Positron states in Si and GaAs

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Positron states in perfect Si and GaAs lattices and at small vacancy-cluster-type defects in these semiconductors are calculated. The method is based on the superposition of free atoms and the solution of the resulting Schrödinger equation by a fully-three-dimensional numerical relaxational method. Positron lifetimes are calculated and compared with available experimental data. The main emphasis is put on the dependence of the positron lifetime on the size of the vacancy cluster and on the role of the lattice relaxation around vacancies.

I. INTRODUCTION

It has recently become evident that positron-annihilation techniques can give a valuable contribution to the technologically important field of defects in semiconductors.[1,2] Positron-lifetime spectroscopy is a unique experimental tool because of its predominant sensitivity to vacancy-type defects. Careful, comprehensive measurements have been performed for Si and GaAs with a wide range of sample conditions, i.e., different controlled doping levels are used, and defects are produced by electron or neutron irradiation. The annealing of the defects has been studied and the change of the defect parameters as a function of temperature has been followed in the positron-lifetime measurements. The method has proved to be sensitive to Fermi-level-controlled processes in the electronic and atomic structure of vacancies.[3]

Insufficient knowledge of positron-defect interaction in semiconductors has hampered the extraction of the defect properties from the accumulated experimental data. The situation is much more difficult (but also much more challenging) than in metals because (i) the variety of the point defects is larger, e.g., different types of vacancies, interstitials, and antisites at different charge states may be present, and, moreover, (ii) the existence of the band gap affects the interaction of the positron with the host system, i.e., the screening of the positron is reduced from that for metals and the mechanism of positron trapping may change due to the lack of low-energy electron-hole excitations.

In this paper we present theoretical results for the annihilation characteristics of positrons both delocalized in perfect Si and GaAs and localized at vacancies and small vacancy clusters in these materials. The calculations lean on the use of non-self-consistent electron structures obtained by superimposing free-atom densities. The potential felt by the positron is then constructed on this basis, and the positron wave function is obtained by a full three-dimensional solution of the corresponding Schrödinger equation. Previously, the positron states in bulk Si and GaAs and at their vacancies have been calculated by Puska *et al.*[4] using self-consistent electron densities. However, these rather heavy calculations assume electron and positron densities and potentials spherically symmetric around the nuclei and interstitial tetrahedral sites [the atomic-sphere approximation (ASA) with empty spheres]. The treatment of lattice relaxation and low-symmetry defects in self-consistent electron-structure methods is difficult, whereas in the present method the positron properties in this kind of cases can be studied rather easily. Judging by the experience gained from previous positron-state calculations[4,5] for metallic systems, the positron lifetime is relatively insensitive to the self-consistency of the electron density, whereas it responds strongly to the ionic relaxation. On the other hand, positron energetics depends remarkably on the details of the electron structure. In the present work these features are clearly found also in the case of semiconductors. Thus, the positron lifetimes predicted are expected to be reliable, whereas the binding energies at defects should be considered as more qualitative ones.

II. THEORETICAL MODEL

The present calculations are performed using the practical calculation method applied first time by Puska and Nieminen[5] in the case of vacancy clusters in metals. The method and the physics behind it have been reviewed recently.[6] The main steps of the method are the following. First, the electron density $n(\mathbf{r})$ and the Coulomb potential V_{Coul} of the host system are obtained by superimposing free-atom densities and potentials,

$$n_-(\mathbf{r})=\sum_{\mathbf{R}} n_-^{\mathrm{at}}(|\mathbf{r}-\mathbf{R}|)\,,$$
$$V_{\mathrm{Coul}}(\mathbf{r})=\sum_{\mathbf{R}} V_{\mathrm{Coul}}^{\mathrm{at}}(|\mathbf{r}-\mathbf{R}|)\,, \tag{1}$$

where $\mathbf{R}$ summations run over the positions of the host nuclei. The potential felt by the positron is then calculated as

$$V(\mathbf{r})=V_{\mathrm{Coul}}(\mathbf{r})+V_{\mathrm{corr}}(n-(\mathbf{r}))\ , \tag{2}$$

