

Positron effective mass in silicon

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The positron effective mass in Si is obtained from the first-principles calculations along various crystallographic directions. The effect of electron-positron correlation on the band mass is examined in this work. A positron pseudopotential scheme is worked out to calculate the isotropic band mass without explicitly solving the band energy. The effective mass $1.46m$ obtained as a sum of band mass and the positron-plasmon interaction compares very well with $1.5m$ obtained from the positron mobility data.

I. INTRODUCTION

The positron in a semiconductor, in analogy with the hole, may be considered as a carrier of positive charge. Apart from its shorter annihilation time (100–300 ps), the few diffusion studies that have been made so far show it to be considerably less mobile than its hole counterpart. This largely arises from the positron's higher effective mass. This mass for Ge was measured by Shullman *et al.* using one-dimensional angular correlation.¹ These workers found a value of $(1.23 \pm 0.17)m$. Working from positron diffusion data, Mäkinen has estimated a value of $(1.5 \pm 0.1)m$ in Si.² Such values are typically ten times those of holes in these semiconductors³ giving rise to acoustic phonon limited mobilities some 100 times smaller through the expected $m^{*-5/2}$ dependence.⁴

The longitudinal acoustic phonon mobility is related to the positron deformation potential and the effective mass through the Bardeen and Shockley formula.⁴ With an accurate value of the positron deformation potential, it is possible to extract the effective mass from these experimental positron mobility (diffusivity) data. Unfortunately there is no accurate method for obtaining the positron deformation potential experimentally. While temperature-dependent positronium work function measurements can in principle yield the deformation potential,^{5,6} the correction for the lattice vibration effect must be obtained from theory and is difficult to compute.⁷ Alternatively E_d can be obtained theoretically.⁸ Using a theoretical deformation potential of -6.19 eV the positron effective mass was found to be $(1.5 \pm 0.1)m$ in Si.² The reliability of this procedure in determining the positron effective mass depends on the accurate estimation of the positron deformation potential. In addition, this method also requires the positron mobility data to be not only free from easily made systematic errors^{9,10} but also limited only by acoustic phonon scattering. The latter condition puts high demands on sample purity because in the low temperature regime positrons not only scatter from impurities but also shallow trap onto ionized acceptors.¹¹

With positron effective masses inferred from mobility data being subject to many systematic errors, direct the-

oretical estimation of the positron effective mass has become quite essential for studying positron diffusion in semiconductors. The band effect, phonon scattering, and positron-plasmon interaction are responsible for changing the positron mass from its bare mass. In metals the band effective mass is close to the bare mass.¹² However, phonon scattering¹³ and the effect of the positron-plasmon contribution¹⁴ have significant effects. With regard to semiconductors, however, there exists practically no such calculation to determine the positron effective mass. The motivation of the present work is to find the effective mass in Si as a test case.

We have used the two-component density functional theory to calculate the positron crystal potential.¹⁵ We have assumed only one positron in a many-electron system. For calculating the anisotropic positron effective mass we have used the full potential in the frozen-core approximation for solving the positron band structure. Moreover, a scheme has been developed to calculate the positron pseudopotential which will yield an isotropic band mass without calculating the positron band structure explicitly.

II. THEORY

The positron potential in the framework of the two-component density functional theory with one positron in a many-electron system is given by¹⁵

$$V_+(\mathbf{r}) = V_{\text{ion}}^+(\mathbf{r}) - e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r' + V_{\text{corr}}(\rho(\mathbf{r})), \quad (2.1)$$

where V_{ion}^+ is the positron ionic potential. The valence electron charge density $\rho(\mathbf{r})$ is obtained from the norm-conserving pseudopotential theory where the ionic pseudopotentials are taken from Ref. 16. In the pseudopotential calculation the exchange-correlation energy is taken as the Ceperly and Alder type with the parametrization of Perdew and Zunger.^{17,18} The second term in Eq. (2.1) represents the electron-positron Coulomb potential. The electron-positron correlation potential (V_{corr}) is cal-

culated in the local density approximation.^{19,20}

The positron-ion interaction potential is calculated in the frozen-core approximation which assumes that the core electrons are not polarized by the positron.²² With the core charge density $\rho_c(\mathbf{r})$ calculated employing Roothan-Hartree-Fock wave functions,²³ the ionic potential is given by

