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Calculation of positron lifetimes in bulk materials

B Barbiellini, P Genoud and T Jarlborg

Département de Physique de la Matière Condensée, Université de Genève, 24 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland

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Abstract. We have calculated positron lifetimes in different bulk materials using the LMTO (linear muffin-tin orbitals) method. Electron-positron correlation effects have been included in the calculation through the enhancement factor calculated within the local density approximation (LDA) by Jarlborg and Singh. Following Jensen and Puska, we apply the enhancement factor identically to all electrons (valence and core), making the approach very general. The overall agreement between the calculated bulk lifetimes and the corresponding experimental values is especially good in the case of 3d transition metals. These calculations constitute a good test for the application of the method to angular correlation data analysis.

1. Introduction

In the calculations of positron annihilation rates, the introduction of electron-positron correlation effects describes the screening charge of the electrons around the positron. The enhancement factor is given by the amplitude of the electron density on the positron site. As the screening length is usually short, this enhancement factor can be well described in a local density approximation (LDA). In this scheme, the pile-up of the electrons corresponds to a homogeneous electron gas with a density depending on the unperturbed electron density at the position of the positron. It turns out that, in spite of strong enhancement, the momentum density $\rho^{2\gamma}(\mathbf{p})$ seen by the positron is reasonably well described by the independent-particle model (IPM) approximation. Moreover the position of the discontinuities in $\rho^{2\gamma}(\mathbf{p})$ due to the Fermi surface is not shifted by the electron-positron (e^-e^+) correlation effects (Majumdar 1965). On the other hand, the calculated positron lifetimes are very sensitive to the enhancement term and so constitute a crucial test for the theory.

Several models for the e^-e^+ interaction in the jellium have been proposed. In each case, the basic idea is to consider that the positron polarizes the homogenous electron gas of density n , leading to a net increase of the electronic density at the site of the positron to $n + \Delta n$. The enhancement factor is then defined as

$$\gamma = 1 + \Delta n/n. \quad (1)$$

As a function of the electron-gas parameter r_s (defined as $(4/3)\pi r_s^3 = 1/n$), Brandt and Reinheimer (1971) have proposed for γ the following expression obtained in the RPA:

$$\gamma = 1 + (r_s^3 + 10)/6. \quad (2)$$

This enhancement factor is valid in the range $2 \leq r_s \leq 6$. Using another theory (boson formalism), Arponen and Pajanne (1979) have described the collective excitations due to a positron immersed in a homogenous electron gas together with the electronic density around the positron. The theory of the Fermi liquid in the hypernetted-chain (HNC) approximation has been used by Kallio *et al* (1982) to study the problem of a charged impurity in the electron gas. This theory has been further improved by Gondzik and Stachowiak (1985) for the positron case. Very similar to the Brandt-Reinheimer formula is the expression proposed by Boronski and Nieminen (1985), interpolated from Fermi liquid results (Chakraborty and Pietiläinen 1982):

$$\gamma = 1 + 1.23r_s + 0.8295r_s^{3/2} - 1.26r_s^2 + 0.3286r_s^{5/2} + \frac{1}{6} r_s^3. \quad (3)$$

Jarlborg and Singh (1987) have obtained their enhancement factor by solving a two-body e^-e^+ Schrödinger equation inside a spherical correlation cell. This model has already been tested by comparison with experimental 2D ACAR (two-dimensional angular correlation of the annihilation radiation) distributions. Analysis of ACAR data has also motivated the introduction of more general enhancement factors which include momentum or energy dependence (Sormann and Puff 1985, Daniuk *et al* 1987, Jarlborg *et al* 1991). These factors are derived from the well known Kahana (1963) formalism based on the resolution of Bethe-Goldstone equations.

As mentioned above, the Jarlborg-Singh approach for the e^-e^+ correlation effects has been confronted with 2D ACAR experimental data. But the influence of these effects is less pronounced in ACAR than in lifetime calculations. Moreover ACAR data consist of relative distributions which prevent an unambiguous scaling of the enhancement factor. To get an initial test of this approach, which is a parameter-free and computationally efficient method, we have performed lifetime calculations, starting from simple materials and then generalizing to more complicated compounds, keeping the same enhancement factor for all electrons (including the core electrons).

