LATTICE LOCATION DETERMINATION OF TRACE AMOUNT CARBON IN GALLIUM ARSENIDE BY THEORETICAL CALCULATION OF CPAA WITH CHANNELING*

Wei Luncun (韦伦存), Bao Shanglian (包尚联), Yang Qixiang (杨其湘) and Yang Xihong (杨熙宏)

(Institute of Heavy Ion Physics, Peking University, Beijing 100871, China)

(Received January 1991)

ABSTRACT

Combining the charged particle activation analysis (CPAA) and the channeling technique, partial concentrations of carbon on different crystal lattice locations of GaAs were calculated. The results show that at lower total concentration ($\approx$0.3 ppm), carbon atoms occupy principally the octahedral and displaced octahedral interstitial positions, but at higher total concentration ($\approx$2 ppm), the substitutional carbon plays a principal role.

Keywords: CPAA Channeling technique Impurity carbon GaAs

I. INTRODUCTION

The study of trace elements in GaAs has been greatly increased in recent years. Carbon residuals of as low as 10 ppm can have significant influence on opto-electronic properties of a GaAs device. CPAA is very sensitive to light elements. The detection limit for C can reach 40 ppb[4,5], even without chemical separation. But CPAA can not give information about lattice location of impurities. Combining CPAA with channeling technique, however, one is able to determine the concentrations of light elements together with their lattice locations. In this respect, M.A.Misdaq *et al* have done some interesting experiments[6,7], but they have not yet made any theoretical calculations. Our work, based on the continuum model with the Moliere screened potential and the assumption of statistical equilibrium in traverse energy shells, is to calculate the partial concentrations of the carbon impurity on different sites in GaAs by using the fluxes of the channeled particles received by atoms on different locations and the ratios of the stopping powers for the channeled and random

* The Project Supported partly by Natural Science Foundation of China and Electronic Science Academy

irradiation particles.

II. BASIC PRINCIPLES

1. Charged particle activation analysis (CPAA)

CPAA is a well-known nuclear method. The quantitative relationship between produced radioactivity and concentration is given by

$$A_0 = k_0 \Phi [C] \int_{E_{th}}^{E_0} \sigma(E)/S(E) dE \quad (1)$$

Where A_0 is radioactivity produced from the element to be analyzed, Φ -flux of the incident particles, $[C]$-concentration of the element to be analyzed, $\sigma(E)$-cross section of the nuclear reaction, $S(E)$-stopping power of sample to the incident particles, E_0-initial energy of the incident particles, E_{th}-threshold of the nuclear reaction, k_0-experimental constant. To analyze the carbon, generally, the following reaction is used:

$$^{12}C(d,n)^{13}N \longrightarrow ^{13}C(\beta^+, 9.98\ min)$$

2. Possible locations of C atoms in GaAs

GaAs crystal has the face-centered cubic ZnS type lattice, with lattice constant a_0 = 0.5654 nm. The interstice of the crystal is composed by the octahedrons with all six atoms being Ga or As (Fig.1). The carbon atoms can be located at the center of these octahedrons: octahedral interstitial carbon (position 1) or on the gallium or arsenic substitutional sites (position 2), the third possibility is the all transitional positions between the above two positions, for simplicity of calculation, we take a position on the mid-point between the positions 1 and 2 to represent them: called displaced octahedral interstitial positon (position 3). It is to note that, CPAA with channeling can't distinguish Ga and As atoms, as a consequence, it can't distinguish Ga substitutional site from that of As, and it is also true for the octahedral interstitial sites.

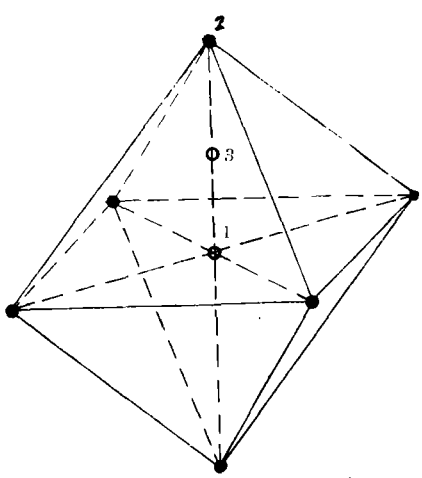


Fig.1 The octahedral interstice in GaAs with all six atoms being Ga or As and the possible C atoms lattice locations

In an experiment of CPAA with channeling, it is necessary to have a high intensity beam and a post-irradiation etching, so, it is impossible to scan principal axis or plan as done in RBS with channeling. As a compromise, we can only irradiate

a sample from several principal axes or plans.

