Computational studies of positron states and annihilation parameters in semiconductors – vacancy-type defects in group-III nitrides –

S Ishibashi¹ and A Uedono²

¹ Nanosystem Research Institute (NRI) “RICS”, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan
² Division of Applied Physics, Faculty of Pure and Applied Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan

E-mail: shoji.ishibashi@aist.go.jp

Abstract. We have computationally studied positron states and annihilation parameters in semiconductors, especially in group-III nitrides. A random alloy system InₐGa₀.₅N was model with the special-quasirandom-structure scheme and distributions of annihilation parameters for cation monovacancies and divacancies were investigated. On GaN, we calculated annihilation parameters considering spin polarization for Ga vacancies with various charge state and demonstrated how the positron annihilation technique is useful to study defect-induced or mediated magnetism in dilute magnetic semiconductors. We also made calculations based on the two-component density functional theory and compared their results with those obtained by the conventional scheme.

1. Introduction

Group-III nitrides are important and promising materials for various applications such as optoelectronics etc. Their properties and functions can be controlled by forming alloys and/or multilayer structures. For group-III nitride based devices, often, defects such as vacancies and dislocations play a critical role in their performances. The positron annihilation technique is known as a powerful tool to study (vacancy-type) defects in various solids including semiconductors [1,2]. We have been applying the positron annihilation technique in characterizing defects in group-III nitrides [3-5]. In this paper, we would like to report our recent progress on the computational side.

Alloys of group-III nitrides such as (Al,Ga)N and (In,Ga)N are frequently used in actual devices. It is thought that two kinds of cations are randomly distributed in these systems. To model atomic arrangements in (In,Ga)N as a random alloy, we utilized the special-quasirandom-structure (SQS) approach [6,7] and calculated positron states and annihilation parameters in bulk In₀.₅Ga₀.₅N, In₀.₅Ga₀.₅N/GaN and \( V_{\text{cation}} \) therein [5]. In the following, results for cation-nitrogen divacancies are reported.

Diluted magnetic semiconductors have been attracting much attention. Although group-III nitrides themselves are nonmagnetic \( sp \) systems, they can be modified to be magnetic. Gd-doped GaN is an example. On this system, Dhar et al. observed a large magnetic moment of 4000 \( \mu_B \) per Gd atom [8]. Dev et al. investigated cation-vacancy induced magnetism in GaN and BN by means of electronic structure calculations [9]. Their results suggest the existence of defect-induced or mediated collective...
magnetism. Gohda and Oshiyama found that $V_{Ga}$ and Gd atoms are ferromagnetically-coupled and that $V_{Ga}$ contribute significantly to the large magnetic moment [10]. Here, we made spin-polarized calculations and obtained magnetic Doppler broadening spectra for $V_{Ga}^0$, $V_{Ga}^1$ and $V_{Ga}^2$ in GaN. To illustrate the uniqueness of the positron annihilation technique in studying vacancy assisted ferromagnetism, we calculated magnetic Compton scattering spectra also and made a comparison.

The density of positron delocalized in the bulk can be regarded as vanishingly small. For such a case, it is a reasonable assumption that positrons do not affect the electronic structure and the atomic arrangement. In the computational procedure, the electronic structure is first obtained and, with clamping it, the positron state is then calculated. In the following, we describe this procedure as the conventional scheme. As for a positron trapped at a defect, its density is finite. The electronic structure and the atomic arrangement should be affected by the trapped positron. To deal with such a case, the two-component density functional theory (TC-DFT) scheme [11,12] is appropriate. Nevertheless, the conventional scheme is frequently applied even for trapped positrons. One reason is that the TC-DFT scheme requires much more computational time than the conventional scheme. So far, we also applied the conventional scheme to calculate positron states trapped at various vacancy-type defects in group-III nitrides. To evaluate their accuracies, we have made calculations for divacancies in group-III nitrides and several other semiconductors by means of the TC-DFT.

2. Computational details

All the calculations in the present paper have been performed with our computational code QMAS (Quantum MAterials Simulator) [13].