$$V_{\text{ion}}^+(\mathbf{r}) = \sum_{\mathbf{R}} [V^+(\mathbf{r} - \mathbf{R} - \boldsymbol{\tau}) + V^+(\mathbf{r} - \mathbf{R} + \boldsymbol{\tau})] , \quad (2.2)$$

where the \mathbf{R} are the nuclear positions of Si, $\boldsymbol{\tau} = (a/8)(1, 1, 1)$, a being the cubic lattice constant, and

$$V^+(\mathbf{r}) = \frac{Ze^2}{|\mathbf{r}|} - e^2 \int \frac{\rho_c(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' , \quad (2.3)$$

where Z is the atomic number of Si. The electron-positron correlation energy in Si is given by

$$V_{\text{corr}}(r) = V_{\text{corr}}^{\text{EG}}(\rho(\mathbf{r})) [f(\epsilon_g, \rho(\mathbf{r}))]^{1/3} , \quad (2.4)$$

where $V_{\text{corr}}^{\text{EG}}$ is the correlation energy for a positron in a homogenous electron gas¹⁹ and $f(\epsilon, \rho(\mathbf{r}))$ is a factor taking into account that the screening is reduced in a semiconductor due to its band gap. In the above equation ϵ_g is the "gap parameter" connected to the band gap (E_g) and Fermi energy (E_F) as E_g/E_F . In the random phase approximation f is given by²⁰

$$f(n, e_g) = 1 - \frac{0.37\epsilon_g}{1 + 0.18r_s} . \quad (2.5)$$

Here $r_s = [\frac{3}{4\pi n}]^{1/3}$. Puska *et al.*²¹ have treated ϵ_g as a free parameter in their positron lifetime calculation and found that the calculation reproduces the experimental bulk lifetimes in most semiconductors when $\epsilon_g = 0.2$. Finally the positron energies are calculated at different \mathbf{k} points in the irreducible part of the Brillouin zone and the positron band masses are obtained by fitting parabolas to the positron band energies calculated in the vicinity of the Γ_1 point along different crystallographic axes.

Kubica and Stott have defined the positron pseudopotential from the full ionic potential and calculated the isotropic positron effective mass of aluminum without calculating the positron band structure in detail.²⁴ Chakraborty and Siegel have modified this scheme to calculate the positron pseudopotential.²⁵ They have fitted the Appelbaum-Hamann form of the pseudopotential²⁶ to the full ionic potential at the Wigner-Seitz sphere to obtain the positron pseudopotential. We have used the same procedure with the positron pseudopotential in the form²⁷

$$V_{\text{ps}}(\mathbf{r}) = \frac{Z_v e^2}{r} \text{erf}\left(\frac{r}{r_c}\right) . \quad (2.6)$$

It is to be mentioned here that Bachelet *et al.*¹⁶ used both Eq. (2.6) and the Appelbaum-Hamann form of the potential to construct the electron nonlocal pseudopo-

tential. A thermalized positron is represented by the $l = 0$ state. Therefore we have avoided the Appelbaum-Hamann form of the pseudopotential which gives the nonlocal contributions. Since both the ionic potential defined in Eq. (2.1) and the pseudopotential V_{ps} have the same $\frac{Z_v e^2}{r}$ dependence at high r , it is easy to obtain the ionic radius r_c by fitting both the potentials at the Wigner-Seitz sphere radius in the same way as done by Chakraborty and Siegel. With the ionic positron pseudopotential being small the ordinary second-order perturbation scheme can be applied to determine the energy eigenvalues without solving the positron band structure. We describe the scheme in the following. For the lowest eigenvalue

$$\begin{aligned} E(\mathbf{k}) &= \frac{\hbar^2 \mathbf{k}^2}{2m} + \langle \mathbf{k} | V_{\text{ps}} | \mathbf{k} \rangle \\ &+ \sum_{\mathbf{G} \neq 0} \frac{|\langle \mathbf{k} | V_{\text{ps}} | \mathbf{k} + \mathbf{G} \rangle|^2}{\hbar^2/2m[\mathbf{k}^2 - (\mathbf{k} + \mathbf{G})^2]} \\ &= \frac{\hbar^2 \mathbf{k}^2}{2m} + V_{\text{ps}}(0) - \sum_{\mathbf{G} \neq 0} \frac{|V_{\text{ps}}(\mathbf{G})|^2}{\hbar^2/2m[\mathbf{G}^2 + 2\mathbf{k} \cdot \mathbf{G}]} , \end{aligned} \quad (2.7)$$