2. Method

In the present local density scheme, the positron annihilation rate $\lambda = 1/\tau$ can be expressed as an overlap between the positron and the electron density through the simple relation (see for example Boronski and Nieminen 1985):

$$\lambda = \pi r_e^2 c \int |\psi_+(r)|^2 n(r) \gamma(r) d^3r \quad (4)$$

where r_e is the classical electron radius, c the speed of light, $n(r)$ and $|\psi_+(r)|^2$ the electron and the positron density and $\gamma(r)$ an enhancement factor which is related to the e^-e^+ pair correlation function $g(r, r')$ by

$$\gamma(r) = g(r, r) \quad (5)$$

The enhancement factor γ tested in this work has been proposed by Jarlborg and Singh (1987) for 2D ACAR calculations in transition metals. It is obtained by solving a two-body problem (a positron and an electron) in a local scheme. The two particles are considered as interacting inside a sphere of radius r_s (depending on the local

density). The value of r_s defines the mean radius of an exchange–correlation hole around the electrons. The e^-e^+ interaction is then described in the LDA as an impurity problem defined inside a Wigner–Seitz sphere of radius r_s . Previously, the reduced mass μ of the system has been treated as a free parameter. Here we take the natural choice $\mu = 1/2$. This leads to γ -values that are close to the improved Kahana solutions calculated by Rubaszek *et al* (1984) in the case of the homogeneous electron gas.

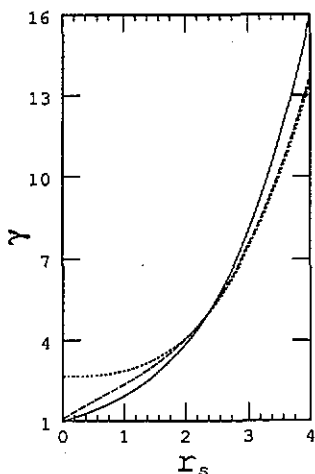


Figure 1. The enhancement factor γ as a function of the electron-gas parameter r_s for the three different models presented in the text. Short-dashed line: Brandt–Reinheimer formula. Dashed line: Boronski–Nieminen formula. Solid line: Jarlborg–Singh approach.

In figure 1 we compare the Jarlborg–Singh (JS) enhancement factor $\gamma(r_s)$ with that obtained using the Brandt–Reinheimer (BR) and the Boronski–Nieminen (BN) formulae. The latter two ensure the proper behaviour for the positronium limit ($r_s \rightarrow \infty$). This is not the case for the JS approach which was initially conceived for the density range of transition metals and this explains some shortcomings at low densities (see below). However, the method is sufficiently general to allow further improvement. Near $r_s = 2$ all the models predict almost the same result. For smaller r_s -values (corresponding to core densities), the BR curve is much higher than the others. This may explain why the use of this formula requires separate treatment of the core states in order to fit the experimental data (Puska and Nieminen 1983).

After the electron density is known, the potential seen by the positron is constructed as

$$V^+(r) = V_{\text{test}}(r) + V_c(r) \tag{6}$$

where V_{test} is the potential for a positron as a test charge and where V_c is the correlation potential describing the positron perturbation. The correlation potential represents the electronic polarization due to the positron impurity and can be written via the Hellmann–Feynman theorem (Hodges and Stott 1973) as

$$V_c(r) = - \int_0^1 dZ \int d^3r' \frac{n(r')(g(r, r', Z) - 1)}{|r - r'|} \tag{7}$$

where $n(r')(g(r, r', Z) - 1)$ is the screening cloud density around a positron with fractional charge Z . When V_c is included in our calculations we use the parametrization proposed by Boronski and Nieminen (1985). In the LDA picture the e^-e^+ (Boronski and Nieminen 1985) and the electron-electron (Vosko *et al* 1980) correlation potentials vary slowly in the region of valence electrons. This would be also the case in a non-local density theory since the effect of the non-locality is to average $n(r)$ over the region of the screening cloud. Therefore in simple materials the positron wave function shape is mainly determined by the repulsive interaction with the positive ion charge and the polarization effects due to the positron play only a minor role. A similar conclusion was reached by Pennetta and Baldereschi (1989) in Si using a different approach.