2.1. Structural modelling

To calculate positron states and annihilation parameters in group-III nitride systems containing defects or in alloys, we used orthorhombic supercells which are equivalent to $4 \times 4 \times 2$ hexagonal unit cells of the wurzite structure. For cubic semiconductors, we used $2 \times 2 \times 2$ and $3 \times 3 \times 3$ supercells. For $In_{0.5}Ga_{0.5}N$, in which two kinds of cations are randomly distributed, we used the special-quasirandom-structure (SQS) approach [6,7]. This is a method to provide realistic structural modeling for random alloys using periodic supercells. With this method, two kinds of atoms $A$ and $B$ are arranged so that pair-correlation functions become as close to those for an infinite random alloy as possible. Practically, an atomic arrangement, which gives the lowest Warren-Cowley parameter for several neighboring shells, is chosen. The Warren-Cowley parameter for the $j$-th nearest neighbor shell is expressed as

$$\alpha_j = 1 - \frac{P_B(j)}{x_B},$$

(1)
where $P_B(j)$ is the probability of finding a $B$ atom on the $j$-th nearest neighbor shell about an $A$ atom as the origin. In the present study, shells up to the 7-th are taken into account and the following quantity should be minimized:

$$ T = \sum_{j=1}^{7} \alpha_j^2. $$

Although the supercell dimensions are also optimized in the original SQS approach, we fixed them in the present work. In figure 1, the SQS-modelled In$_{0.5}$Ga$_{0.5}$N supercell is shown. From this structure, an initial structure for a defect system was prepared by removing (an) atom(s).

2.2. Electronic structure calculation

Electronic structures were calculated based on the DFT within the generalized gradient approximation using the exchange-correlation functional of Perdew, Burke and Ernzerhof (PBE) [14]. Electronic wave functions are described with the plane-wave basis in the framework of the projector augmented-wave (PAW) method [15]. The PAW method is adequate to obtain the momentum density distribution of annihilation quanta accurately even in a higher momentum region [16,17]. It is also known to be more efficient than the norm-conserving pseudopotential method. The plane-wave energy cutoff and the force convergence criterion were set to be 20 Ha and $5 \times 10^{-5}$ Ha/bohr, respectively, for all the calculations with the conventional scheme. As for $k$ point sampling, only the $\Gamma$ point was used except for spin-polarized calculations on the GaN supercell, where $2 \times 2 \times 2$ $k$ points were used.

2.3. Positron state and annihilation parameters

The positron effective potential was constructed using core electron wave functions from isolated atom calculations and valence electron wave functions described in the PAW formalism [15]. As for the positron-electron correlation potential term, we used that proposed by Boroński and Nieminen [11]. The positron wave function is also described with the plane-wave basis and optimized in the reciprocal space iteratively. With the obtained positron and electron wave functions, the momentum distribution of annihilation quanta $\rho(p)$ and positron lifetimes $\tau$ were calculated with the following equations:

$$ \rho(p) \propto \sum_j \int \psi_+^*(r) \psi_j^*(r) \sqrt{n_+(r)} \exp(-ip \cdot r) dr^2, $$

$$ \frac{1}{\tau} = \lambda = \pi r_0 c \int n_+(r) n_-(r) \gamma_0(r) n_-(r) dr, $$

where $\psi_+, \psi_j, n_+$ and $n_-$ are the positron wave function, the $j$-th electron wave function, the positron density and the electron density, respectively. $r_0$ represents the classical electron radius and $c$ is the speed of light. $\gamma$ is the enhancement factor. We used the Boroński-Nieminen enhancement factor

$$ \gamma_{\text{LDA}} = 1 + 1.23 r_s + 0.8295 r_s \sqrt{r_s} - 1.26 r_s^2 + 0.3286 r_s^2 \sqrt{r_s} + r_s^3 / 6, $$

where $r_s = [3/(4\pi n_+)]^{1/3}$ is the density parameter, with a small modification to deal with semiconductors [18]. Here, in analogy with the GGA enhancement factor [19], and to be consistent with the positron-electron correlation energy, we used the expression

$$ \gamma_{\text{semi}} = 1 + (\gamma - 1)(1 - 1/\varepsilon_\infty). $$

$\varepsilon_\infty$ is the dielectric constant of the target system. Although it can be determined by first-principles calculations, we adopted the experimental values for convenience. In case of alloys, linearly-interpolated values were used. For reference, the expression in the original semiconductor model [18] is
\[ \gamma_{\text{sen}} = 1 + \frac{(1 - 1/\epsilon_{\infty})r_{s}^{3} + 10}{6}. \]  

