Advanced Materials '93, I / B: Magnetic, Fullerene, Dielectric, Ferroelectric,
Diamond and Related Materials, edited by M. Homma et al.
Trans. Mat. Res. Soc. Jpn., Volume 14B

Defects in HB-GaAs probed by positron annihilation

A. Uedono[a], T. Kawano[b], L. Wei[a], S. Tanigawa[a] and S. Fujii[c,*]

[a]Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305, Japan

[b]Isotope Center, University of Tsukuba, Tsukuba, Ibaraki 305, Japan

[c]Opto-Electronics R&D Laboratories, Sumitomo Electric Industries Ltd., 1 Taya-cho, Sakae-ku,
Yokohama 244, Japan

Defects in as-grown GaAs were studied by positron annihilation. From measurements of Doppler broadening profiles of the annihilation radiation, vacancy-type defects were observed in Si-doped and undoped GaAs grown by horizontal Bridgman (HB) method. Lifetime spectra of positrons were analyzed by a numerical integral transform method. From the analysis of the lifetime spectra, vacancy-type defects in Si-doped and undoped HB-GaAs were identified as monovacancy-type defects. For undoped GaAs grown by liquid-encapsulated Czochralski method and Zn-doped HB-GaAs, it was found that the lifetime of positrons trapped by defects was shorter than that of positrons annihilated in bulk GaAs.

1. INTRODUCTION

The positron annihilation technique has made important contributions for the study of point defects in semiconductors [1,2]. By using this technique, the concentration of point defects for a detectable response is about 0.1 ppm, and there are no restrictions regarding specimen conductivity nor specimen temperature [2]. For compound semiconductors, the positron trapping in such defects has been found to strongly depend on a position of the Fermi level [3]. Because of this unique character, the study of defects in GaAs by the positron annihilation technique is a subject of increasing interest [4-7].

A positron implanted into the specimen eventually annihilates with an electron producing annihilation γ rays. A Doppler broadening of such γ rays provides the momentum distribution of the annihilating electrons. The lifetime of positrons in materials reflects the density of electrons where the positron annihilates. Since a positron is positively charged, it is repelled from ion cores by a Coulomb interaction. Thus, if a specimen contains vacancy-type defects, there is a finite probability of positrons being trapped in these regions. Due to a reduced electron density and a reduced overlap of positrons with core electrons in vacancy-type defects, the lifetime of trapped positrons increases and the Doppler broadening profile narrows. The change in Doppler broadening spectra is characterized by a line shape parameter, S, which divides total counts into the counts in a central region of the spectrum [1]. A relationship between the lifetime of positrons and the species of defects has been well established [2]. In the present paper, we report the application of the positron annihilation technique to the study of native defects in GaAs wafers grown by horizontal Bridgman (HB) method and by liquid-encapsulated Czochralski (LEC) method.

2. EXPERIMENTAL

The specimens used in the present experiment were Si-doped, undoped and Zn-doped HB-GaAs and undoped LEC-GaAs. Characteristics of these specimens are listed in Table I. The positron lifetime spectra were obtained by the fast-fast system with BaF_2 scintillators attached to

---

[*] Present address: Itami Research Laboratories, Sumitomo Electric Industries Ltd., 1-1-1 Koyakita Itami 664, Japan.

Table I. Characteristics of the GaAs specimens grown by HB method and by LEC method.

specimen	growth condition	dopant	carrier concentration (/cm^3)	etch pit density (/cm^2)
HB-Si	HB	Si	2.5×10^{18}	$<2.0\times10^4$
HB	HB	undoped	1.8×10^{12}~5.5×10^{14} (n-type)	$<1.0\times10^5$
HB-Zn	HB	Zn	5.0×10^{19}	$<1.0\times10^5$
LEC	LEC	undoped	semi-insulating	$<5.0\times10^4$

XP2020Q (Philips) photomultiplier tubes. The full width at half maximum (FWHM) of the time resolution curve was about 215 ps. Each lifetime spectrum contained 8×10^6 counts. The positron source was 8×10^5 Bq of ^{22}NaCl deposited on kapton foils.