The self-consistent calculation of the electronic structure has been performed using the LMTO method. The potentials and the charge densities are spherical averages inside Wigner-Seitz spheres centred both at nuclei and, in the case of open structures, at interstitial sites (the so-called empty spheres). The electron charge density is evaluated self-consistently and relativistic effects, except spin-orbit coupling, are always included for the valence states. The core states are fully relativistic and, in achieving self-consistency, the core states are not frozen. The positron states are calculated using the same LMTO method. The positron potential is taken as the inverse of the electron Coulomb potential, except for in some test cases where the LDA V_c is used. The positron is assumed to be thermalized when annihilating and its wave function is then calculated only at $k = 0$. Previously Singh and Jarlborg (1985) had applied LMTO for calculations of positron states in bulk materials. They showed that this method describes well the momentum distribution in the first Brillouin zone (BZ) but that for the Umklapp processes an overlap correction is needed. In simple metals, comparing positron wave functions for different potentials (with and without the correlation term) shows minor differences, meaning that the positron wave function is mainly determined by the repulsive interaction with the nuclear charge. However, in CoSi_2 Garreau *et al* (1991) have observed that when the potential contains the correlation term then the empty sphere loses a significant amount of charge. The positron charge transfer seems too drastic for an improvement and this is confirmed by our lifetime calculations (see below). Thus our conclusion is that with the LMTO method, e^-e^+ correlation potential may give some incorrect charge transfer from empty to atomic spheres in the case of compounds. The effect of the e^-e^+ correlation potential has also been studied with FLAPW (full potential linear APW) method by Singh *et al* (1989) in the copper oxides.

In the present lifetime calculations all electrons are treated in the same way and the JS LDA enhancement factor $\gamma(r_s(r))$ is used. For previous comparison with 2D ACAR experimental results (Jarlborg and Singh 1987, Garreau *et al* 1991), the dependence on the reduced mass μ (of the e^-e^+ system) has been tested without a definite answer being obtained. Here we have taken $\mu = 1/2$ which is the natural choice for interactions between two free particles of equal mass. Using $\mu = 1$ gives lifetimes that are much too small. For instance in 3d transition metals the lifetimes calculated using $\mu = 1$ amount to about 35 ps, without significant variation. This corresponds to values three or four times smaller than those from the experiment. So large a disagreement is not observed in a 2D ACAR analysis.

Our lifetime calculations are similar to those (also using LMTO formalism) tested by Puska *et al* (1986) in Al, Si and GaAs for bulk and vacancy positron lifetimes. However, these authors have divided the total annihilation rate into two components

(due to valence and core electrons), following the prescription given by Puska and Nieminen (1983). This requires the use of the BR enhancement factor for valence *s* and *p* electrons and of a constant factor $\gamma = 1.5$ for core and *d* valence electrons (in the case of transition metals). Jensen (1989) has shown that it is not necessary to treat core and valence electrons separately and has given a prescription where the BN LDA enhancement factor is used. His calculated positron lifetimes has been obtained using non-self-consistent electron densities. Very recently Puska (1991) has used the same prescription with LMTO self-consistent electron structures, but in the frozen-core approximation.

3. Results and discussion

The lifetimes calculated in several bulk materials are presented in table 1 together with the corresponding experimental values collected by Seeger *et al* (1989), together with those for Ce (Boring *et al* 1983), CoSi₂ (Garreau *et al* 1991), MgO and NiO (Forster *et al* 1989). For the calculated values, both JS and BN enhancement factors are used. In order to get a uniform picture of our results, we give in this table only the lifetimes obtained without including the correlation potential of Boronski and Nieminen as discussed above. The overall agreement between experiment and theory is good, particularly when considering that these calculated values result from a fully *ab initio*, all-electron approach.