(7)

When we make comparisons with results obtained from TC-DFT calculations, we used

\[ \gamma_{\text{sen}} = 1 + 1.23r_{s} + 0.9889r_{s} \sqrt{r_{s}^{2} - 1.4820r_{s}^{2} + 0.3956r_{s}^{2} \sqrt{r_{s}^{2} + (1 - 1/\epsilon_{\infty})r_{s}^{3}}/6}, \]  

(8)

which is compatible with that used in the TC-DFT calculations. The enhancement factor expressed in (8) corresponds to that in the vanishing \( n \) limit for the TC-DFT scheme. Doppler broadening spectra were calculated by integrating equation (3)

\[ J(p_{z}) = \iint \rho(p)dp_{x}, dp_{y}. \]  

(9)

If spin sign is distinguished, it is expressed as

\[ J(p_{z}) = \iint \left( \rho_{\uparrow}(p) + \rho_{\downarrow}(p) \right)dp_{x}, dp_{y}. \]  

(10)

From magnetic Doppler broadening measurements,

\[ J_{\text{mag}}(p_{z}) = \iint \left( \rho_{\uparrow}(p) - \rho_{\downarrow}(p) \right)dp_{x}, dp_{y}. \]  

(11)

Then, we can obtain

\[ J_{\uparrow}(p_{z}) = \frac{1}{2} \left( J(p_{z}) + J_{\text{mag}}(p_{z}) \right) = \iint \rho_{\uparrow}(p)dp_{x}, dp_{y}, \]  

(12)

\[ J_{\downarrow}(p_{z}) = \frac{1}{2} \left( J(p_{z}) - J_{\text{mag}}(p_{z}) \right) = \iint \rho_{\downarrow}(p)dp_{x}, dp_{y}. \]  

(13)

To calculate Compton scattering spectra, the following expression is used instead of equation (3):

\[ \rho(p) \propto \sum_{j} \left| \int \psi_{-j}(r) \exp(-ip \cdot r)dr \right|^2. \]  

(14)

2.4. Two-component density functional (TC-DFT) scheme

According to [12], we made calculations with following steps:

(1) The electronic structure is calculated neglecting the presence of positron.

(2) The positron state is calculated with the results obtained in the (1) or (3) step.

(3) The electronic structure is calculated considering the positron state obtained in (2).

(4) Steps (2) and (3) are repeated to obtain the convergence of the electron and positron states.

(5) The atomic positrons are optimized calculating forces considering the positron effect.

Steps (1)-(5) are repeated to obtain the converged result. Because of steps (2)-(4), more computational time is required compared with the conventional method. The force convergence criterion was set to $5 \times 10^{-5}$ Ha/bohr.

As for the electron-positron correlation energy and potentials, we used the expressions and interpolation scheme in [12]. Correspondingly, we used the enhancement factor evaluated by the interpolation scheme in [11,12] with a modification for semiconductors [20].

