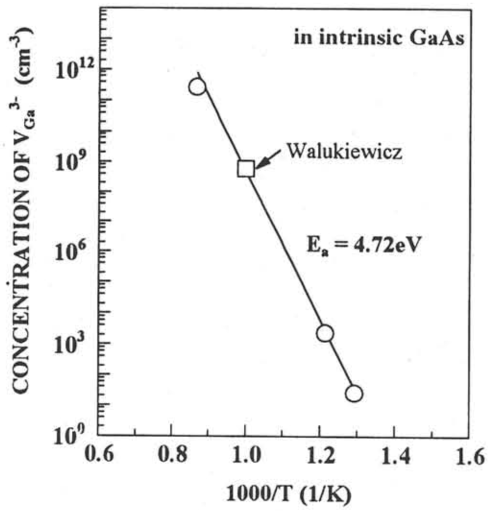

Fig. 5 Thermal equilibrium concentration of V_{Ga}^{3-} in intrinsic GaAs as a function of reciprocal temperature

Moreover, our study was directed to the previously presented results for annealed GaAs samples with three doping levels of 2.5×10^{18} cm^{-3}, 5×10^{18} cm^{-3} and 7.5×10^{18} cm^{-3}. The structure of the samples was the same as shown in Fig. 1. The experimental procedure was described in detail in Ref. 5. Figure 4 shows the decrease in carrier concentration by annealing at 880℃ as a function of the doped layer thickness. In calculating the decrease, we subtracted the calculated percentage decrease at the growth temperature from that at the annealing temperature because in such highly doped layers some electrical deactivation already occurred during MBE growth, as shown in Fig. 2. The calculated results were found to be overlayed with the experimental data in Fig. 4. The agreement is excellent at each doping level. Thus, our analysis on the quantification of electrical deactivation in n-GaAs can be applied to a wide temperature range of comprehensive thermal processing. Also, we found thinning n-GaAs layers to be effective for alleviating the annealing-induced carrier concentration decrease. This is due to the Fermi energy effect described above.

Furthermore, we can easily calculate the thermal equilibrium concentration of V_{Ga}^{3-} in intrinsic GaAs ($[V_{Ga}^{3-}(i)]$) by using the derived value of c in Eq. (4), because the concentration is expressed by

$$\left[V_{Ga}^{3-}(i)\right]=c\cdot\exp\left(\frac{3\cdot E_I}{k_B T}\right) \qquad (5)$$

where E_I is the Fermi energy in the case of intrinsic GaAs. Here, we assumed that E_I is correspondent to the stabilized Fermi level (E_{Fs}) which is proposed by Walukiewicz.[4)] We also supposed that the energy level of E_{Fs} is maintained to be E_V+0.4Eg (E_V: energy of valence band edge, Eg: bandgap energy) at all temperatures. Figure 5 shows the thermal equilibrium concentration of V_{Ga}^{3-} in intrinsic GaAs as a function of reciprocal temperature. In Fig. 5, the value of $[V_{Ga}^{3-}(i)]$ at 1000K was quoted from Ref. 4. The data can be fitted by

$$\left[V_{Ga}^{3-}(i)\right]=1.73\times10^{32}\exp\left(\frac{-4.72eV}{k_B T}\right)\quad cm^{-3}. \qquad (6)$$

4. Conclusion

In conclusion, we have successfully demonstrated the quantification of electrical deactivation in n-GaAs thin layers grown by MBE. Our results and theoretical calculation methods are useful for estimating electrical deactivation in n-GaAs channels in practical devices after various forms of thermal processing, such as epitaxial growth and annealing.

References

1) A. Uedono and S. Tanigawa: Jpn. J. Appl. Phys. **29** (1990) L. 346.
2) M. Uematsu and K. Maezawa: Jpn. J. Appl. Phys. **29** (1990) L. 527.
3) G. A. Baraff and M. Schlüter: Phys. Rev. Lett. **55** (1985) 1327.
4) W. Walukiewicz: Appl. Phys. Lett. **54** (1989) 2094.
5) S. Matsushita, E. Fujii, D. Inoue, S. Terada, S. Banba, K. Matsumura, M. Sawada and Y. Harada: Jpn. J. Appl. Phys. **35** (1996) 1198.
6) J. S. Blakemore: J. Appl. Phys. **53** (1982) R123.
7) E. F. Schubert, A. Fischer and K. Ploog: IEEE Trans. Electron Devices **33** (1986) 625.