where $V_{\mathrm{corr}}(n)$ is the electron-positron correlation energy[7] depending on the local electron density n. For semiconductors V_{corr} is calculated as

$$V_{\mathrm{corr}}(n)=V_{\mathrm{corr}}^{\mathrm{EG}}(n)[f(n,\varepsilon_g)]^{1/3}\ , \tag{3}$$

where $V_{\mathrm{corr}}^{\mathrm{EG}}$ is the correlation energy for a positron in a homogeneous electron gas,[7] and f is a factor taking into account that the screening is reduced due to the band gap. For f, the form

$$f(n,\varepsilon_g)=1-\frac{0.37\varepsilon_g}{1+0.18r_s},\quad r_s=\left[\frac{3}{4\pi n}\right]^{1/3} \tag{4}$$

with $\varepsilon_g=0.2$, is used. This reduction is found to reproduce the experimental positron lifetimes in several IV- and III-V-type semiconductors.[4,6] The positron wave function $\Psi_+(\mathbf{r})$ and the energy eigenvalue corresponding to the potential (2) are then solved by a numerical relaxation method. Using the superimposed electron density (1), the positron-annihilation rate λ is calculated as the integral

$$\lambda=\pi r_0^2 c\int d\mathbf{r}\,|\Psi_+(\mathbf{r})|^2[n_v(\mathbf{r})\Gamma_v(n_v(\mathbf{r}))+n_c(\mathbf{r})\Gamma_c]\ , \tag{5}$$

where Γ_v is the enhancement factor for the valence electrons[8]

$$\Gamma_v(n_v)=\left[1+\frac{r_s^3+10}{6}f(n,\varepsilon_g)\right]\ . \tag{6}$$

In Eq. (5), Γ_c is the enhancement factor for the core electrons, and the value of 1.5 is used for it.

The present model assumes that the electronic (excluding the short-range screening of the positron) and the ensuing ionic structures of vacancies do not change due to the presence of the trapped positron. Indeed, the model calculations[9] for localized positron states performed by the two-component density-functional theory have shown that the annihilation characteristics are not drastically affected if the positron and electron densities are solved simultaneously self-consistently. This result is expected to remain valid also for semiconductors, because the valence electrons in semiconductors screen the positron nearly as effectively as conduction electrons in metals. Moreover, the trapped positron states in semiconductors are rather delocalized. The second important assumption in the model used is the local description of the correlation effects in Eq. (2). This means that in the vacancy clusters neither positronium formation nor positron trapping into a surface state are taken into account. This assumption can be defended again by the delocalized character of the positron wave function at the compact small vacancy clusters considered in this work.

III. RESULTS AND DISCUSSION

A. General

The superimposed electron density in a perfect GaAs lattice is shown in Fig. 1. Naturally, the superimposed

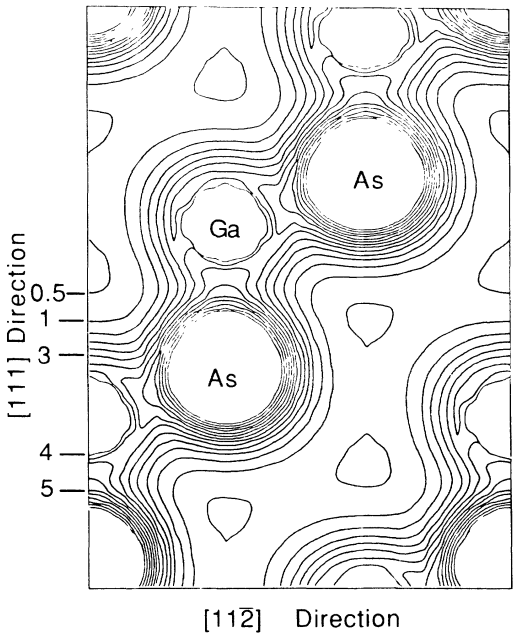

FIG. 1. Valence-electron density in GaAs. Atomic superposition is used. The unit is $0.01a_0^{-3}$, and the contour spacing is 0.5 units. The rapid oscillations of the valence-electron density at ion cores are not shown.