3. Results and discussion

Measured Doppler broadening spectra are often analysed through \( S \) and \( W \) parameters. As shown in figure 2, the \( S \) parameter is defined as the ratio of the center area to the total spectrum area while the \( W \) parameter is that for the higher momentum areas. Positrons trapped at a defect usually give a higher \( S \) value and a lower \( W \) value since an increase of the open volume size results in narrowing of the
spectrum. For all the calculations in the present study, $S$ is evaluated in the momentum region between $\pm 0.419$ a.u. while $W$ is evaluated in the regions of $\pm (1.828\sim3.688)$ a.u. Plotting $S$ and $W$ together on a two-dimensional map is useful to identify defect species. If there is only one type of defect in the system, observed parameters $S_{\text{obs}}$ and $W_{\text{obs}}$ should be described with the parameters for the bulk $S_b$ and $W_b$ and those for the defect $S_d$ and $W_d$ as $S_{\text{obs}} = f_b S_b + f_d S_d$ and $W_{\text{obs}} = f_b W_b + f_d W_d$ ($f_b + f_d = 1$). The point $(S_{\text{obs}}, W_{\text{obs}})$ should be located on the line connecting $(S_b, W_b)$ and $(S_d, W_d)$ shown in figure 3(a). If there are two types of defects, denoting parameters for the second defect as $S_{d'}$ and $W_{d'}$, $S_{\text{obs}} = f_b S_b + f_d S_d + f_d' S_{d'}$ and $W_{\text{obs}} = f_b W_b + f_d W_d + f_d' W_{d'}$ ($f_b + f_d + f_d' = 1$). In this case, the point $(S_{\text{obs}}, W_{\text{obs}})$ should be located inside the triangle connecting $(S_b, W_b)$, $(S_d, W_d)$ and $(S_{d'}, W_{d'})$ shown in figure 3(b). In practical situations, the point $(S_{\text{obs}}, W_{\text{obs}})$ moves by, for example, annealing. In a certain case, vacancies aggregate to form vacancy clusters, while, in another case, vacancies form complexes with impurity atoms. Theoretical predictions are expected to be useful to distinguish them.

**Figure 2.** Definition of $S$ and $W$. $S$ and $W$ are given as ratios of the shaded areas to the total area.

**Figure 3.** Schematic $S$–$W$ plots for the positron annihilation from the defect-free state $(S_b, W_b)$ and the trapped state by defects which show different $(S, W)$ values: $[(S_d, W_d)$ and $(S_{d'}, W_{d'})]$.

### 3.1. Divacancy in (In$_{0.5}$Ga$_{0.5}$)N

In our previous work [5], we calculated $S$ and $W$ parameters for 64 types of cation vacancies in (In$_{0.5}$Ga$_{0.5}$)N (a supercell modelled by the SQS approach [6,7]) and found an extended distribution of $S$ in the $S$–$W$ plot. Tuomisto et al. also reported similar finite spreads of positron annihilation parameters ($S$, $W$ and the positron lifetime) for cation monovacancies in (In,Ga)N systems [21].

In the present work, we calculated $S$ and $W$ parameters for 104 types of cation-nitrogen divacancies, which are randomly selected among 256 possibilities, in (In$_{0.5}$Ga$_{0.5}$)N. The results are plotted together with those for the bulk and cation monovacancies in figure 4. As for the $S$ parameter, significant variation has been observed and there is a finite overlap in the $S$–$W$ plot between two types of defects. We also plot each $S$, $W$ and the positron lifetime $\tau$ in figure 5 as a function of $x_{\text{Ga}}$, which represents the gallium concentration of the neighboring cation shells containing 12 sites. Although it is somewhat obscure, there seems to be positive correlation.
Figure 4. $S-W$ plot for bulk In$_{0.5}$Ga$_{0.5}$N cation monovacancies and cation-nitrogen divacancies.

![Image: S-W plot for bulk In$_{0.5}$Ga$_{0.5}$N cation monovacancies and cation-nitrogen divacancies.](image)

Figure 5. Positron annihilation parameters (a) $S$, (b) $W$, (c) $\tau$ for cation vacancies (○) and cation-nitrogen divacancies (×) as a function of neighbouring gallium concentration $x_{Ga}$.

3.2. **Vacancy assisted ferromagnetism in GaN**

First, spin-polarized calculations were made on the 4×4×2 supercell containing a gallium monovacancy (Ga$_{0}$N$_{64}$) with optimizing the atomic positions. In figure 6, obtained spin density distributions around $V_{Ga}^0$, $V_{Ga}^{-1}$ and $V_{Ga}^{-2}$ are shown. Dumbbell-like spin density distributions are observed. Each of them corresponds to the 2$p$-like orbital of nitrogen. The gallium vacancy is surrounded by four major dumbbells. The calculated net magnetic moment values are 3 $\mu_B$, 2 $\mu_B$ and 1 $\mu_B$ for $V_{Ga}^0$, $V_{Ga}^{-1}$ and $V_{Ga}^{-2}$, respectively.