The observed lifetime spectrum of positrons, $y(t)$, can be represented by the convolution of the decay curve of positrons, $C(t)$, and the instrument resolution function, $R(t)$:

$$y(t) = N_s R(t) * C(t), \quad (1)$$

where N_s is the total number of annihilation events [8]. $C(t)$ is represented by

$$C(t) = \sum_{i=1}^{n} \alpha_i \lambda_i \exp(-\lambda_i t), \quad (2)$$

where α_i is the fraction of positrons annihilating with i-th lifetime, τ_i $(=1/\lambda_i)$. $y(t)$ can be analyzed by the least-square method using eq. (2). This analysis can be performed by using codes (PATFIT and RESOLUTION) developed by Kirkegaard *et al.* [9]. However, we usually have no prior knowledge of n in eq. (2). Since the number of components obviously has ramifications for physical interpretations, one must consider limits of the statistical accuracy for which various types of analyses are possible [4].

Equation (2) can be expressed in a continuous decay form:

$$C(t) = \int_0^{\infty} \alpha(\lambda)\, \lambda \exp(-\lambda t)\, d\lambda. \quad (3)$$

In eq. (3), $C(t)$ is a Laplace transformation of the decay probability density function (pdf), $\alpha(\lambda)\lambda$. The deconvolution by a Laplace inversion technique was first developed by Provencher [10] into a computer code named CONTIN for the numerical solution of the integral equation. CONTIN was modified by Gregory *et al.* [11] for the analysis of the lifetime spectra of positrons (CONTIN (PALS-2)). The exact solution of $\alpha(\lambda)$ and λ in eq. (3) is a difficult mathematical problem since $R(t)$ is not known exactly. In CONTIN (PALS-2), pdf is obtained by using a reference spectrum of the specimen with the known positron lifetime. In the present experiment, the lifetime spectrum of a well-annealed Ni specimen was used for the reference spectrum.

Doppler broadening profiles of the annihilation radiation were also measured using an intrinsic Ge detector with FWHM of 1.2 keV at 512 keV γ-line of ^{106}Ru. A total of 2×10^8 counts was recorded for each spectrum. The obtained spectrum was characterized by the S parameter.

3. RESULTS AND DISCUSSION

Figure 1 shows the S parameter for Si-doped, undoped and Zn-doped HB-GaAs and undoped LEC-GaAs, respectively. For Si-doped and undoped HB-GaAs specimens, the value of S was found to be larger than that for Zn-doped HB-GaAs. It is generally accepted that the characteristic value of S for the positron annihilation in vacancy-type defects is larger than that in the bulk [1]. Thus the observed increase in the value of S can be attributed to the annihilation of positrons in vacancy-type defects.

Figures 3 and 4 show distributions of the

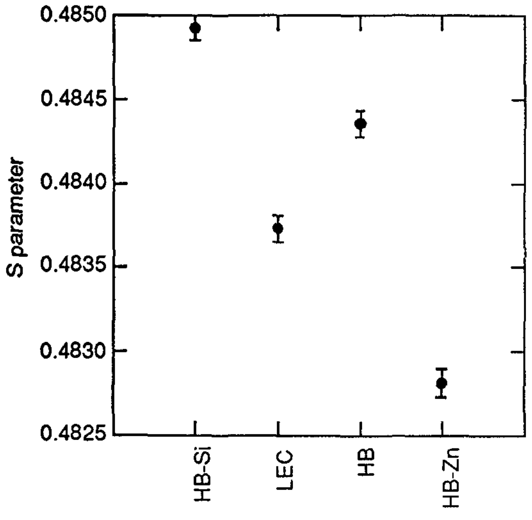

Figure 1. The line shape parameter *S* for Si-doped, undoped and Zn-doped HB-GaAs and undoped LEC-GaAs.