The best results for the JS factor concern the 3d transition metals (V, Cr, Fe, Ni), the noble metals (Cu, Ag, Au) and metals with filled *d* shells (Zn, Pb). Both JS and BN calculations predict that Nb (4d) and Ta (5d) positron lifetimes should be longer than the V (3d) one, but this effect is not confirmed by the experiment. We notice a similar discrepancy for Cr (3d) as against Mo (4d) and for Ni (3d) as against Pd (4d).

The disagreement exhibited by the alkali metals is much more pronounced and is explained by their very low electronic density. At these densities the JS method overestimates the Coulomb cusp near the positron (see figure 1), leading to annihilation rates that are much too high. This effect becomes more and more dramatic when going from Li to Cs (i.e. to lower electronic densities).

We have compared the JS and BN lifetime values with the corresponding ones (still in the LDA) obtained by applying to all the electrons the IPM ($\gamma = 1$) and the BR enhancement. This is illustrated in table 2 by the results obtained for Cs (alkali), V (3d transition metal), Pd (4d), Pt (5d) and γ -Ce (4f rare earth). This table reflects the differences noted in the enhancement curves of figure 1. It also shows the influence of the LDA correlation potential V_c : the lifetimes calculated by including the correlation potential are systematically lower than when it is neglected. When we consider the positron wave function obtained with $V_c \neq 0$ and the BN enhancement factor, our calculated lifetimes compare well with those of Jensen (1989), who used a non-self-consistent method. The corresponding values of Puska (1991), who determined the valence states self-consistently but with a frozen core, agree better with the experiment. Recently, Daniuk *et al* (1991) showed that the core positron annihilation characteristics can be sensitive to various details of the electron and positron models. Moreover the effect of the self-consistency should be more appreciable in compounds where important charge transfers occur, rather than in simple metals.

Coming back to table 1, one can notice the good agreement between experimental and calculated lifetimes for Al and Pb. In contrast, the calculations fail for Ce. The

Table 1. Bulk positron lifetimes (in ps) calculated for different materials using the Jarlborg–Singh (JS) and the Boronski–Nieminen (BN) approach together with the corresponding experimental values (Expt.). The experimental values are from Seeger *et al* (1989) or ^a Boring *et al* (1983), ^b Garreau *et al* (1991), and ^c Forster *et al* (1989). The crystal structure and the volume per atom used in the calculations (normalized to the Bohr's volume) are also given. No electron–positron correlation potential has been included in the calculations.

Element	Structure	Volume per atom	τ (ps)		
			JS	BN	Expt.
Li	BCC	34.0	281	299	291
Na	BCC	60.7	287	328	338
K	BCC	114.9	271	374	397
Rb	BCC	140.1	266	383	406
Cs	BCC	177.8	246	394	418
V	BCC	22.4	128	115	130
Cr	BCC	19.2	112	99	120
Fe	BCC	18.9	113	101	106
Ni	FCC	17.5	108	96	110
Cu	FCC	19.0	119	107	110
Zn	HCP	24.2	146	133	148
Nb	BCC	29.0	134	121	119
Mo	BCC	25.2	117	104	103
Pd	FCC	23.5	115	102	96
Ag	FCC	27.5	136	123	131
Ta	BCC	29.1	128	116	116
W	BCC	25.5	111	99	105
Pt	FCC	24.3	107	94	99
Au	FCC	27.2	122	109	117
Al	FCC	26.7	174	163	163
Pb	FCC	47.4	194	184	194
α -Ce	FCC	45.7	180	171	232 ^a
γ -Ce	FCC	55.4	208	197	235 ^a
C	Diamond	9.1	101	88	115
Si	Diamond	32.3	207	202	219
Ge	Diamond	36.5	211	209	230
α -Sn	Diamond	55.0	231	245	289
GaAs	ZnS	36.1	211	211	231
GaP	ZnS	32.6	202	197	223
CoSi ₂		20.7	152	141	155 ^b
MgO	NaCl	15.1	134	121	155 ^c
NiO	NaCl	14.9	119	107	110 ^c

explanation is probably related to the difficulties encountered in the band methods in describing this rare-earth element. In the light of LMTO calculations and 2D ACAR measurements in γ -Ce, Jarlborg *et al* (1989) proposed that the position of the f states relative to the Fermi level should be different from what is obtained in LDA.

