Evaluation of some basic positron-related characteristics of SiC

G. Brauer, W. Anwand, and E.-M. Nicht

Arbeitsgruppe Positronen-Annihilations-Spektroskopie der Technischen Universität Dresden, c/o Forschungszentrum Rossendorf,
Postfach 510119, D-01314 Dresden, Germany

J. Kuriplach,* and M. Šob

Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Zizkova 22, CZ-61662 Brno, Czech Republic

N. Wagner

Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06108 Halle/Saale, Germany

P. G. Coleman

School of Physics, University of East Anglia, Norwich NR4 7TJ, United Kingdom

M. J. Puska and T. Korhonen

Laboratory of Physics, Helsinki University of Technology, SF-02150 Espoo, Finland

First-principles electronic structure and positron-state calculations for perfect and defected 3C- and 6H-SiC polytypes of SiC have been performed. Monovacancies and divacancies have been treated; the influence of lattice position and nitrogen impurities have been considered in the former case. Positron affinities and binding energies have been calculated; trends are discussed, and the results compared with recent atomic superposition method calculations. Experimental determination of the electron and positron work functions of the same 6H-SiC allows an assessment of the accuracy of the present first-principles calculations, and to suggest further improvements. [S0163-1829(96)01828-0]

I. INTRODUCTION

The current interest in silicon carbide (SiC) as a semiconductor for device technology is based on its outstanding chemical and physical properties. However, the identification of the chemical nature or atomic and electronic structures of defects in SiC, which exists in many different crystallographic structures (polytypes), is in its infancy.[1,2]

Positron annihilation spectroscopy (PAS) is now a well-established tool for the study of electronic and defect properties of solids.[3–5] Radiation damage caused by ion implantation in 6H-SiC has recently been studied by monoenergetic positron beam techniques in combination with theoretical calculations.[6] It has been shown that the main defect produced by Ge$^+$ implantation is the divacancy. Ge$^+$ ions were chosen for implantation because (a) Si or C ions would disturb stoichiometry, (b) the available Si ion beam is not free of N$_2$ admixture (N would act as a dopant impurity), and (c) Ge$^+$ ions have the same valency as Si and C and therefore do not disturb the electrical behavior of the target. The atomic superposition method used in Ref. 6 allowed the evaluation of positron lifetimes in different polytypes of bulk SiC, in carbon and silicon monovacancies, and in vacancy agglomerates consisting of up to four Si-C divacancies. The lifetimes calculated in this way correspond to neutral, unrelaxed defects; however, vacancies might be in different charge states, and this would affect the corresponding positron lifetime through modified electrostatic potentials and changes in the atomic relaxation around the vacancy.[7–9] Moreover, the degree of relaxation around a defect is expected to increase

with the number of vacancies in the agglomerate. A positron bound in a vacancy also interacts electrostatically with the surrounding ions, and this affects their positions; this effect has been documented in the case of GaAs.[8,9]

Any theoretical investigation of lattice relaxations due to open volume defects and positrons trapped therein is a very complex problem which has not, to date, been resolved. There is, however, a standard *ab initio* calculational method which neglects lattice relaxation around a defect; this method has been shown to form a reasonable foundation for the interpretation of data from experimental positron trapping studies.[10]

Recently, from first-principles electronic structure and positron-state calculations linear muffin-tin orbital atomic-sphere approximation (LMTO-ASA), positron affinities A_+ and lifetimes τ have been presented for perfect and vacancy-defected transition-metal carbides and nitrides.[11] These self-consistent calculations led to a discussion of the possible trapping of positrons in precipitates formed in alloys by thermal treatment, as well as in precipitates in reactor pressure vessel steels induced by neutron irradiation.[12] The application of improved LMTO-ASA calculations to different polytypes of SiC allows a more reliable treatment, compared to the atomic superposition method, of the following: (i) bulk positron lifetimes; (ii) positron lifetimes in monovacancies and divacancies and the influence of an impurity atom in the vicinity of these defects; and (iii) positron trapping in clusters of Si or Ge atoms, which might be formed by ion implantation. This last calculation was prompted by the fact that the bulk positron lifetimes given in the literature[13] for Si

(218 ps) and Ge (230 ps) are both close to the experimental lifetime (235±3) ps found after ion implantation.[6]

In connection with studies of ion implantation of 6H-SiC, it has been found that SiC may form the basis of an important moderator/remoderator for the production of slow positron beams.[14] The positron work function ϕ_+ of 6H-SiC was measured to be (-3.0 ± 0.2) eV. Measurement of the electron work function ϕ_- allows an experimental determination of the positron affinity A_+ for SiC. ϕ_- can also be calculated from the electronic band structure of SiC, and a comparison can thus be made between experiment and theory for this fundamental materials property.