![Image: Spin density distribution around (a) $V_{Ga}^0$, (b) $V_{Ga}^{-1}$ and (c) $V_{Ga}^{-2}$.](image)

Figure 6. Spin density distribution around (a) $V_{Ga}^0$, (b) $V_{Ga}^{-1}$ and (c) $V_{Ga}^{-2}$. Each dumbbell-like distribution corresponds to the 2$p$-like orbital of nitrogen. The gallium vacancy is surrounded by four major dumbbells.

Magnetic Doppler broadening and Compton scattering spectra were calculated along the [1100] direction for three systems mentioned above. The obtained results are shown as $(\rho_{up}\rho_{down})/(\rho_{up}+\rho_{down})$. 

The International Workshop on Positron Studies of Defects 2014 IOP Publishing
Journal of Physics: Conference Series 674 (2016) 012020
doi:10.1088/1742-6596/674/1/012020
in figure 7. It is clearly shown that the magnetic Doppler spectra are approximately 20 times enhanced than the magnetic Compton ones. This is because positrons are selectively trapped at \( V_{Ga} \). The positron annihilation Doppler broadening technique is expected to be uniquely sensitive for vacancy-assisted ferromagnetism. It is also noted that curve intervals are more or less similar to each other reflecting the magnetic-moment difference in the graph of the Compton scattering spectra while it is not the case with the Doppler broadening spectra. It should be attributed to the positron density distribution localized at \( V_{Ga} \). A detailed analysis is ongoing. For reference, the \((S, W)\) values were evaluated from the spin-integrated spectra as \((0.471, 0.0163), (0.474, 0.0146)\) and \((0.474, 0.0135)\) for \( V_{Ga}^0, V_{Ga}^{-1} \) and \( V_{Ga}^{-2} \), respectively. The \( S \) parameter is almost unchanged while the \( W \) parameter decreases slightly with the charge state varying from neutral to doubly negative.

![Graph](image)

**Figure 7.** One-dimensional projection of spin density distribution along [1100] for \( V_{Ga}^0, V_{Ga}^{-1} \) and \( V_{Ga}^{-2} \): (a) Doppler broadening and (b) Compton scattering.

### 3.3. Two-component density functional theory scheme

First, we would like to mention our calculations for monovacancy (\( V \)) and divacancy (\( V_2 \)) in Si. The calculated lifetime values are listed in table 1. It is clearly shown that there is a strong supercell-size dependence for the conventional scheme. The main reason is the difference in the atomic arrangement in the vicinity of \( V \) or \( V_2 \). The larger supercell, the larger inward relaxation is observed. This tendency and the defect structures are consistent with the previous studies [22, 23]. On the other hand, for the TC-DFT scheme, the resultant lifetimes are longer than those obtained with the conventional scheme and show a much smaller supercell-size dependence. The monovacancy is surrounded by four Si atoms (1~4) showing the \( T_d \) point symmetry in the unrelaxed structure. Six distances between two of them \((d_{12}, d_{13}, d_{14}, d_{23}, d_{24}, d_{34})\) are equivalent to each other in this case and the value is 3.84 Å. After structural relaxation, with the 2×2×2 supercell, the distance decreases to 3.67 Å (−4.4%) for the conventional scheme while it increases to 4.00 (+4.2%) for the TC-DFT scheme. With the 3×3×3 supercell, the point symmetry becomes \( D_{2d} \). There are four equivalent distances \((d_{13}, d_{14}, d_{23}, d_{24})\) of 3.45 Å (−10.1%) and two distances \((d_{12}, d_{34})\) of 3.00 Å (−21.9%) for the conventional scheme while four distances of 3.93 Å (+2.4%) and two distances of 3.70 Å (−3.7%) for the TC-DFT scheme. The presence of positron suppresses the inward relaxation around \( V \). A similar situation is observed for \( V_2 \) as described below together with results of other semiconductors. This has been already found and reported by Saito and Oshiyama [24] although they used a different version of TC-DFT [25]. They obtained 279 ps for \( V \) and 309 ps for \( V_2 \) with the 2×2×2 supercell. Considering that they did not modify the enhancement factor with \( \varepsilon_\infty \), their values seem to be slightly overestimated. In other words, the positron effect seems to be slightly overestimated.
Table 1. Calculated positron lifetimes (in ps) for monovacancy ($V$) and divacancy ($V_2$) in Si with the conventional scheme and the TC-DFT scheme on different-sized supercells.