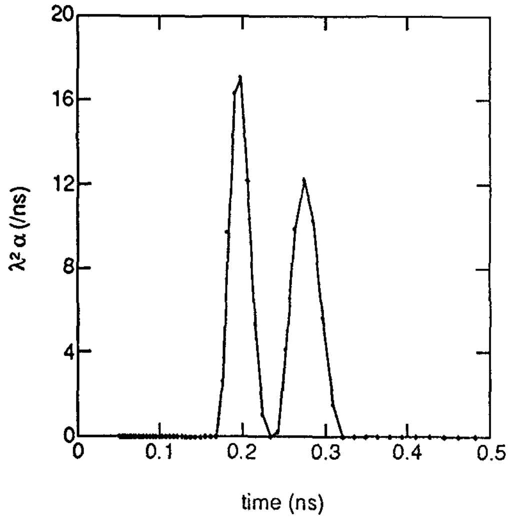

Figure 3. The positron lifetime distribution function for undoped HB-GaAs obtained by the numerical Laplace transform technique. The weight average of the peak in the region between 220 ps and 320 ps was calculated as 276 ps.

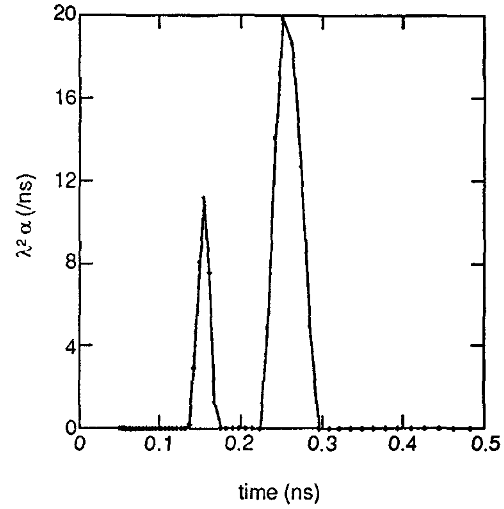

Figure 2. The positron lifetime distribution function for Si-doped HB-GaAs obtained by the numerical Laplace transform technique. The weight average of the peak in the region between 220 ps and 300 ps was calculated as 258 ps.

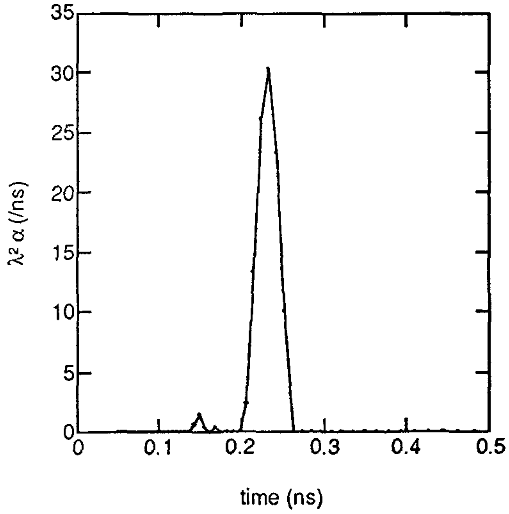

Figure 4. The positron lifetime distribution function for LEC-GaAs. The weight average of the peak in the region between 220 ps and 280 ps was calculated as 232 ps.

positron lifetime for Si-doped and undoped HB-GaAs, respectively. In Figs. 3 and 4, it was found that the lifetime spectra consist of two components. The weight averages of the component in the region between 220 ps and 320 ps were calculated as 258 ps and 276 ps for Si-doped and undoped HB-GaAs, respectively. These values are in good agreement with the lifetime of positrons trapped by monovacancy-type defects [3,4]. Since it is generally accepted that As-vacancies are positively charged and Ga-vacancies, V_{Ga}, are negatively charged [13], only V_{Ga} is detectable by the positron annihilation technique. Thus, the major type of defects in these specimens can be identified as monovacancy-type defects such as V_{Ga} or monovacancy-impurity complexes.