In the case of semiconductors, the experimental lifetimes are 10 to 20 ps higher than the calculated values. This could be corrected to some extent if gap corrections were taken into account: Puska *et al* (1986) predict an increase of about 10 ps for the lifetimes calculated including the effect of the gap. In the open part of the unit cell the diamond structure contains two empty spheres whose density decreases with

Table 2. The Jarlborg–Singh (JS) and Boronski–Nieminen (BN) lifetime values (in ps) are compared with the corresponding ones (still in the LDA) obtained by applying to all the electrons the IPM ($\gamma = 1$) and the Brandt–Reinheimer (BR) factors. For the JS and BN cases, the influence of the Boronski and Nieminen LDA correlation potential V_c is shown.

	Cs	V	Pd	Pt	γ -Ce
IPM	5466	359	301	273	861
BR	401	106	92	85	196
BN	394	115	102	94	200
BN and $V_c \neq 0$	383	113	100	93	194
JS	246	128	115	107	208
JS and $V_c \neq 0$	245	126	113	105	204
Experiment	418	130	96	99	235

increasing unit cell volume. As for alkali metals, the annihilation rate calculated by JS is overestimated in low-density regions ($r_s > 3$). This is illustrated by the case of α -Sn which is a metal of low density in the interstitial region and for which the BN approach is more appropriate than the JS one. On the other hand diamond is at the high- r_s limit and the JS factor gives a good result.

Concerning the metal oxides, we notice a good agreement for NiO, but in the case of MgO a gap correction seems to be needed. To end the overview of table 1, we notice the good result obtained for CoSi₂ when the JS factor is used. In this compound the silicon atoms form a diamond-like lattice, with Co on one of the two empty sites. Including the LDA correlation potential V_c for the positron drastically modifies the calculated lifetime: τ falls from 155 ps to 119 ps. As we mentioned previously, this effect is due to the fact that the correlation potential drastically reduces the amount of positron charge in the empty sphere. Calculations with different reduced masses in the JS approach have already been confronted with the corresponding experimental 2D ACAR results (Garreau *et al* 1991). As regards lifetime ($\tau = 30$ ps when using $\mu = 1$), the 2D ACAR analysis favours the enhancement factor obtained with a reduced mass $\mu = 1/2$. But in 2D ACAR the discrimination is not so clear.

As the experimental lifetimes of table 1 have been measured at different temperatures, we have estimated the influence due to the volume variations on the τ calculated by JS. This is shown in figure 2 where the lifetime values calculated for V, diamond and Ce are reported as functions of the lattice parameter. We deduce an increase of lifetime of about 1 ps for V over a 300 K temperature range and even less for diamond. A similar study has been reported by Gupta and Siegel (1977) for Al. This value of 1 ps is comparable to the time needed by the positron to thermalize (Perkins and Carbotte 1970). Therefore if there is a small difference between the effective lattice parameter and the one used in the calculation, the resulting error remains within the experimental uncertainty. It is quite satisfactory to see the rather small spread of different calculations of τ in high-density materials. The results of Jensen (1989), Puska (1991) and our results (using BN or JS enhancement) give acceptable values in view of experimental uncertainty in τ .