When an irradiation is along the <100> axis, the described three positions have the projections shown in Fig.2. The positions 1 and 2 are both on *B*, but the position 3 has 2/3 possibility on *A* and 1/3 on *B*. For <110> axis direction, their projections are in Fig.3: the position 1 on *A*, the position 2 on *B* and the position 3 has 2/3 possibility on *C*, 1/6 on *A* and 1/6 on *B*. When irradiation direction is far from the principal axes, these three positions are equivalent. So when a sample is irradiated, from <100>, <110> and random directions, three different radioactivities $A_{<100>}$, $A_{<110>}$ and A_r can be obtained.

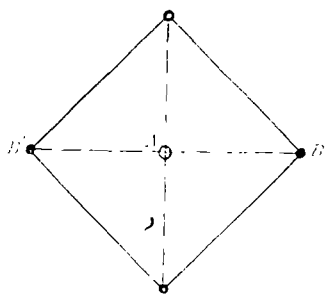


Fig.2 The projection of the positions 1,2 and 3 in <100> channel

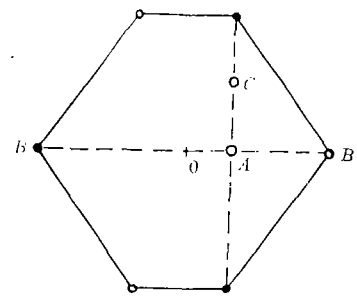


Fig.3 The Projection for the positions 1,2 and 3 in <110> channel

3. CPAA with channeling[8]

The channeling effect is twofold: (1) flux peaking: the beam flux is redistributed in the channel: in the center (lower potential), the flux is larger; near the axes (higher potential), the flux is smaller; (2) reduction of stopping power: target has lower stopping power for the channeled particles than that for the random incident particles.

CPAA uses relatively light ions, such as p, d, ^{3}He, α , *etc*, and relatively high energy (> 0.5 MeV), the irradiation damages produced during an analysis are very limited, therefore, for simplicity, we ignore the dechanneling effect caused by irradiation damages.

Supposing the carbon concentrations on the octahedral interstitial position, the substitutional position and the displaced octahedral interstitial position being $[C_1]$, $[C_2]$, $[C_3]$ respectively, the formula (1) can be rewritten:

$$A_r = k_0\Phi\,([C_1]+[C_2]+[C_3]\int {}^{\varphi}{}_{E_0}\sigma\,(E)/S_r(E)\mathrm{d}E \qquad (2)$$

where the subscript "r" stands for random direction irradiation, the other parameters are the same as in formula (1).

If the irradiation direction is <100>, then one gets:

$$A_{<100>} = k_0\Phi\,(k_1[C_1]+k_2[C_2]+k_3[C_3])\int {}^{\circ}{}_{E_0}\sigma\,(E)/S_{<100>}(E)\mathrm{d}E$$
$$= k_0\Phi\,(k_1[C_1]+k_2[C_2]+k_3[C_3])\int {}^{\circ}{}_{E_0}\sigma\,(E)/S_r(E)R_{\mathrm{sb}<100>}(E)\mathrm{d}E \qquad (3)$$

where "$<100>$" stands for $<100>$ direction irradiation. $R_{sb<100>}(E)$ ($S_{<100>}(E)/S_r(E)$) is the ratio of the stopping power of $<100>$ channeled particles to that of random irradiation, and k_1, k_2, k_3 are respectively ratios of the flux of the channeled particles to that of random incident on positions 1,2 and 3, caused by flux peaking. $A_{<100>}$ is the radioactivity produced from this direction irradiation.