electron density does not show the pileup of the valence-electron density at the covalent bonds between the neighboring atoms. However, when compared with the self-consistent calculations,[10] the superposition describes the electron density in the interstitial regions rather well and also the rise of the density near the atom chains is reproduced reasonably well. The description of the electron density in the interstitial regions and the volume of the open interstitial space are the most important aspects for the positron-state calculations because the positron wave function is mainly located in the interstitial regions between the atoms as shown in Fig. 2 for GaAs. Figure 2 shows also that the positron wave function does not clearly distinguish between the Ga and As atoms. The positron wave function in a perfect Si lattice is qualitatively similar to the wave function in GaAs.

The calculated positron lifetimes in bulk Si and GaAs are 219 p and 229 ps, respectively. The value is shorter for Si than for GaAs, reflecting the higher electron density in the interstitial regions in Si than in GaAs. These lifetimes are in agreement with the experimental results for Si (Refs. 11 and 12) and GaAs (Refs. 3 and 13). The agreement gives credence to the use of the universal description of Eq. (4) for all semiconductors.[6] Moreover, the present values calculated using the atomic superposition are in agreement with the linear-muffin-tin-orbital (LMTO) atomic-sphere-approximation (ASA) calculations[4] in which the electron density is self-consistent. When the same electron gap parameter $\varepsilon_g=0.2$ was used in the latter, positron lifetimes of 221 and 235 ps were found for Si and GaAs, respectively.

In the present calculations the electronic structures

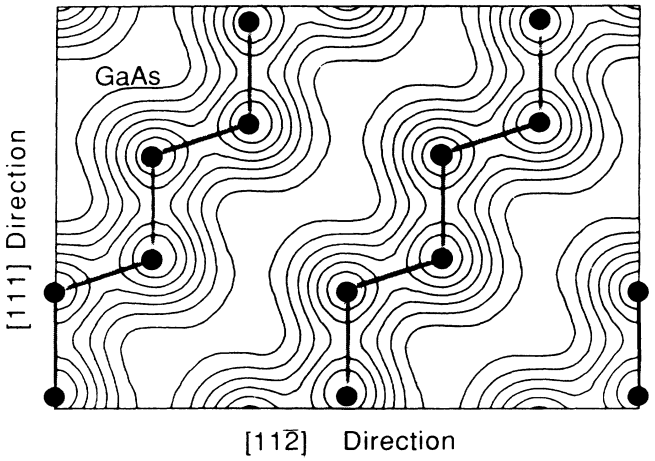

FIG. 2. Delocalized positron wave function in perfect GaAs. The ion positions are denoted by solid circles. The upper of the nearest neighbors in the [111] direction is Ga and the lower one As. The wave function is at a maximum in the interstitial regions between the ion chains and vanishes at the nuclei. The contour spacing is one-seventh of the maximum value.

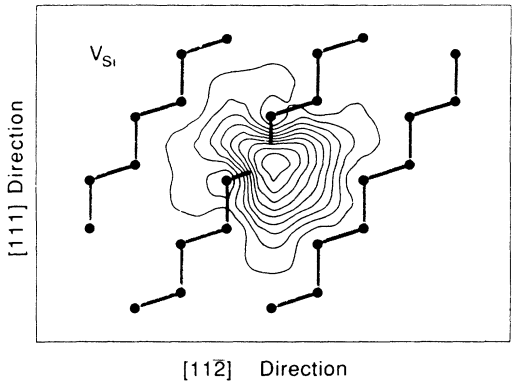

FIG. 3. Localized positron wave function in the Si vacancy. The ion positions are denoted by solid circles. The contour spacing is one-tenth of the maximum value.