The paper is organized as follows. Sections II and III outline the experimental and theoretical methods used. The results are presented and discussed in Sec. IV, and conclusions are drawn in Sec. V.

II. EXPERIMENTAL METHODS

A. Electron affinity, band gap, and electron work function

The electronic properties of the 6H-SiC specimen were determined by use of the contact potential (CP) method, which has already been successfully applied to TiC,[15] and photoacoustic spectroscopy.[16] The CP between the tungsten cathode and SiC gives the electron affinity χ_{SiC} of SiC.

In determining the energy gap E_g, photoacoustic spectroscopy was employed, having an advantage over optical spectroscopy in that any error caused by light scattering is avoided. The phase-sensitive lock-in amplifier signal was monitored with a chopper frequency of 420 Hz which was chosen in light of the specimen thickness in order to give the best signal-to-noise ratio. The combination of χ and E_g then gives the electron work function ϕ_-.

B. Doppler-broadened annihilation linewidths

The mean Doppler-broadened annihilation line-shape parameter S was measured as a function of incident positron energy E for Si, Ge, and implanted 6H-SiC. This was done using the computer-controlled magnetically guided slow positron beam at UEA Norwich.[17] Positrons of energies controllable in the range 0.1–30 keV are guided to the target sample through an evacuated flight tube; the beam diameter was apertured to 4-mm diameter. For a more detailed description of the measuring system as well as data evaluation procedures, see Ref. 17.

III. THEORETICAL METHOD: POSITRON LIFETIMES AND AFFINITIES

The atomic superposition method[18] used recently to calculate positron lifetimes in SiC (Ref. 6) utilizes only an approximate electronic charge density. This is constructed from atomic charge densities of free Si and C atoms, and charge transfer between the atoms (and also between atoms and vacancies) is completely neglected. In general, charge transfer causes a redistribution of electrons, and this can affect the positron lifetime.

In the present paper we employ the tight-binding linear muffin-tin orbital method (TB-LMTO),[19] and thereby calculate the electronic charge self-consistently. The computations are performed within the atomic-sphere approximation

TABLE I. Structure data for the polytypes 3C-SiC and 6H-SiC used in the present calculations (Ref. 22). a and c denote the unit-cell dimensions in the corresponding crystallographic directions, W_0 the unit-cell volume, p the number of atoms per unit cell, and ε_∞ the high-frequency dielectric constant. The lattice constants and the unit-cell volume are given in atomic units (1 a.u. $=52.9177\times10^{-12}$ m).

Polytype	a (a.u.)	c/p (a.u.)	W_0/p (a.u.^{3})	ε_∞
3C-SiC	5.826	4.756	139.83	6.7
6H-SiC	5.822	4.762	139.76	6.7

(ASA)—i.e., the electron and positron potentials are spheridized within overlapping atomic spheres which have the same volume as Wigner-Seitz cells. The lattice relaxation in the neighborhood of a vacancy is neglected. Furthermore, in the calculation of positron annihilation characteristics, the influence of electron-positron interaction is taken into account in the limit of small positron density.[20] This limit, which is exact in the case of positron annihilation in perfect solids with delocalized positrons, may not be appropriate for positrons localized in vacancies, where the positron density is relatively high. As discussed in Ref. 6 in more detail, this simplification does not affect the results appreciably.

Improvement has also been made with regard to the symmetry of the lattice. Whereas in the earlier calculations the 6H-SiC polytype was simulated by the simpler orthorhombic structure, the proper hexagonal symmetry of this polytype is now taken into account.