The calculations for Ce have been motivated by the fact that in this element an isostructural γ - α phase transition, accompanied by a large ($\sim 18\%$) volume contraction, occurs for temperatures lower than 100 K (at atmospheric pressure) or for pressures higher than 8 kbar (at room temperature). The calculations predict a

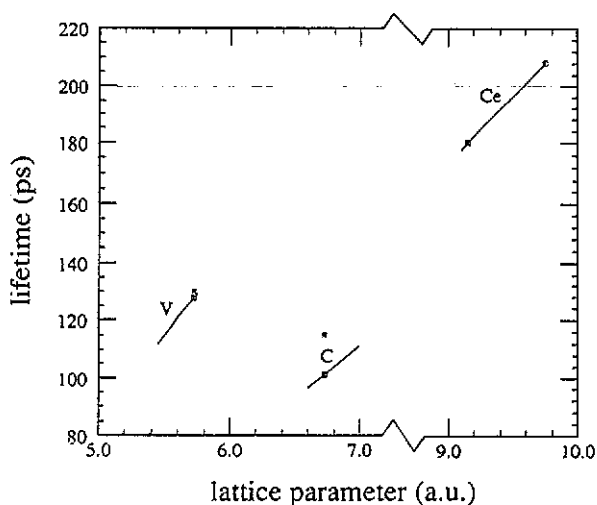


Figure 2. Bulk lifetimes calculated in the Jarlborg-Singh approach for V, diamond and Ce as a function of the lattice parameter a . At room temperature the values of a used in the calculations and represented by a square on the graph are 5.72 for V, 6.73 for diamond, 9.15 for α -Ce and 9.75 for γ -Ce (atomic units). The experimental values are indicated by asterisks for V and diamond. In the case of Ce, the experimental values fall outside the figure and it is not yet clear whether the γ - α transition can be seen experimentally from the positron annihilation lifetime.

significant effect on the lifetime due to the volume contraction alone (see table 1). Experimental values reported by Boring *et al* (1983) have shown a constant mean lifetime of 233 ps in both phases. These authors conclude that positron annihilation is insensitive to the electronic γ - α transition in Ce. This conclusion is, however, in conflict with the results of Gustafson *et al* (1969) and of Bharathi *et al* (1987) who found a lifetime in α -Ce about 8% shorter than in γ -Ce.

4. Conclusion

We have computed bulk lifetimes in different materials using the self-consistent LMTO method. In order to include e^-e^+ correlation effects in the calculation of the annihilation rates, we have considered the enhancement factor calculated within the LDA proposed by Jarlborg and Singh (1987). This enhancement factor has been applied identically to all electrons (valence and core), making the approach very general. The motivation of this work was to test the JS model with the aim of being able to apply it confidently to 2D ACAR analysis. The result is that these enhancement factors can be used for rather dense metallic systems using $\mu = 1/2$. The question of whether a reduced mass $\mu = 1$ or $\mu = 1/2$ should be used in the determination of the enhancement factor has been unambiguously answered by these lifetime calculations, which was not the case with ACAR results.

For high-density systems (in particular for 3d transition metals, CoSi_2 and diamond) the agreement between the calculated lifetimes and the corresponding experimental values is better when the JS enhancement factor is used. The BN approach is certainly more appropriate for low-density systems like the alkali metals. In view of

these results one should obtain the best overall agreement by always using the lowest enhancement factor $\gamma(r_s) = \min(\gamma_{JS}(r_s), \gamma_{BN}(r_s))$. In this way the high-density factors of JS would be replaced at low density by the BN factors, thus ensuring the correct positronium limit. Such semi-empirical calculations are under way and will be presented elsewhere (Barbiellini *et al* 1991).

In Ce the experimental situation is not yet clear and further theoretical improvements for correlations of *f* electrons are also needed. The results obtained in semiconductors could be improved by including gap corrections in the calculations as suggested by Puska *et al* (1986). The lifetimes obtained in CoSi₂ and in NiO are encouraging for further *ab initio* calculations in more complicated materials like the copper oxides (Jarlborg *et al* 1991).