of vacancies and vacancy clusters are treated simply by omitting atoms in the superposition. No attempts to describe the different charge states are made. As far as only positron annihilation rates are considered, this is not even necessary, because the annihilation rate is not sensitive to the corresponding changes in the electron density provided that the ionic positions are not varied. This was demonstrated clearly in the LMTO ASA Green's-function calculations,[4] which are able to deal with different charge states of defects. On the other hand, a reliable determination of the positron energetics, including the positron binding energies at defects, requires self-consistent electron densities.[6]

B. Vacancy clusters in Si

The wave function for a positron trapped at a vacancy in Si (V_{Si}) is shown in Fig. 3. The localization of the wave function is not as strong as seen in similar plots for metal vacancies.[5] Now the contours of equal values are strongly affected by the nearest Si atoms, and the positron wave function has a tendency to leak far into the interstitial regions. The rather delocalized character of the positron wave function is seen also in the calculated positron lifetime. It is 254 ps, which is longer than the bulk lifetime by a factor of 1.16, only. For metals the corresponding ratio is typically about 1.5–1.6, reflecting a much more localized positron wave function in a close-packed lattice. Also, the positron-trapping energy at the V_{Si} can then be predicted to be low. The present model gives the value of 0.4 eV, which is less than half of the value[4] obtained by the LMTO ASA Green's-function method for neutral or negative vacancies. For the reasons discussed above the latter values should be considered more reliable. The present positron lifetime of 254 ps is in a good agreement with the previous LMTO ASA Green's-function calculation,[4] which gave 259 ps for the neutral vacancy. The experimental values of 266–270 ps (Refs. 11 and 12) are slightly longer, presumably due to the lattice relaxation that has been omitted in the calculations thus far.

One of the main aims of this work was to study the response of the positron lifetime on the size of the vacancy cluster. We have performed calculations for the nearest-neighbor clusters in Si. The results are collected in Table I. The positron lifetime of 306 ps for the divacancy is remarkably longer than the 254 ps found for the monovacancy. The large difference becomes understandable by comparing the positron wave functions for the di- and monovacancies shown in Figs. 4 and 3, respectively. In the case of the divacancy the positron wave function is more like that in a metal vacancy, i.e., rather localized and isotropic. Table I also shows how the positron lifetime increases rapidly as a function of the cluster size and starts to saturate towards 500 ps, which is the upper limit for positron lifetime in the present model.

The positron-lifetime measurements for the annealing of the neutron-[14] or electron-[11] irradiated Si have been interpreted in terms of the positron lifetime as a function of the number of vacancies in the cluster. The deduced positron lifetime at a divacancy is 320–325 ps. This is in a reasonable agreement with the present theoretical predic-

TABLE I. Calculated positron-annihilation characteristics in Si. λ_v and λ_c are the annihilation rates due to the valence and core electrons, respectively. τ_v is the positron lifetime and E_b is the positron binding energy at the defect.

Number of vacancies	λ_v (ns^{-1})	λ_c (ns^{-1})	τ_v (ps)	E_b (eV)
bulk	4.48	0.10	219	
1	3.89	0.05	254	0.42
2	3.25	0.03	306	1.33
4	2.82	0.01	354	2.27
5	2.66	0.01	376	2.57
8	2.50	0.01	399	3.04

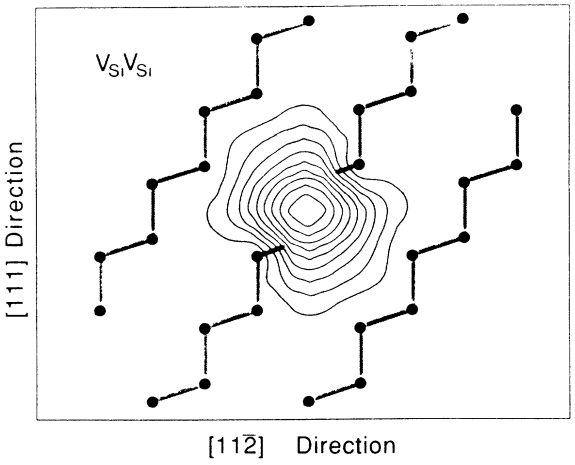

FIG. 4. Localized positron wave function in the Si divacancy. The ion positions are denoted by solid circles. The contour spacing is one-tenth of the maximum value.