In Fig. 1, the value of the S parameter for LEC-GaAs was found to be larger than that for Zn-doped HB-GaAs. The lifetime spectra for LEC-GaAs and Zn-doped HB-GaAs were analyzed by RESOLUTION. It was found that the lifetime spectra for these specimens can be analyzed assuming only one component, and the obtained lifetimes were 231.5±0.2 ps and 230.8±0.2 ps for LEC-GaAs and Zn-doped HB-GaAs, respectively. These values are in good agreement with the lifetime of positrons annihilated in bulk GaAs obtained by Corbel *et al.* [3] However, since the value of the S parameter for LEC-GaAs is different from that for Zn-doped HB-GaAs, it can be concluded that the annihilation characteristics of positrons in LEC-GaAs is different from those in Zn-doped GaAs. The distribution of the positron lifetime for LEC-GaAs is shown in Fig. 4. The weight average of the peak in the region between 200 ps and 260 ps was calculated as 232 ps. This value agrees with the lifetime obtained by RESOLUTION. In Fig. 4, a week peak was observed at ~150 ps. The similar peak at $t \cong 110$ ps was also observed for Zn-doped HB-GaAs. Dannefaer [2] reported that positrons can be trapped by interstitial oxygen clusters in Czochralski-grown Si and the lifetime of positrons trapped by such defects is shorter than that of positrons annihilated in the bulk. Thus, the difference of the value of S for LEC-GaAs and Zn-doped HB-GaAs might be attributed to the annihilation of positrons trapped by such interstitial-type defects.

4. CONCLUSIONS

We have presented the study of native defects in GaAs by the positron annihilation technique. The numerical Laplace transform technique was successfully used to analyze the lifetime spectra of positrons. For Si-doped and undoped HB-GaAs, the main species of defects was identified as monovacancy-type defects. The annihilation characteristics of positrons in LEC-GaAs is found to be different from those in Zn-doped GaAs, while no drastic change in the value of the lifetime was observed. This difference might be attributed to the annihilation of positrons trapped by interstital-type defects.

REFERENCES

1. P. Hautojärvi (ed.), Positrons in Solids, Springer-Verlag, Berlin, 1979.
2. S. Dannefaer, Defect Control in Semiconductors, K. Sumino (ed.), North-Holland, Amsterdam, 1990, p. 1561.
3. C. Corbel, M. Stucky, P. Hautojärvi, K. Saarinen and P. Moser, Phys. Rev. B, 38 (1988) 8192.
4. S. Dannefaer, P. Mascher and D. Kerr, J. Phys. Condens. Matter, 1 (1989) 3213.
5. A. Uedono and S. Tanigawa, Jpn. J. Appl. Phys., 29 (1990) L346.
6. P. Mascher, S. Dannefaer and D. Kerr, Can. J. Phys., 69 (1991) 298.
7. K. Saarinen, P. Hautojärvi, P. Lank and C. Corbel, Phys. Rev. B, 44 (1991) 10585.
8. R.B. Gregory and Y. Zhu, Positron and Positronium Chemistry, Y.C. Jean (ed.), World Scientific, Singapore, p.136.
9. P. Kirkegaard, N.J. Pedersend and M. Eldrup, RISO-M-2740, Riso National Lab., Roskilde, Denmark, 1989.
10. S.W. Provencher, Comput. Phys. Commun., 27 (1982) 213.
11. R.B. Gregory and Y. Zhu, Nucl. Instr. and Meth., A290 (1990) 172.
12. M.J. Puska, S. Mäkinen, M. Manninen and R.M. Nieminen, Phys. Rev. B, 39 (1989) 7666.
13. G.A. Baraff and M. Schlüter, Phys. Rev. Lett., 55 (1985) 1327.