For the sake of comparison, two SiC polytypes, i.e., 3C- and 6H-SiC, were investigated. It is possible to describe the structure of both polytypes within the hexagonal representation,[21] and the corresponding lattice parameters are given in Table I. For all calculations a supercell created by doubling the elemental cell in the a and b directions, i.e., in the basal plane, was used; the reason for this is that large distances between vacancies for a structure with defects are needed in order to reduce their mutual interactions. Thus there are 24 (48) atomic sites in the supercell in case of the 3C (6H) SiC polytype for the calculation of bulk properties. As the structures are open, the same number of empty spheres into the supercell is incorporated in order to describe better the interstitial charge distribution. If vacancies are included in the lattice, the number of atomic sites lowers correspondingly. In the basis s, p, and d orbitals were included, the d orbitals being downfolded.[19]

As in Ref. 6, the positron lifetime τ was calculated as the reciprocal value of the positron annihilation rate λ by

$$1/\tau = \lambda = \int |\Psi_+(r)|^2 \Gamma(n_-(r)) dr. \quad (1)$$

Here $|\Psi_+(r)|^2$ is the positron density, and $\Gamma(n)$ denotes the annihilation rate for a positron in a homogeneous electron gas.[6,20] The high-frequency dielectric constant ε_∞ enters into the expression for $\Gamma(n)$.[6] Values of ε_∞ differ slightly for 3C and 6H modifications.[22] Nevertheless, a value of $\varepsilon_\infty=6.7$ has been used for both 3C and 6H SiC polytypes in the present calculations to make results comparable with those in Ref. 6.
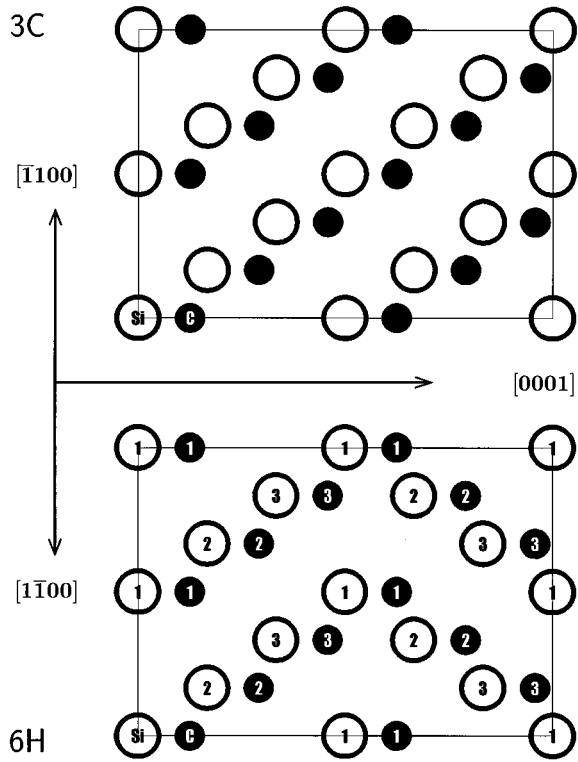
FIG. 1. Atomic positions in the $(11\bar{2}0)$ plane for 3C-SiC and 6H-SiC polytypes. In the lower part, numbers inside circles (atoms) mark crystallographically nonequivalent positions of C and Si atoms for 6H-SiC. The rectangular area in both diagrams corresponds to the intersection of the $(11\bar{2}0)$ plane with the supercell used in the calculations; the only exception is for the 3C-SiC polytype, where the size of the supercell in the [0001] direction (c axis) is two times smaller. Structural data for both polytypes are given in Table I.

In the 6H-SiC polytype there exist three nonequivalent lattice positions for Si and C atoms, and correspondingly three nonequivalent positions for monovacancies. This is illustrated in Fig. 1. In the case of Si monovacancies the changes in the calculated positron parameters are negligibly small. Therefore, the calculations were restricted to one geometrical type of C monovacancy.

IV. RESULTS AND DISCUSSION

A. Bulk and defect positron lifetimes

Theoretical results for positron lifetimes, positron-defect binding energies, and positron affinities are presented in Table II. If we compare the values from Table II with the corresponding results from the atomic superposition method calculations,[6] we arrive at the following conclusions.

(a) For the bulk material a slightly smaller positron lifetime is found for 3C-SiC, whereas for 6H-SiC exactly the same value has been calculated. The small difference between 3C-SiC and 6H-SiC values reflects the larger interstitial space in the 6H-SiC compared to the 3H-SiC structure.