Similarly, for the $<110>$ axis irradiation, one gets:

$$A_{<110>} = k_0\Phi\,(k_4[C_1]+k_5[C_2]+k_6[C_3])\int {}^{\circ}_{E_0}\sigma\ (E)/S_{<110>}(E)\mathrm{d}E$$
$$= k_0\Phi\,(k_4[C_1]+k_5[C_2]+k_6[C_3])\int {}^{\circ}_{E_0}\sigma\ (E)/(S_r(E)R_{sb<110>}(E))\mathrm{d}E \qquad (4)$$

where k_4, k_5, k_6, $R_{sb<110>}(E)$, $A_{<110>}$ have the similar significance as in formula (3), except the irradiation direction along $<110>$.

The parameters k_1 *to* k_6, $R_{sb<100>}(E)$, $R_{sb<110>}(E)$ need to be calculated.

Ⅲ. THEORETICAL CALCULATIONS

1. Calculations of K_i

The continuum model with the Moliere screened potential[9] was used to calculate the equipotential contours in channel. For an axis, the continuum potential is

$$U(r) = (1/d)\int_{-\infty}^{+\infty} V(r^2+z^2)^{1/2}\mathrm{d}z \qquad (5)$$

where d is inter-atom distance on the axis, $r=(x^2+y^2)^{1/2}$ distance between point (x,y) to the axis, z-coordinate on the axis, $V(r)$-Moliere screened potential.

The potential of a point (x, y) in a channel contents contributions of all axes around this channel at this point:

$$U_T\ (x,\ y) = \Sigma_i U(r_i) \qquad (6)$$

Where $r_i=[(x_i-x)^2+(y_i-y)^2]^{1/2}$ is distance from ith axis, $(x_i,\ y_i)$ to the point $(x,\ y)$.

According to the assumption of the statistical equilibrium, when the incident particles move to a certain depth (about several hundred Angstroms) into a channel, the flux will reach statistical equilibrium, and it obeys to

$$F(E_0\varphi^2,\ x,\ y) = \int_{E_r\geq U_T(x,\ y)} dA\ (x_{in},\ y_{in})/A(E_T) \qquad (7)$$

$$E_r = E_0\varphi^2 + U_T(x_{in},\ y_{in}) \qquad (8)$$

where E_0 is initial particles energy, φ -angle between incident direction and that of the axis, $(x_{in},\ y_{in})$-impact point coordinates of incident particle, $U_T(x_{in},\ y_{in})$-potential at the impact point, $A(x_{in},\ y_{in})$-area inside the potential $U_T(x_{in},\ y_{in})$, $A(E_T)$-area inside the potential E_T.

The fluxes, which are interesting for us, are those at the points A, B in the channel $<100>$ and A, B, C in $<110>$. They should be averaged over all possible thermal vibration positions. For lack of the thermal vibration parameter, we take the

Debye Temperature for C in GaAs to be $\theta_c = \theta_{Host}(m_{GaAs}/m_c)^{0.5}$, so the unidimensional vibration amplitude for carbon in GaAs at the room temperature (298K) is $u = 0.017$ nm. therefore, one gets

$$F_{th}(E_0\varphi^2) = \int\int_{-\infty}^{+\infty} F(E_0\varphi^2, x, y)\, G(u^2, x_0)\, G(u^2, y_0)\, dxdy \qquad (9)$$

where (x_0, y_0) is impurity atom equilibrium position; $G(u^2, x_0)$, $G(u^2, y_0)$ are Gaussian position distributions of a thermally vibrating impurity atom.

A real ion beam has always some angle divergence, characterized by its angle distribution variance (σ_φ^2), so when the irradiation is parallel to the axis direction chosen, there are still a part of particles which have some angle differences with that axis. Supposing the beam angle distribution obeys the Gaussian law with a variance of σ_φ^2, real flux received by an atom at a special point as function of the variance of the beam's angle distribution, σ_φ^2 was calculated with the following formula

$$F_b(\sigma_\varphi) = \int_{-\infty}^{+\infty} F_{th}(E_0\varphi^2)\, G(\sigma_\varphi, 0)d\varphi \qquad (10)$$

where $G(\sigma_\varphi, 0)$ is Gaussian angle distribution of the incident beam, "0" means the irradiation is parallel to the axis; σ_φ is variance of beam angle distribution.