|       | Conventional | TC-DFT |
|-------|--------------|--------|
|       | $2\times2\times2$ | $3\times3\times3$ | $2\times2\times2$ | $3\times3\times3$ |
| $V$   | 232.5        | 222.8  | 267.7  | 268.6  |
| $V_2$ | 282.7        | 247.4  | 314.8  | 315.2  |

Table 2. Distance between atoms neighbouring divacancy (in Å). In parentheses, relative changes from the unrelaxed values are shown (in %).

|       | Conventional | TC-DFT |
|-------|--------------|--------|
|       | cation       | anion  | cation       | anion  |
| C     |              |        |              |        |
| $2\times2\times2$ | 2.69 (+6.7) | 2.75 (+9.2)
| $3\times3\times3$ | 2.65 (+5.2) | 2.73 (+8.4) |
| Si    |              |        |              |        |
| $2\times2\times2$ | 3.62 (-5.7) | 3.85 (+0.2)
| $3\times3\times3$ | 3.01 (-21.7), 3.04 (-20.9), 3.55 (-7.5) | 3.69 (-3.9) |
| Ge    |              |        |              |        |
| $2\times2\times2$ | 3.40 (-14.9) | 3.50 (-12.4)
| $3\times3\times3$ | 3.16 (-20.9) | 3.40 (-14.8) |
| 3C-SiC|              |        |              |        |
| $2\times2\times2$ | 3.88 (+1.0) | 4.15 (+8.1) | 3.99 (+3.9) | 4.20 (+9.5) |
| $3\times3\times3$ | 3.08 (-0.2) | 3.29 (+6.8) | 3.16 (+2.6) | 3.35 (+8.6) |
| AlN   |              |        |              |        |
| $4\times4\times2$ | 3.67 (+18.0) | 3.36 (+8.0) | 3.76 (+20.9) | 3.32 (+6.7) |
| GaN   |              |        |              |        |
| $4\times4\times2$ | 2.98 (-6.5) | 3.39 (+6.4) | 3.05 (-4.4) | 3.35 (+4.9) |
| InN   |              |        |              |        |
| $4\times4\times2$ | 3.43 (-3.1) | 3.56 (+0.6) | 3.50 (-1.1) | 3.47 (-2.1) |

Thus, the conventional scheme is thought to be not very accurate at least for $V$ and $V_2$ in Si, and we made calculations for divacancies in several semiconductors including group-III nitrides (C, Si, Ge, 3C-SiC, AlN, GaN and InN). Each anion (cation) vacancy forming a divacancy has three nearest neighbor cation (anion) atoms. For elemental semiconductors, although there is no distinction between cation and anion, there are similar $3\times2$ neighbor atoms. In table 2, distances between two of three atoms are listed. Except for the case of Si with the $3\times3\times3$ cell and the conventional scheme, three distances are almost equal to each other. Correspondingly, positron annihilation parameters $S$, $W$ and $\tau$ were calculated and the results are plotted in figure 8 as a function of bulk modulus. Roughly speaking, the softer material with the smaller $B$ gives the larger difference between the results of the conventional and TC-DFT schemes. For the cubic materials, it is also confirmed that the supercell-size dependence is larger in softer materials. In figure 8(c), for Si and Ge, it looks that the conventional-scheme results with the smaller ($2\times2\times2$) cell are better than those with the larger ($3\times3\times3$) cell. As mentioned above, the inward relaxation is suppressed in the smaller cell. This is because the supercell size is too small for complete relaxation. For the TC-DFT case, the inward relaxation is suppressed by the presence of positron. The mechanism is different. The better agreement for the smaller cell is not essential.

For 3C-SiC, Wiktor et al. reported a TC-DFT lifetime of 195 ps for $V_C$ (217 ps with the different version TC-DFT [25]) and also a value of 154 ps obtained with the conventional scheme [20]. We also made a TC-DFT calculations on for $V_C$ in 3C-SiC and obtained a lifetime of 142 ps. Our value is quite different from the value by Wiktor et al. The reason is not clear yet.
Figure 8. Positron annihilation parameters for the annihilation of positrons trapped by divacancies in various semiconductors. Calculated values of (a) $S$, (b) $W$ and (c) $\tau$ are plotted as a function of bulk modulus.