(b) In the case of C and Si monovacancies, generally somewhat larger positron lifetimes are found for both SiC polytypes. The differences are most significant in case of the Si vacancy, which indicates a large redistribution of charges at atomic sites and in the interstitial region if a Si atom is removed. This was verified by comparing the charges at atomic sites and empty spheres for bulk and Si monovacancy cases. As in the case of bulk materials, a longer positron lifetime is found in 6H-SiC, which again reflects the larger interstitial space existing in this structure. Except for the C vacancy, generally much larger positron binding energies have been calculated for 6H-SiC.

TABLE II. Positron lifetime τ, positron binding energy E_b (the difference between the positron energies in the bulk and the defect), and positron affinity A_+ calculated for bulk and various defects in 3C-SiC and 6H-SiC. In the case of 6H-SiC there exist three different lattice positions for the Si vacancy marked by (n) with $n=1, 2,$ and 3 (for details, see text). The values calculated by the atomic superimposed method (Ref. 6) are given in parentheses.

Positron state	τ (ps)	E_b (eV)	A_+ (eV)
	3C-SiC		
bulk	138(141)		−5.57
C vacancy	153(150)	+1.05(+0.28)	−4.39
Si vacancy	191(185)	+2.66(+1.69)	−8.22
Si+C divacancy	212(216)	+3.17(+2.39)	−8.18
Si+Si divacancy	194	+2.69	−8.93
C+C divacancy	160	+1.29	−4.92
Si vacancy+N	191	+2.73	−8.56
	6H-SiC		
bulk	141(141)		−5.91
C vacancy (1)	153(150)	+0.26(+0.28)	−4.30
Si vacancy (1)	194(183)	+2.46(+1.73)	−8.27
Si vacancy (2)	192	+2.30	−8.17
Si vacancy (3)	192	+2.32	−8.16
Si+C divacancy	214(214)	+2.95(+2.44)	−8.10
Si+Si divacancy	196	+2.64	−8.91
C+C divacancy	161	+0.58	−4.72
Si vacancy+N	194	+2.52	−8.75

(c) For the SiC divacancy the positron lifetime is slightly smaller (3C-SiC) or equal (6H-SiC) than in the earlier calculations, but a generally larger positron binding energy has been calculated.

(d) It is interesting to note that a Si-Si divacancy is more or less seen as two isolated monovacancies by the positron, according to the calculated positron lifetime. This effect can be understood from Fig. 1; if two nearest-neighbor Si atoms are removed there is still one C atom close to these vacancies which separates them. Therefore we have two isolated vacancies rather than one larger vacancy. In the case of the C-C divacancy the situation is similar, but the difference between the monovacancy and divacancy is more noticeable.

(e) To account for the effect of nitrogen doping, the location of a nitrogen atom in the vicinity of a Si monovacancy has been considered. This does not influence the corresponding positron lifetime in either SiC polytype, although it causes a slight increase in the positron binding energy.

(f) In general the more realistic LMTO-ASA calculations, while able to provide the positron affinity, are unable to remove the difference in positron lifetimes for the Si-C divacancy in 6H-SiC between the experimental value of 235 ± 3 ps and that calculated using the atomic superposition

TABLE III. Positron lifetime τ, and positron affinity A_+ for 6H-SiC, Si, and Ge. r_c is the critical radius of Si and Ge clusters in 6H-SiC necessary for positron trapping, calculated using Eq. (5).

Material	τ (ps)	A_+ (eV)	r_c (nm)
6H-SiC	141	−5.91	
Si	218	−7.20	0.27
Ge	219	−7.62	0.24

method.[6] The (small) difference between the measured and calculated values suggests that there may be lattice relaxation around this defect, or that perhaps an impurity atom such as nitrogen located on a lattice site near the defect. However, it should be pointed out that the improved calculations shown in Table II do not cast doubt on the interpretation of the positron annihilation studies of ion-implanted 6H-SiC given in Ref. 6.

B. Positron trapping in Si or Ge precipitates in SiC

A positron will be trapped by a precipitate if the difference ΔA_+ between the positron affinity of the host and the precipitate is positive, and the radius of the precipitate exceeds the critical radius r_c given by[23]

$$r_c = 0.31/(\Delta A_+)^{1/2}. \qquad (2)$$

Here the proportionality constant is in units of nm $(\text{eV})^{1/2}$, ΔA_+ is in eV, and r_c is in nm (a spherical precipitate is assumed). Although the positron lifetimes and affinities for Si and Ge are already known from the literature,[23] they were calculated once more on equal footing with the ones for 6H-SiC. The results are given in Table III together with the critical sizes of precipitates estimated from Eq. (2).