tion, especially if one considers only the experimental and theoretical relative differences between the values for mono- and divacancies. For the larger vacancy clusters the comparison is less satisfying. Namely, according to the interpretation of the experiments the positron lifetime rises linearly with the number of vacancies without saturation: the positron lifetime of 435 ps (Ref. 14) has been connected with quadrivacancies, and that of 505 ps (Ref. 15) with clusters consisting of five vacancies. The interpretation of the experiments has, however, raised doubts.[16] It has been argued that the values extracted from lifetime spectra cannot uniquely be connected with a certain number of vacancies. Namely, in the original interpretations[11,14] it is assumed that during the vacancy-migration stage only divacancies are formed and the migration of divacancies generates purely quadrivacancies. However, it has been stated[16] that during these annealing processes larger clusters are possible products, too, and these larger clusters are responsible for the rather long positron lifetimes. Figure 5 shows the calculated positron wave function in the quadrivacancy. It is seen that the extent of the wave function is not essentially larger than in the case of the divacancy in Fig. 4. In both vacancy clusters a positron has a large probability of being in the interstitial space close to the neighboring perfect Si chains. The increase of the positron lifetime between the divacancy and the quadrivacancy is then 48 ps, which is much less than the value of 110 ps obtained in the experimental interpretation.

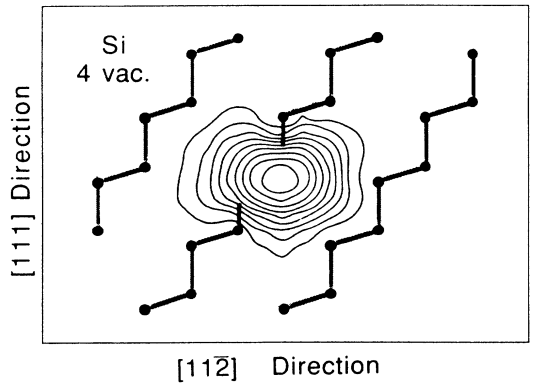

FIG. 5. Localized positron wave function in the Si quadrivacancy. The ion positions are denoted by solid circles. The contour spacing is one-tenth of the maximum value.

C. Vacancies in GaAs: The role of lattice relaxation

The results of the calculations for defects in GaAs are listed in Table II. The positron lifetimes in the As (V_{As}) and Ga (V_{Ga}) vacancies are 266 and 263 ps, respectively. They are very close to each other, and they are longer than the lifetime at a V_{Si} due to the larger lattice constant. According to the LMTO ASA Green's-function calculations[4] the lifetime at the neutral V_{As}^0 is longer, 279 ps, whereas the value of 267 ps for the neutral V_{Ga}^0 is in good agreement with the present results. The disagreement of ~ 10 ps in the case of the V_{As} may reflect the role of the charge transfer from Ga towards As. In the self-consistent electron structure the Ga atoms nearest the As vacancy contribute less to the electron density inside the vacancy than the free atoms used in the superposition. The value of the positron lifetime in the vacancy pair ($V_{As}V_{Ga}$) is again about 50 ps longer than in single vacancies.

In positron-lifetime experiments for n-type GaAs a Fermi-level-controlled process is seen.[1,3] In this process the lifetime of trapped positrons decreases from 295 to 260 ps when the Fermi level in the band gap rises over a certain value. The position of the Fermi level is close to the bottom of the conduction band and can be controlled by changing the measuring temperature or the doping. Two models have been proposed to explain the process. In the first model, that of Corbel *et al.*,[3] the change is due to the change of the charge state of V_{As} from singly negative V_{As}^- to doubly negative V_{As}^{2-}. The corresponding ionization level $(2-,-)$ deduced from the positron-lifetime measurements is in good agreement with other experimental and theoretical estimations. The model can also successfully predict the ionization level $(-,0)$ by assuming that neutral vacancies are not efficient traps for positrons. The second model[1,3] suggests that the process

TABLE II. Calculated positron-annihilation characteristics in GaAs. λ_v and λ_c are the annihilation rates due to the valence and core electrons, respectively. τ_v is the positron lifetime and E_b is the positron binding energy at the defect.