As shown in figure 8, for C and SiC, the conventional-scheme results are very close to the corresponding TC-DFT ones. On the other hand, there are large deviations for the positron lifetime in Si and Ge between the two schemes. For the other cases, it depends on the situation whether or not the conventional scheme is sufficient to obtain reasonable results. For group-III nitrides, judging from the $(S,W)$ or $\tau$ variation shown in figures 4 and 5, the conventional-scheme results can be used for our purpose identifying defect species.

4. Summary
We have made computational studies on defects in semiconductors, especially those in group-III nitrides. Variations of positron annihilation parameters $S$, $W$ and $\tau$ for cation monovacancies and cation-nitrogen divacancies in $(\text{In}_{0.5}\text{Ga}_{0.5})\text{N}$ were examined utilizing the SQS approach to reproduce its random-alloy nature. Magnetic positron annihilation Doppler broadening spectra were calculated for gallium monovacancies with various charge states. The obtained results were compared with magnetic Compton scattering spectra to demonstrate the uniqueness and usefulness of the positron annihilation technique in studying vacancy-assisted ferromagnetism in diluted magnetic semiconductors. For divacancies in several semiconductors, positron annihilation parameters $S$, $W$ and $\tau$ were calculated using the conventional scheme as well as using the TC-DFT scheme. The validity of the conventional scheme has been examined and discussed for various cases.

References
[1] Krause-Rehberg R and Leipner H S 1999 Positron Annihilation in Semiconductors (Berlin: Springer)
[2] Tuomisto F and Makkonen I 2013 Rev. Mod. Phys. 85 1583
[3] Uedono A, Ishibashi S, Oshima N and Suzuki R 2013 Jpn. J. Appl. Phys. 52 08JJ02
[4] Uedono A, Sumiya S, Ishibashi S, Oshima N and Suzuki R 2014 J. Phys.: Conf. Ser. 505 012009
[5] Ishibashi S and Uedono A 2014 J. Phys.: Conf. Ser. 505 012010
[6] Zunger A, Wei S-H, Ferreira L G and Bernard J E 1990 Phys. Rev. Lett. 65 353
[7] Mäder K A and Zunger A 1995 Phy. Rev. B 51 10462
[8] Dhar S, Brandt O, Ramsteiner M, Sapega V F and Ploog K H 2005 Phys. Rev. Lett. 94 037205
[9] Dev P, Zue Y and Zhang P 2008 Phys. Rev. Lett. 100 117204
[10] Gohda Y and Oshiyama A 2008 Phys. Rev. B 78 161201(R)
[11] Boroński E and Nieminen R M 1986 Phys. Rev. B 34 3820
[12] Puska M J, Seitsonen A P and Nieminen R M 1995 Phys. Rev. B 52 10947
[13] http://qmas.jp
[14] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[15] Blöchl P E 1994 Phys. Rev. B 50 17953
[16] Ishibashi S 2004 Mater. Sci. Forum 445-446 401
[17] Makkonen I, Hakala M and Puska M J 2006 Phys. Rev. B 73 035103
[18] Puska M J, Mäkinen S, Manninen M and Nieminen R M 1989 Phys. Rev. B 39 7666
[19] Barbiellini B, Puska M J, Torsti T and Nieminen R M 1995 Phys. Rev. B 51 7341
[20] Wiktor J, Jomard G, Torrent M and Bertolus M 2013 Phys. Rev. B 87 235207 (Note that the sign of the fourth term in their equation (A9) is wrong.)
[21] Tuomisto F, Norrman V and Makkonen I 2014 J. Phys.: Conf. Ser. 505 012042
[22] Puska M J, Pöykkö S, Pesola M, and Nieminen R M 1998 Phys. Rev. B 58 1318
[23] Iwata J, Shiraishi K and Oshiyama A 2008 Phys. Rev. B 77 115208
[24] Saito M and Oshiyama A 1996 Phys. Rev. B 53 7810
[25] Gilgien L, Galli G, Gygi C and Car R 1994 Phys. Rev. Lett. 72 3214