

INVESTIGATION OF NATIVE VACANCIES IN GaAs USING POSITRON ANNIHILATION AND OTHER MEASUREMENTS

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Abstract. Positron lifetime measurements are used in combination with electrical (Hall and resistivity) investigation to study native point defects and their complexes in as-grown GaAs crystals. We explained the characteristic of the defects in GaAs. The lifetime spectra measured in different positions on the GaAs slice are not one-component spectra, but they can be well fitted by three exponentials. The vacancy concentration observed by us gives an underestimate of the deviation δ from the stoichiometry. Concentration of divacancy (I_2) as well as EPD variation along the radial of the slice takes W-shape profile, while the concentration of monovacancy or/and complexes of monovacancy with impurities takes M-shape profile. EPD as well as multi-vacancy clusters is closely related with the deviation δ from the stoichiometry (melt composition).

1. Introduction

Positron annihilation technique is well established to investigate properties of open volume defects like vacancies, their agglomerates and dislocations in metals and alloys. [Dlubek, G.: Positronenannihilation in : Ausgewählte Untersuchungsverfahren der Metallskunde (Autorenkollektiv), Leipzig: VEB Dt. Verl. f. Grundstoffindustrie 1983, P. 266] Recent studies have shown that it is a potential tool also in semiconductors. However, the interaction of positrons with the various types of defects formed in compound semiconductors is not yet well understood. [Cheng, L.J.; et al, J. Appl. Phys. 50(1979)2962. Dannefaer, S.: J. Phys. C15(1982)599.] This paper reports experimental results of a positron lifetime study on the interaction and relationships among point defects, micro-defects, dislocations and impurities in GaAs. We see strong positron trapping in doped GaAs and attribute τ_1 to DV_{Ga}^- and τ_2 to As vacancies produced by non-stoichiometry.

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2. Experimental details

The standard positron-lifetime measurement technique was used. The experiment was performed at room temperature by using a fast coincidence device with a time resolution of 380ps(FWHM). Each lifetime spectrum contains $1.0E+6$ counts. A $^{22}\text{NaCl}$ positron source of $6.0E+5\text{Bq}(15\mu\text{Ci})$ deposited and sealed between two $1\mu\text{m}$ thick nickel foils, was sandwiched by two identical pieces of the sample under study. In case of the Si-doped GaAs slices ($40\text{mm}\times 1\text{mm}$) the positron lifetime was studied in several different positions on the slice (compare Fig.1).

Van der Pauw method was used to obtain free carrier concentration and resistivity combined with Chemical etching to obtain Etching Pit Density (EPD).

The samples used were polished (100)-oriented crystal wafers grown by LEC. The specification of the crystals investigated is shown in Table I.

Table I. A specification of the samples investigated and results of positron lifetime, chemical etching as well as electrical measurements. The specific positron trapping rate here is $2.0E-9\text{cm}^3/\text{s}$, σ is the conductivity of the Si-doped GaAs. τ_1, τ_2, τ_3 are the lifetimes measured at different positions on the same slice which was cut from the same ingot as HS5.

	τ_1	τ_2	τ_3	I1	I2	I3	$\bar{\tau}$	τ_b	K	EPD	σ	d	n	$\log \sigma$
	(ps)	(ps)	(ps)	(%)	(%)	(%)	(ps)	(ps)	($1.0E+9/\text{s}$)	($1.0E+14/\text{cm}^3$)	($1.0E+18/\text{cm}^3$)	($1.0E+16\text{cm}^{-3}$)		
HS5	177	275	1850	75.25	24.33	1.425	206.94	193.88	0.43	0.15	1.37	1.215	54.82	1.869
HS6	179	372	1751	64.36	30.72	4.88	241.36	215.05	0.94	1.56	1.73	1.470	286.1	2.075
HS7	171	360	1806	60.06	35.10	4.84	240.72	212.07	1.13	1.67	1.70	1.565	286.1	2.075
HS8	187	306	1882	86.38	12.65	0.52	189.53	196.77	0.27	1.2	1.56	1.135	286.1	2.075
HS9	190	335	2044	90.78	8.720	0.50	202.57	197.53	0.20	0.06	1.70	1.100	286.1	2.075
H10	189	342	2478	89.94	9.540	0.53	203.38	198.46	0.22	0.07	1.72	0.11	286.1	2.075
H11	177	293	2288	79.21	20.27	0.53	200.64	192.50	0.46	0.07	1.52	0.23	286.1	2.075

The PA spectra are dissociated to three components by multi-exponential fitting method. From the lifetime τ_i and relative intensi-

ties I_1 also the average positron lifetime $\bar{\tau}=(I_1\tau_1+I_2\tau_2)/(I_1+I_2)$ was calculated. The concentration of vacancy defects N_d (interpreted as neutral As divacancy) is estimate from $\bar{\tau}$ with the aim of eq. (1) and assuming a specific positron trapping rate of $=2.0E-9\text{cm}^3/\text{s}$.

$$K=\mu N_d=I_2/(1-I_2)*(1/\tau_b - 1/\tau_d)=1/\tau_b*(\bar{\tau}-\tau_b)/(\tau_d-\tau_b) \quad (1)$$

$$(\tau_b)^{-1}=(I_1/\tau_1(I_1+I_2)+I_2/\tau_2(I_1+I_2)) \quad (2)$$

Here τ_b and τ_d denote the bulk lifetime of positrons annihilation from defects. τ_d can be read directly from the lifetime spectrum $\tau_2=\tau_d$. K is positron trapping rate.