The results collected in Table III would support the idea of positron trapping in Si and Ge clusters if formed in 6H-SiC due to ion implantation. However, the similarity of positron lifetimes in Si, Ge, and 6H-SiC after ion implantation—as mentioned in Sec. I—is not sufficient evidence of such trapping. At least one other positron method reflecting the momentum distribution of electrons participating in the annihilation process needs to be considered. Therefore, Doppler broadening of the annihilation linewidth, as reflected in the line-shape parameter S, was measured by slow positron implantation spectroscopy for pure Si and Ge, as well as Ge$^+$-implanted 6H-SiC, and the results are presented in Fig. 2.

For all three materials the influence of the surface properties on the mean S parameter is reflected at very low incident positron energies. However, at incident positron energies above about 7 keV this influence vanishes, and the bulk properties are reflected through the corresponding S values (means of the high-energy results): Si: 0.4934±0.0003; Ge: 0.4795±0.0009; 6H-SiC: 0.4929±0.0006. As measured S values in Ge$^+$-implanted SiC are considerably *higher* than that for bulk 6H-SiC,[6] it would appear that trapping in open-volume defects dominates trapping at precipitates, although the latter clearly needs to be studied in more detail in the future.
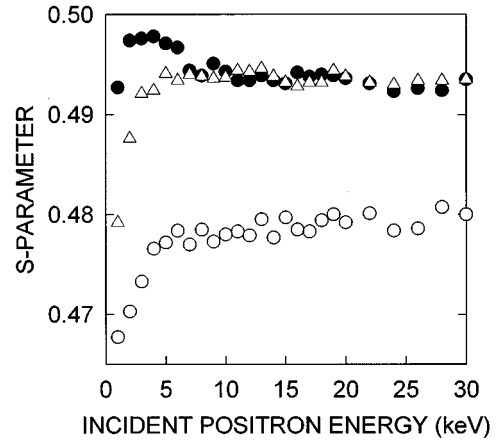

FIG. 2. Mean S parameter vs incident positron energy for Si ($\triangle$), Ge($\bigcirc$), and 6H-SiC ($\bullet$).

C. Electronic properties

The electron affinity χ_{SiC} of SiC was measured using the method outlined in Sec. II: the CP between the tungsten cathode [4.50 eV (Ref. 15)] and the SiC anode (−1.16±0.05 eV) gives

$$\chi_{\text{SiC}} = (-1.16 \pm 0.05) + 4.50 = (3.34 \pm 0.05) \ \text{eV}. \qquad (3)$$

The data presented in Fig. 3 lead to the result for the band gap E_g,

$$E_g = (3.17 \pm 0.12) \ \text{eV}. \qquad (4)$$

The value E_g depends on the SiC polytype. In the case of 6H-SiC values of E_g between 2.9 and 3.08 eV have been reported,[23,24] whereas for 4H-SiC a value of 3.2 eV has been quoted.[23] Taking this into consideration, we cannot exclude the possibility that our specimen might contain a small admixture of the polytype 4H-SiC, from which the local characteristic could be determined by use of a transmission mapping.[25]

Taking the experimental results [Eqs. (3) and (4)] together, the electron work function ϕ_- is given by
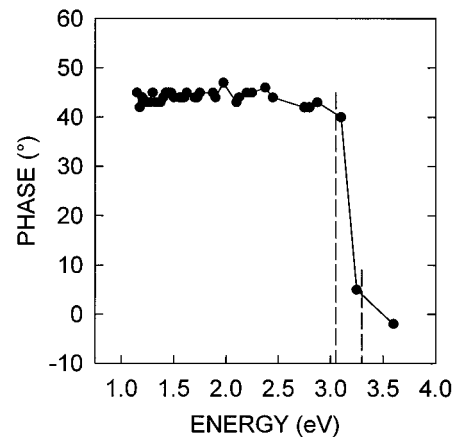

FIG. 3. Photoacoustic phase-indicated gap absorption spectrum of 6H-SiC.