Defect	λ_v (ns^{-1})	λ_c (ns^{-1})	τ_v (ps)	E_b (eV)
bulk	4.03	0.34	229	
V_{As}	3.53	0.23	266	0.24
V_{Ga}	3.63	0.17	263	0.37
$V_{As}V_{Ga}$	3.05	0.12	316	1.03
$V_{As}As_{Ga}$	3.57	0.21	265	0.30

is a conversion of V_{Ga} to an As-vacancy–As-antisite pair $V_{As}As_{Ga}$. Indeed, a positron lifetime of 260 ps has experimentally[17] been connected with V_{Ga}, and the positron lifetime in $V_{As}As_{Ga}$ is expected to be nearly the same as in V_{As}. From the two vacancies only for V_{As} has the value of 295 ps been suggested[1,3,13] (in addition to the value of 260 ps). The bistability of V_{Ga} has been proposed also on the basis of first-principles theoretical calculations.[18] Recently, Dannefaer and Kerr[19] suggested that the value of 295 ps corresponds to divacancies $V_{As}As_{Ga}$. However, this assignment disagrees with the present results, which predict that the positron lifetime in $V_{As}As_{Ga}$ is 316 ps or even more due to an outward relaxation. The outward relaxation is expected, e.g., on the basis of the comparison of theoretical and experimental lifetimes for the divacancy in Si.

The LMTO ASA Green's-function calculations[4] give a ~ 10 ps longer positron lifetime at V_{As} than at V_{Ga}. This is along the lines of the second model, although the experimental change in the lifetime is 30 ps. In this work we have calculated the positron lifetime for $V_{As}As_{Ga}$ to be 265 ps, i.e., only 1 ps less than for the "normal" V_{As} (see Table II). The LMTO ASA Green's-function calculations have shown that a change of the charge state of the defect without changing the ionic configuration does not greatly affect the positron lifetime. The other of the two main aims of this work is to study how much different types of relaxations around vacancies affect the positron lifetime and to clarify if reasonable changes in the relaxations can account for the 30-ps change needed in the first model.

According to the present understanding,[20,21] the relaxation of a vacancy in a semiconductor depends on the charge state of the vacancy. When there are no electrons localized in deep levels in the band gap, the rotation symmetry group of the vacancy is T_d, i.e., the same as for a lattice point in the perfect diamond structure. Thus, only the symmetry-conserving breathing relaxation [Fig. 6(a)] is possible. If there is one electron in a deep level a tetragonal relaxation [Fig. 6(b)] lowers the symmetry to D_{2d}. The driving force behind the relaxation is the Jahn-Teller effect, in which the symmetry lowering removes the spatial degeneracy of the occupied deep levels and the total energy of the defect decreases. The second electron added has the opposite spin as the first one and the two electrons are occupying the same energy level. Therefore the symmetry remains D_{2d}, although the magnitude of the displacements may change. The third bound electron causes a further symmetry lowering. The relaxation is a mixture of tetragonal and trigonal [Fig. 6(c)] relaxations and the resulting point group is C_{2v}. When the Fermi level rises in the band gap, the occupancy of the deep levels increases one by one and the processes described above take place. However, this is not the whole truth, if the vacancy forms a so-called negative-effective-U system. For example, in the case of a Si vacancy it is proven both experimentally and theoretically that due to the change of the relaxations the total energy of V_{Si}^0 is lower than that of V_{Si}^+. Therefore the stable single positive vacancy does not exist in Si. The negative-effective-U behavior is not seen in the case of vacancies in GaAs (Ref. 22). For different vacancies the different charge states correspond to different numbers of bound electrons on the deep levels. For example, the neutral vacancy in Si has two bound electrons, whereas in GaAs V_{Ga}^0 and V_{As}^0 have three and one electrons, respectively. It is interesting to note that in the case of the As vacancy the change from the tetragonal relaxation to the mixture of tetragonal and trigonal relaxations happens between V_{As}^- and V_{As}^{2-}, which are both active traps for positrons. On the other hand, in Si and Ga vacancies this change takes place, when the vacancies are positive or neutral and thus assumed to be unable to trap positrons. Two values of positron lifetimes are reported for As vacancies but not for Si or Ga vacancies.