The real fluxes received by carbon at the points A, B in $<100>$ and those at A, B, C in $<110>$, during a channeling experiment, are shown in Figs. 4 and 5. In other way, the fluxes for all points are same, taken as unit, when the incident direction is random. Therefore, $F_b(\sigma_\varphi)$ is the flux ratio of a channeling irradiation to the random one at a special point.

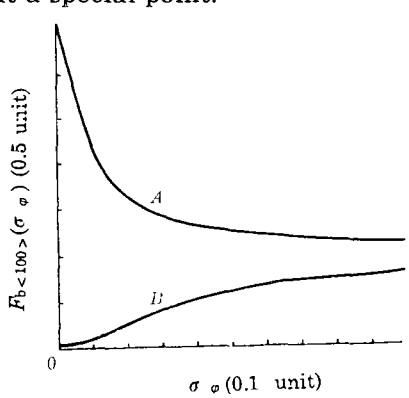


Fig.4 Real flux ($F_{b<100>}(\sigma_\varphi)$) received by carbon at A, B in $<100>$ vs. angle distribution variance (σ_φ) for a 2.7 MeV deuteron beam parallel to $<100>$

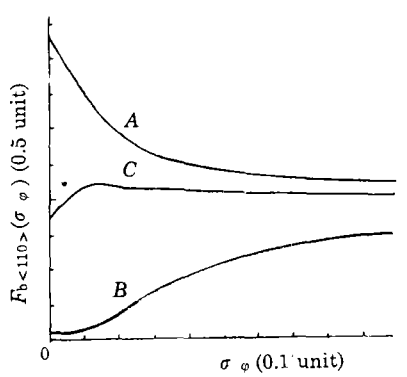


Fig.5 Real flux ($F_{b<100>}(\sigma_\varphi)$) received by carbon at A, B, C in $<110>$vs. angle distribution variance (σ_φ) for a 2.7 MeV deuteron beam parallel to $<110>$

As described carlier, carbon on position 1 and 2 (Fig.1) are both on point B in $<100>$ channel, but that on position 3 (Fig.1) has 2/3 possibility on A and 1/3 on B, therefore, one gets:

$$k_1(\sigma_\varphi) = F_{b,A<100>}(\sigma_\varphi) \tag{11}$$

$$k_2(\sigma_\varphi) = F_{b,B<100>}(\sigma_\varphi) \tag{12}$$

$$k_3(\sigma_\varphi) = (2/3)F_{b,A<100>}(\sigma_\varphi) + (1/3)F_{b,B<100>}(\sigma_\varphi) \tag{13}$$

For $<110>$ channel, position 1 is on A, position 2 on B and position 3 has 2/3 possibility on C, 1/6 on A, 1/6 on B. That is:

$$k_4(\sigma_\varphi) = F_{b,A<110>}(\sigma_\varphi) \tag{14}$$

$$k_5(\sigma_\varphi) = F_{b,B<110>}(\sigma_\varphi) \tag{15}$$

$$k_6(\sigma_\varphi) = (2/3)F_{b,C<110>}(\sigma_\varphi) + (1/6)F_{b,A<110>}(\sigma_\varphi) + (1/6)F_{b,B<100>}(\sigma_\varphi) \tag{16}$$

2. Calculation of R_s

The major contribution to the stopping powers of GaAs for the channeled deuterons in the energy region of 1.0 MeV $< E_d <$ 2.7 MeV is the electronic stopping power. According to Lindhard's formula for channeling electronic stopping power, the ratios of the stopping power for the channeled and random irradiation particles as function of the channeled particle incident angles can be calculated:

$$R_s(E, E_0\varphi^2) = 1-\alpha\ (1-\int\int_{A_0} F(E_0\varphi^2, x, y)\varepsilon\ (x, y)\,dxdy)/\,(dE/dx)_{ch}(E)/A_0 \tag{17}$$

where A_0 is area of channel's cross section, N number of target atoms in unit volume, Z_2 nuclear charge number of target atom, $\varepsilon\ (x, y)$ electron density at point (x, y), where the incident particles move through, $F(E_0\varphi^2, x, y)$ given by formula (7), and α about 0.5. So, it is only necessary to calculate $\varepsilon\ (x, y)$.