TABLE IV. Experimental positron (ϕ_+) and electron (ϕ_-) work functions, ''experimental'' positron affinity $A_{+,\text{expt}}$ [Eq. (6)], and theoretical $A_{+,\text{theor}}$ for W and 6H-SiC.

Material	ϕ_+ (eV)	ϕ_- (eV)	$A_{+,\text{exp}}$ (eV)	$A_{+,\text{theor}}$ (eV)
6H-SiC	-3.0	$+6.51$	-3.51	-5.91
W	-3.0 (Ref. 13)	$+4.15$ (Ref.14)	-1.5	-1.31 (Ref. 23)

$$\phi_- = (6.51 \pm 0.17) \text{ eV}. \qquad (5)$$

D. Positron affinity A_+

The positron affinity A_+ is defined by[23]

$$A_+ = \mu_- + \mu_+ . \qquad (6)$$

A_+ is a pure bulk quantity which does not depend on the surface orientation of a crystalline sample. The values presented in Table II have been calculated using the electron chemical potential μ_- and the positron chemical potential μ_+, assuming that μ_- corresponds to the top of the valence band. It is natural to use such a definition in order not to invoke any experimental numbers; moreover, the position of the electron chemical potential is not always known experimentally.

The 6H-SiC specimen used for the positron reemission measurements[14] is the same as that used for the electron work-function measurements. The valence band is found to be positioned 6.51 eV below the vacuum level. This value has been used in determining the positron work function from Eq. (6). Thereby

$$\phi_+ = -(A_+ + \phi_-) = -[-5.91 + (6.51 \pm 0.17)] \text{ eV}$$
$$= -(0.60 \pm 0.17) \text{ eV} \qquad (7)$$

for 6H-SiC. The theoretical value for ϕ_+ of about -1 eV mentioned in Ref. 14 was estimated using an early calculation of the positron affinity for 3C-SiC in 1994.[26]

It is encouraging that the theory already predicts a relatively large negative positron work function, in agreement with experimentally observed positron work-function emission from 6H-SiC which suggests that this material may find use as a positron moderator in the future.[13] On the other hand, the experimental estimation of both positron and electron work functions for the same material offers the unique possibility by use of Eq. (6) to evaluate the ''experimental'' positron affinity and compare it to the ''pure'' theoretical value. The present work on 6H-SiC and earlier work on W (Ref. 15) allows this comparison for two different materials (see Table IV). It is evident that in case of W an excellent agreement between theoretical and experimental positron affinity values is found, which is not the case for 6H-SiC. However, it is generally clear that the local-density approximation, widely used in electronic structure calculations, usually yields large errors for electron and positron energy levels for systems having an energy gap.[27,28] To overcome this problem in the future, an improved approach to obtain reasonable gap and positron level values from first principles

should be used. This would require the inclusion of self-interaction correction terms as well as modification of the electron-positron correlation potential. Such work is already in progress.

V. CONCLUSIONS

First-principles electronic structure and positron-state calculations for different SiC polytypes in perfect and defected states have been performed. The quantities studied are the positron lifetime and affinity and thereby the positron-defect binding energy has been derived. The results show that the positron lifetime is rather sensitive to the size of a defect. Compared to these rather large differences, the influence of the difference in polytype (3C-SiC and 6H-SiC) as well as of different lattice positions in the case of the Si monovacancy in 6H-SiC is negligibly small, at least with respect to the achievable accuracy in any positron measurement. However, it is remarkable that Si-Si and C-C divacancies may both be regarded as isolated monovacancies, in contrast to the Si-C divacancy. In general, much larger positron binding energies have been found compared with those calculated using the atomic superposition method for the same defect configurations.

Positron affinity calculations allow consideration of the case of positron trapping in Si and Ge clusters in 6H-SiC. In general a critical size can be estimated for such clusters, above which they would be attractive to positrons. However, slow positron beam measurements performed on Si, Ge, and 6H-SiC suggest that the formation of and positron trapping in such clusters due to Ge^+ implantation is unlikely.

An experimental estimation of the electron work function of 6H-SiC, combined with independent positron work-function measurements on the same 6H-SiC specimen,[13] allows the evaluation of the positron affinity for this sample and its comparison with the theoretical value. Whereas excellent agreement was seen for W in earlier work,[15] the less satisfactory result for 6H-SiC has prompted suggestions for improvements in the theoretical calculations which need to be confirmed by future work.