3. Results and discussions

The results of our positron lifetime study are presented in Table I. The appearance of the second lifetime component indicated evidently that positrons annihilate not only as a Bloch particle in GaAs bulk but also highly localized at a vacancy-type defect. In this case the overlap of the electron and positron density is reduced which leads to an increase in the positron lifetime being characteristic for the types(size) of defect. Candidates of defects trapping positrons are such open volume defects like vacancies, their agglomerates or complexes with other native defects or with impurities and dislocations. For positron trapping the defects must be in a neutral or negatively charged state. Positively charged defects repel positrons. τ_1 is the positron lifetime of free state, monovacancy, complexes of monovacancy with impurities, dislocations, interstitial and interstitial cluster. τ_2 is the positron lifetime of multi-vacancy cluster and microcavity. I_1 and I_2 is relative intensity with lifetime τ_1 and τ_2 respectively. The long-lifetime component τ_3 is most likely due to annihilations at the surfaces of the sample and source rather than in the bulk of the sample.

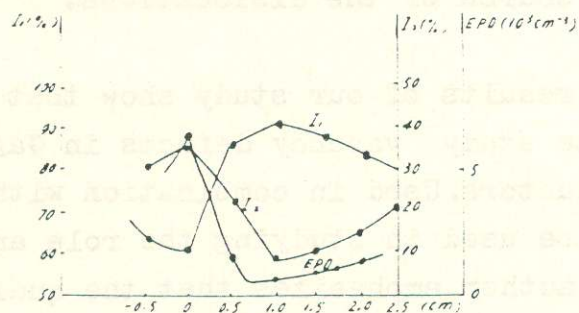
The sensitivity of the positron method ranges from $2.0E+7$ to $2.0E+10$ dislocations per cm^3 . The dislocation density does not exceed

$1.0E+5 / \text{cm}^2$ in the single crystals investigated. Therefore, we can exclude positron trapping by dislocations and grain boundaries.

From electron and neutron irradiation experiments (Dannefaer, S.; et al : Phys. Rev. B14(1976)2709, Fuhs, W., et al : phys. stat. sol.(b) 89(1978)69.) it was found that this ratio (τ_a/τ_b) in Si is 1.22 ± 0.10 for a monovacancy, 1.46 ± 0.12 for a divacancy and 1.93 ± 0.12 for a quadrivacancy. In the light of these values it is reasonable to conclude that defects trapping positrons (τ_2) in Si-doped GaAs are of divacancy-type.

Our results show that at least a large if not the dominating fraction of the nonstoichiometry of GaAs is realized by As vacancies. $\delta = [\text{As}]^{-1/2} = -[V_{\text{As}}]$. The local fluctuation of the As vacancy concentration has its origin in a local variation of the composition of the crystal. The vacancy concentrations in Table I and Fig. 1 indicate that the non-stoichiometry δ varies in the range from $1.0E-7$ to $1.2E-5$ as a function of the position on the slice.

Fig.1 Variation of the positron lifetime parameters and EPD versus the position on an Si-doped GaAs slice.



From Fig.1 concentration of divacancy (I_2) as well as EPD variation along the radial of the slice takes W-shape profile while the concentration of monovacancy or/and complexes of monovacancy with impurities (I_1) takes M-shape profile. Likewise, we got positron-lifetime τ_1 and τ_2 and their relative intensity I_1 and I_2 dependence with EPD (see Fig.1). It is noted that τ_1 , τ_2 and I_1 decrease with the increase of dislocation density. During EPD increasing, some of interstitial atoms released were absorbed by dislocations and vacancies, others were merged into interstitial clusters, the concentration of the interstitial atoms increase, the monovacancy's (or complexes of monovacancy with impurities) decrease. On the other hand, with the EPD increasing, more dislo-

cations, isolate interstitial atoms and impurities would interact with vacancies and clusters. These results show that multi-vacancy clusters is the source of the dislocation, while monovacancy, especially complexes of monovacancy with impurities (We think DV_{Ga}^-) resist the creation and motion of the dislocations. The higher the concentration of the complexes of the impurities with impuricancy, the lower the dislocations. EPD as well as multi-vacancy clusters is closely related with the deviation δ from the stoichiometry (melt composition).

4. Conclusion.

In GaAs crystals we have detected vacancy defects which are probably of the type $(V_{As}^0)_2$ and DV_{Ga}^- . The vacancies are inhomogeneously distributed over the sample slice. We also explained the interaction and relationship among point defects dislocations and impurities in GaAs. The higher the concentration of the DV_{Ga}^- the lower the dislocations. Multi-vacancy clusters is probably the source of the dislocations.

The results of our study show that the positron is a useful probe to study vacancy defects in GaAs and related compound semiconductors. Used in combination with other measurements, the method can be used in studying the role and structure of vacancy defects. The author emphasizes that the quality of GaAs single crystals will certainly be improved in many aspects in near future very quickly through fundamental investigations on defects properties and defect-impurities interactions.

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