Acknowledgments

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References

- Arponen J and Pajanne E 1979 *J. Phys. F: Met. Phys.* **9** 2359
- Barbiellini B, Genoud P, Lerch P, Jarlborg T and Peter M 1991 *Positron Annihilation, Proc. ICPA9 (Szombathely, Hungary, 1991)* (Aedermannsdorf: TransTech) submitted
- Bharathi A, Gopinathan K P, Sundar C S and Viswanathan B 1987 *Theoretical and Experimental Aspects of Valence Fluctuations and Heavy Fermions* ed L C Gupta and S K Malik (New York: Plenum) p 641
- Boring A M, Huang C Y, Gschneider K A, McGervey J D, Panigrahi M and Usmar S G 1983 *J. Magn. Magn. Mater.* **37** L7
- Boronski E and Nieminen R N 1985 *Phys. Rev. B* **34** 3820
- Brandt W and Reinheimer J 1971 *Phys. Lett.* **35A** 109
- Chakraborty T and Pietiläinen P 1982 *Phys. Rev. Lett.* **49** 1034
- Daniuk S, Kontrym-Sznajd G, Rubaszek A, Stachowiak H, Mayers J, Walters P A and West R N 1987 *J. Phys. F: Met. Phys.* **17** 1365
- Daniuk S, Šob M and Rubaszek A 1991 *Phys. Rev. B* **43** 2580
- Forster M, Mundy J N and Schaefer H E 1989 *Positron Annihilation, Proc. ICPA8* ed L Dorikens *et al* (Singapore: World Scientific) p 833
- Garreau Y, Lerch P, Jarlborg T, Walker E, Genoud P, Manuel A A and Peter M 1991 *Phys. Rev. B* **43** 14532
- Gondzik J and Stachowiak H 1985 *J. Phys. C: Solid State Phys.* **18** 5399
- Gupta R P and Siegel R W 1977 *Phys. Rev. Lett.* **39** 1212
- Gustafson D R, McNutt J D and Roellig L O 1969 *Phys. Rev.* **183** 435
- Hodges C H and Stott M J 1973 *Phys. Rev. B* **7** 73
- Jarlborg T, Barbiellini B, Boronski E, Genoud P and Peter M 1991 *J. Phys. Chem. Solids* at press
- Jarlborg T, Manuel A A, Peter M, Sanchez D, Singh A K, Stephan J-L, Walker E, Asmuss W and Hermann M 1989 *Positron Annihilation, Proc. ICPA8* ed L Dorikens *et al* (Singapore: World Scientific) p 266
- Jarlborg T and Singh A K 1987 *Phys. Rev. B* **36** 4660
- Jensen K O 1989 *J. Phys.: Condens. Matter* **1** 10595
- Kahana S 1963 *Phys. Rev.* **129** 1622
- Kallio A, Pietiläinen P and Lantto L 1982 *Phys. Scr.* **25** 943
- Majumdar C K 1965 *Phys. Rev. A* **140** 227
- Pennetta C and Baldereschi A 1989 *Positron Annihilation, Proc. ICPA8* ed L Dorikens *et al* (Singapore: World Scientific) p 693

- Perkins A and Carbotte J P 1970 *Phys. Rev. B* **1** 101
- Puska M J 1991 *J. Phys.: Condens. Matter* **3** 3455
- Puska M J, Jepsen O, Gunnarsson O and Nieminen R N 1986 *Phys. Rev. B* **34** 2695
- Puska M J and Nieminen R N 1983 *J. Phys. F: Met. Phys.* **13** 333
- Rubaszek A, Stachowiak H, Boronski E, Szotek Z 1984 *Phys. Rev. B* **30** 2490
- Seeger A, Banhart F and Bauer W 1989 *Positron Annihilation, Proc. ICPA8* ed L Dorikens et al (Singapore: World Scientific) p 275
- Singh A K and Jarlborg T 1985 *J. Phys. F: Met. Phys.* **15** 727
- Singh D, Pickett W E, Cohen R E, Krakauer H and Berko S 1989 *Phys. Rev. B* **39** 9667
- Sormann H and Puff W 1985 *Positron Annihilation, Proc. ICPA7* ed P C Jain et al (Singapore: World Scientific) p 161
- Vosko S H, Wilk L and Nusair M 1980 *Can. J. Phys.* **58** 1200