[*]Also at Department of Low Temperature Physics, Charles University, V Holešovickach 2, CZ-18000 Prague, Czech Republic.

[1]G. Pensl and R. Helbig, in *Festkörperprobleme/Advances in Solid State Physics*, edited by U. Rössler (Vieweg, Braunschweig, 1990) Vol. 30, p. 133.

[2]G. Pensl and W. Choyke, Physica B **185**, 264 (1993).

[3]Positrons in Solid-State Physics. *Proceedings of the International School of Physics ''Enrico Fermi,'' Course LXXXIII, Varenna, 1981*, edited by W. Brandt and A. Dupasquier (North-Holland, Amsterdam, 1983).

[4]P. J. Schultz and K. G. Lynn, Rev. Mod. Phys. **60**, 701 (1988).

[5]Positron Annihilation: *Proceedings of the 10th International Conference on Positron Annihilation, Beijing, 1994* [Mater. Sci. Forum **175-178** (1995)].

[6]G. Brauer, W. Anwand, P. G. Coleman, A. P. Knights, F. Plazaola, Y. Pacaud, W. Skorupa, J. Störmer, and P. Willutzki, Phys. Rev. B (to be published).

[7]K. Laasonen, R. M. Nieminen, and M. J. Puska, Phys. Rev. B **45**, 4122 (1992).

[8]L. Gilgien, G. Galli, F. Gygi, and R. Car, Phys. Rev. Lett. **72**, 3214 (1994).

[9]M. J. Puska, A. P. Seitsonen, and R. M. Nieminen, Phys. Rev. B **52**, 10 947 (1995).

[10]M. J. Puska and R. M. Nieminen, Rev. Mod. Phys. **66**, 841 (1994).

[11]M. J. Puska, M. Šob, G. Brauer, and T. Korhonen, Phys. Rev. B **49**, 10 947 (1994).

[12]G. Brauer, M. J. Puska, M. Šob, and T. Korhonen, Nucl. Eng. Design **158**, 151 (1995).

[13]R. Krause-Rehberg, M. Brohl, H. S. Leipner, Th. Drost, A. Polity, U. Beyer, and H. Alexander, Phys. Rev. B **47**, 13 266 (1993).

[14]J. Störmer, A. Goodyear, W. Anwand, G. Brauer, P. G. Coleman, and W. Triftshäuser, J. Phys. Condens. Matter **8**, L89 (1996).

[15]G. Brauer, W. Anwand, E.-M. Nicht, P. G. Coleman, A. P. Knights, H. Schut, G. Kögel, and N. Wagner, J. Phys. Condens. Matter **7**, 9091 (1995).

[16]N. Wagner (unpublished).

[17]N. B. Chilton and P. G. Coleman, Meas. Sci. Technol. **6**, 53 (1995).

[18]M. J. Puska and R. M. Nieminen, J. Phys. F **13**, 333 (1983).

[19]For a recent review, see O. K. Andersen, O. Jepsen and M. Šob, in *Electronic Band Structure and its Applications*, edited by M. Yussouff (Springer, Berlin, 1987), p. 1.

[20]See, e.g., P. Käckell, B. Wenzien, and F. Bechstedt, Phys. Rev. B **50**, 17 037 (1994).

[21]L. Patrick and W. L. Choyke, Phys. Rev. B **2**, 2255 (1970)

[22]M. J. Puska, P. Lanki, and R. M. Nieminen, J. Phys. Condens. Matter **1**, 6081 (1989).

[23]J. A. Powell and L. G. Matus, in *Amorphous and Crystalline Silicon Carbide and Related Materials*, edited by G. L. Harns and C. Y.-W. Yong, Springer Proceedings in Physics, Vol. 34 (Springer, Berlin, 1989), p. 2.

[24]H. Matsunami, K. Shibakara, N. Kuroda, W. Yoo, and S. Niskina, in *Amorphous and Crystalline Silicon Carbide and Related Materials* (Ref. 23), p. 34.

[25]P. A. Glasow, in *Amorphous and Crystalline Silicon Carbide and Related Materials* (Ref. 23), p. 13.

[26]M. J. Puska (private communication).

[27]J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).

[28]M. J. Puska and R. M. Nieminen, Phys. Rev. B **46**, 1278 (1992).