Ziegler *et al* have calculated the electron distributions for all elements[10], But our interest is the average electron density in channel cross section, therefore we used the differentiation of the Molière screened potential, because it is this electron screening effect which makes the atom screened potential to be different from the nuclear potential. According to Poisons equation, for an axis, we got:

$$\varepsilon\ (x, y) = [d^2U(r)/dr^2 + (1/r)dU(r)/dr]/Z_1c \tag{18}$$

where, $U(r)$ is given by formula (6), and $r = (x^2+y^2)^{1/2}$ is the distance from the axis to point (x, y). The electron density at point (x, y) in a channel contains contributions of all axes around this channel:

$$\varepsilon_T(x, y) = \Sigma_i\ \varepsilon\ (r_i) \tag{19}$$

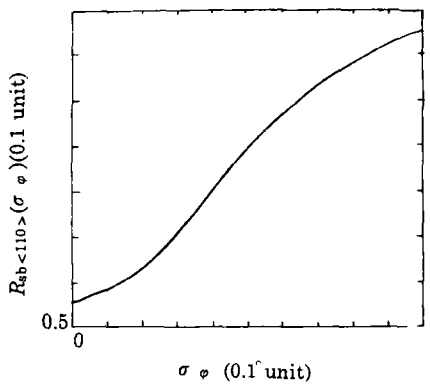
where $r_i = [(x_i-x)^2+(y_i-y)^2]^{0.5}$ is distance from point (x, y) to ith axis (x_i, y_i)

For a real beam with a certain angle divergence, R_{sb} should be averaged over this angle distribution by following formula

$$R_{sb}(\sigma_\varphi) = \int_{-x}^{x} R_s(E_0\varphi^2)\ G(\sigma_\varphi, 0)\,d\varphi \tag{20}$$

where the "0" in $G\ (\sigma_\varphi, 0)$ means that the irradiation is parallel to the axis, and the

final results of calculation are shown in Fig.6 and 7.



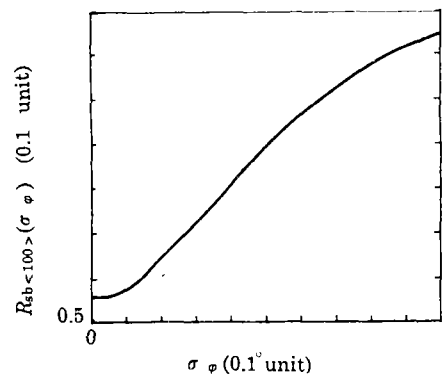


Fig.6 $R_{sb<100>}$ (σ_φ^2) **ratio of stopping powers of GaAs to a 2.7 MeV deuteron beam parallel to <100> and random irradiation vs. beam angle distribution variance (σ_φ)**

Fig.7 $R_{sb<110>}$ (σ_φ^2) **ratio of the stopping powers of GaAs to a 2.7 MeV deuteron beam parallel to <110> and random irradiation vs. beam angle distribution variance (σ_φ)**

3. The combined effect of the flux peaking and the reduction of the stopping power of channeling

The radioactivity produced by an irradiation from random direction is given by formula (2), and those produced by $<100>$ and $<110>$ irradiations with a certain angle divergence are given by the following formulas:

$$A_{<100>}(\sigma_\varphi) = k_0\Phi\,(k_1(\sigma_\varphi)[C_1] + k_2(\sigma_\varphi)[C_2] + k_3(\sigma_\varphi)[C_3]) \times \int_{E_0}^{0} \sigma(E)/(S_r(E)R_{sb<100>}(\sigma_\varphi))\mathrm{d}E$$

$$= k_0\Phi\,(k_1(\sigma_\varphi)[C_1] + k_2(\sigma_\varphi)[C_2] + k_3(\sigma_\varphi)[C_3](\int_{E_0}^{0} \sigma(E)/S_r(E)\mathrm{d}E \qquad (21)$$