We have studied the effects of the different types of lattice relaxations on the positron-state and annihilation characteristics in the case of Si vacancies. The effects are similar for the vacancies in GaAs as shown by our results for the breathing relaxation of V_{As}. We have moved the Si atoms nearest the vacant site according to the modes shown in Fig. 6. All the Si atoms are moved by the same amount, either 5% or 10% of the bond length. This is a typical amplitude found in theoretical approaches.[23,24] The results are listed in Table III. It is seen that the out-

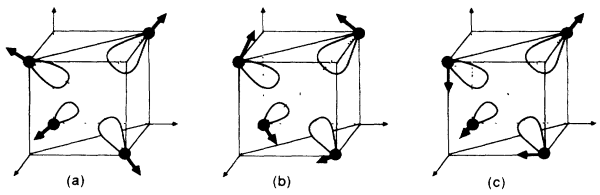

FIG. 6. Relaxation modes of a vacancy in the diamond or zinc-blende structure. The vacant site is the center of the cube. The displacements of the four atoms nearest to the vacant site are denoted in the (a) breathing, (b) tetragonal, and (c) trigonal modes.

TABLE III. Effects of lattice relaxation on positron-annihilation characteristics at a Si vacancy. The different relaxation modes are explained in Fig. 6. The magnitudes of the displacements are given relative to the bond length. λ_v and λ_c are the annihilation rates due to the valence and core electrons, respectively. τ_v is the positron lifetime and E_b is the positron binding energy at the defect. The results for breathing relaxation at V_{As} are shown too.

Relaxation	λ_v (ns^{-1})	λ_c (ns^{-1})	τ_v (ps)	E_b (eV)
	V_{Si}			
breathing 5%	3.67	0.04	270	0.69
tetragonal 5%	3.92	0.03	254	0.54
tetragonal 10%	3.91	0.03	253	0.54
trigonal 5%	3.92	0.05	252	0.39
trigonal 10%	3.89	0.05	254	0.41
	V_{As}			
breathing 5%	3.31	0.20	286	0.45

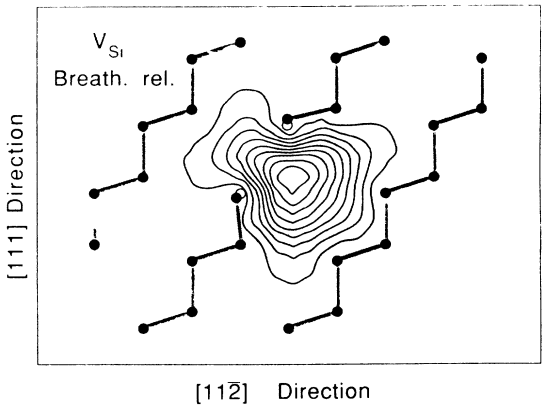

FIG. 7. Effect of the breathing relaxation on the positron wave function at the Si vacancy. The ion positions are denoted by solid circles. The unrelaxed positions of the atoms nearest the vacant site are given as open circles. The contour spacing is one-tenth of the maximum value.