$$A_{<110>}(\sigma_\varphi) = k_0\Phi\,(k_4(\sigma_\varphi)[C_1] + k_5(\sigma_\varphi)[C_2] + k_6(\sigma_\varphi)[C_3]) \times \int_{E_0}^{0} \sigma(E)/(S_r(E)R_{sb<110>}(\sigma_\varphi)\mathrm{d}E$$

$$= k_0\Phi\,(k_4(\sigma_\varphi)[C_1] + k_5(\sigma_\varphi)[C_2] + k_6(\sigma_\varphi)[C_3]) \times \int_{E_0}^{0} \sigma(E)/S_r(E)\mathrm{d}E \qquad (22)$$

Taking the ratios of formulas (21), (22) to (2), one gets:

$$A_{<100>}(\sigma_\varphi)/A_r = (K_1(\sigma_\varphi)[C_1] + K_2(\sigma_\varphi)[C_2] + K_3(\sigma_\varphi)[C_3])/[C_T] \qquad (23)$$

$$A_{<110>}(\sigma_\varphi)/A_r = (K_4(\sigma_\varphi)[C_1] + K_5(\sigma_\varphi)[C_2] + K_6(\sigma_\varphi)[C_3])/[C_T] \qquad (24)$$

$$[C_T] = [C_1] + [C_2] + [C_3] \qquad (25)$$

where

$$K_i(\sigma_\varphi) = k_i(\sigma_\varphi)/R_{sb<100>}(\sigma_\varphi) \qquad i = 1, 2, 3 \qquad (26)$$

$$K_i(\sigma_\varphi) = k_i(\sigma_\varphi)/R_{sb<110>}(\sigma_\varphi) \qquad i = 4, 5, 6 \qquad (27)$$

The calculated $K_i(\sigma_\varphi)$ values are shown in Table 1. When the values of A_r, $A_{<100>}$

and $A_{<110>}$ are measured experimentally, with the formulas (23), (24) and (25), $[C_1]$, $[C_2]$ and $[C_3]$ can be calculated.

Table 1

Calculated values of $K_i(\sigma_\varphi)$ for carbon in GaAs

σ_φ	$K_1(\sigma_\varphi)$	$K_2(\sigma_\varphi)$	$K_3(\sigma_\varphi)$	$K_4(\sigma_\varphi)$	$K_5(\sigma_\varphi)$	$K_6(\sigma_\varphi)$
0.00°	0.094	0.094	4.637	4.133	0.062	1.756
0.01°	0.090	0.090	4.434	4.110	0.064	1.763
0.02°	0.090	0.090	4.094	4.069	0.068	1.781
0.03°	0.091	0.090	3.742	3.977	0.067	1.804
0.04°	0.094	0.094	3.439	3.853	0.068	1.825
0.05°	0.098	0.098	3.191	3.720	0.070	1.839
0.06°	0.105	0.105	2.989	3.590	0.074	1.850
0.07°	0.115	0.115	2.824	3.468	0.078	1.850
0.08°	0.128	0.128	2.687	3.355	0.085	1.845
0.09°	0.146	0.146	2.573	3.252	0.093	1.845
0.10°	0.167	0.167	2.477	3.157	0.105	1.838

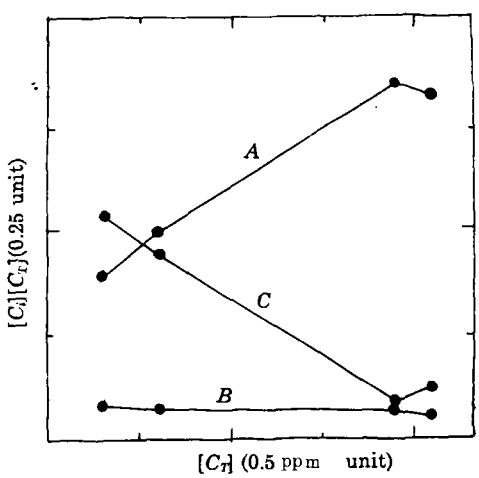


Fig.8 Variation of the carbon concentration on the octahedral interstitial (*B*), the substitutional (*A*) and the displaced octahedral interstitial (*C*) positions as function of the total concentration ([*G*])

IV. DETERMINATION OF CARBON LATTICE LOCATIONS IN GaAs

Study of the carbon atoms lattice locations in GaAs has made some progress. The substitutional carbon[12], the carbon acceptors and the interstitial carbon[7] are all confirmed recently. Taking a group of results of M.A.Misdaq[6] (Table 2), obtained using a 2.7 MeV deuterons beam with a beam angle distribution variance (σ_φ^2) of about 0.03°, using our calculated $K_i(\sigma_\varphi)$, the ratios: $[C_1]/[C_T]$, $[C_2]/[C_T]$ and $[C_3]/[C_T]$ have been calculated, and the results are also shown in table 2 and in Fig.8.

From Fig.8, it is easy to see that, as the total carbon concentration $[C_T]$ increases from 0.3 ppm to 2.1 ppm, the proportion of the octahedral interstitial carbon decreases from 8% to 6%, with its absolute concentration increased slightly; but the proportion on the displaced octahedral interstitial position decreases from about 50% to about 10%, with its absolute concentration kept almost constant; finally, the concentration on the substitutional site increases from about 40% to about 80%, its absolute concentration increases continuously. So, at lower $[C_T](\approx 0.3$ ppm), the

carbon atoms mainly occupy the octahedral and displaced octahedral interstitial positions, but at higher $[C_T](\approx 2$ ppm), the substitutional carbon is the principal component.

Table 2

The calculated concentration ratios for carbon in GaAs

Samples	WYK 537	WYK 466	WYK 456	WYK 478
$[C_T]$(ppm)	0.30+0.03	0.60+0.03	1.90+0.05	2.10+0.04
$A_{<100>}/A_r$	2.0	1.7	0.40	0.55
$A_{<110>}/A_r$	1.3	1.1	0.50	0.52
$[C_1]/[C_T]$	0.08	0.07	0.07	0.06
$[C_2]/[C_T]$	0.39	0.49	0.84	0.81
$[C_3]/[C_T]$	0.53	0.44	0.09	0.13

It is worthwhile to note that, a relative error of about $\pm 15\%$ is estimated, taken into accounts the approximations made in our calculation.

V. CONCLUSION

By using a theoretical calculation of CPAA with channeling, and with the experimentally measured values of the radioactivity by irradiations along different axial directions, the variation of carbon concentration on the different lattice locations has been calculated. The results of the calculation show us that the CPAA with channeling is very useful for light elements lattice location determination, even in trace amounts (about 1 ppm weight).

ACKNOWLEDGEMENTS

One author of this paper (Wei) would like to thank the group of CPAA of French CNRS at Orleans, and especially Prof. J.L.Debrun for the permission to use their experimental results.

REFERENCES

[1] M.Valladon *et al., J. Radioanal. Chem.*, **58** (1980), 169.

[2] G.Blondiaux *et al., IEEE Trans. Nucl. Sci.*, **NS—28** (1980), 2:1675.

[3] L.C.Wei *et al., Nucl. Instr. Meth.*, **B24/25** (1987), 999.

[4] C.Koemmerer, Thesis of Orleans University, 1982.

[5] M.Valladon, Thesis of Orleans University, 1980.

[6] M.A.Misdaq, Thesis of Orleans University, 1985.

[7] M.A.Misdaq *et al., Nucl. Instr. Meth.*, **B15** (1986), 328.

[8] L.C.Feldman *et al.*, Materials analysis by ion channeling, Academic Press, New York, 1982.

[9] R.J.Jaszczak *et al., Phys. Rev.*, **181** (1969), 1428.

[10] J.S.Williams *et al., Nucl. Instr. Meth.*, **B30** (1988), 480.

[11] J.F.Ziegler ed., The stopping and ranges of ions in matter various volumes, 1977, 1980 and 1985, Pergamon Press, New York.

[12] W.M. Theis *et al., Appl. Phys. Lett.*, **41** (1982), 1:70.