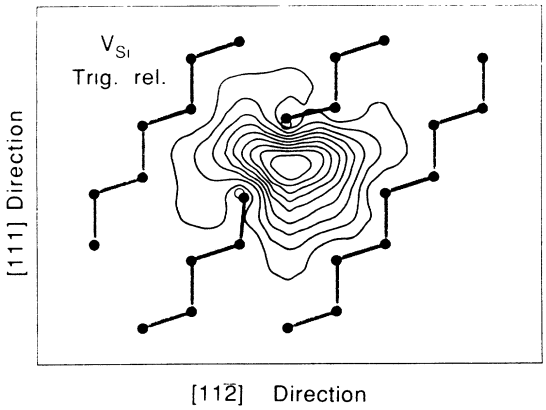

FIG. 9. Effect of the trigonal relaxation on the positron wave function at the Si vacancy. The ion positions are denoted by solid circles. The unrelaxed positions of the atoms nearest the vacant site are given as open circles. The contour spacing is one-tenth of the maximum value.

ward breathing relaxation rapidly increases the positron lifetime, whereas the positron characteristics are nearly unchanged due to the pure tetragonal or trigonal relaxations. The reason for the different types of behavior can be understood from Figs. 7–9. The breathing relaxation clearly increases the open volume available for the trapped positron, whereas the pure tetragonal and trigonal relaxations only distort the positron wave function. The present calculations cannot *quantitatively* support or disprove the first model for the Fermi-level-controlled process, because the exact relaxation patterns are not known. For instance, there is a breathing component in the tetragonal mode and the mixing ratio of the tetragonal and trigonal modes is not quantitatively known. However, the message of the present calculations is that changes in the open volume available for the positron are needed to explain the changes in the positron lifetime detected experimentally. An increase of a few percent in the breathing relaxation can increase the positron lifetime of the order of 30 ps, which is seen in the experiments. Moreover, in the present calculations the electron-positron correlation is the same for the all charge states. In the LMTO ASA Green's-function calculations, this approximation predicted that the positron lifetime is rather insensitive to the charge state of the unrelaxed vacancy. If the correlation changes, it may still increase the differences in the positron lifetimes for different charge states.

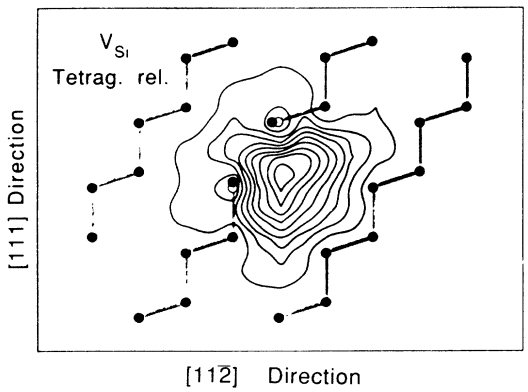

FIG. 8. Effect of the tetragonal relaxation on the positron wave function at the Si vacancy. The ion positions are denoted by solid circles. The unrelaxed positions of the atoms nearest the vacant site are given as open circles. The contour spacing is one-tenth of the maximum value.

IV. CONCLUSIONS

We have studied the positron states at defects in Si and GaAs using a practical calculation method based on the superposition of free-atom densities and the three-dimensional solution of the positron Schrödinger equation. The method is shown to be accurate to describe the positron-annihilation rate. The rather large and open interstitial regions in semiconductors determine the characteristic features of the positron states. The localization of the positron states at vacancies is much weaker than in metals, leading to the rather small ratio between the positron vacancy and bulk lifetimes. The two main aims of this work were to study the dependence of the positron lifetime on the size of the vacancy cluster and in the case of vacancies the effect of the lattice relaxation. The positron lifetime at vacancy clusters increases as a function of the cluster size, saturating rapidly towards the model limit of 500 ps. The result extracted from positron-lifetime measurements,[11,14] i.e., the linear dependence of the positron lifetime on the number of vacancies in the cluster, cannot be reproduced in the present model. The results for the effects of the relaxation around vacancies show that reasonable changes ($\sim 5\%$ in the breathing relaxation) in the atomic displacements may cause positron lifetime to decrease or increase even by the amount of ~ 30 ps. According to the model by Corbel *et al.*,[3] changes of this size take place due to the different relaxations in different charge states of the As vacancy in GaAs.

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