where

$$\begin{aligned} V_{\text{ps}}(\mathbf{G}) &= \frac{4\pi e^2}{\Omega_{\text{at}} G^2} \sum_{\alpha} Z_{\alpha} \exp(-\frac{1}{4} r_{\alpha}^2 G^2) S_{\alpha}(\mathbf{G}) \\ &- \frac{4\pi e^2 \rho(\mathbf{G})}{G^2} + V_{\text{corr}}(\mathbf{G}) , \end{aligned} \quad (2.8)$$

where $S_{\alpha}(\mathbf{G}) = \exp(i\mathbf{G} \cdot \boldsymbol{\tau}_{\alpha})/N_{\alpha}$ is the structure factor, N_{α} being the number of basis atoms. The above equation takes the electron charge density from a pseudopotential band structure calculation. Since the positron wave function is not very sensitive to the accuracy of the valence charge density the electron charge density can also be calculated from the superposition of the free-atom model thus eliminating the need for any band structure calculation. With the positron band mass evaluated close to the center of the Brillouin zone, the quantity $(\mathbf{G}^2 + 2\mathbf{k} \cdot \mathbf{G})^{-1}$ can be expanded using the binomial theorem:

$$\begin{aligned} E(\mathbf{k}) &= V(0) - \sum_{\mathbf{G} \neq 0} \frac{|V_{\text{ps}}(\mathbf{G})|^2}{G^2} + \frac{\hbar^2 \mathbf{k}^2}{2m} \\ &\times \left[1 - 4 \sum_{\mathbf{G} \neq 0} \left\{ \frac{|V_{\text{ps}}(\mathbf{G})| \cos \theta}{\hbar^2 G^2/2m} \right\}^2 + \dots \right] \end{aligned} \quad (2.9)$$

where $\cos \theta = \frac{\mathbf{k} \cdot \mathbf{G}}{kG}$. Following the definition of the band effective mass, we obtain

$$\frac{m_b}{m} = \left[1 - 4 \sum_{\mathbf{G} \neq 0} \frac{|V_{\text{ps}}(\mathbf{G})|^2 \cos^2 \theta}{\{\hbar^2 G^2/2m\}^2} \right]^{-1} . \quad (2.10)$$

Substituting $\cos^2 \theta = \frac{1}{3} + \frac{2}{3} P_2(\cos \theta)$ (P_2 is the second Legendre polynomial) and averaging, we find that

$$\frac{m_b}{m} = 1 + \frac{4}{3} \sum_{\mathbf{G} \neq 0} \left\{ \frac{|V_{\text{ps}}(\mathbf{G})|}{\hbar^2 G^2/2m} \right\}^2 . \quad (2.11)$$

The summation over $P_2(\cos \theta)$ is zero because the potential $V_{ps}(\mathbf{G})$ has cubic symmetry at Γ_1 .

III. RESULTS AND DISCUSSIONS

The *ab initio* pseudopotential calculation was carried out using 300 plane waves exactly and another 400 plane waves treated in the second-order perturbation scheme. The positron band structure using the frozen-core approximation was solved using 500 plane waves.

Aourag *et al.* have calculated the positron band structure in the point-core approximation using the charge density obtained from an empirical pseudopotential calculation.²⁸ However, the positron band structure obtained by Pennetta and Baldereschi in the frozen-core approximation is quite different from that obtained in the point-core approximation.²² Neither group took the contribution of the electron-positron correlation potential into account. Pennetta and Baldereschi considered the contribution of the valence electron polarization term.

In order to resolve the difference we have plotted the positron energy bands in Fig. 1 with and without the electron-positron correlation potential. Since the average value of the potential energy is assumed to be zero in our calculation, the absolute position of the bands is not meaningful in making comparisons with earlier cal-

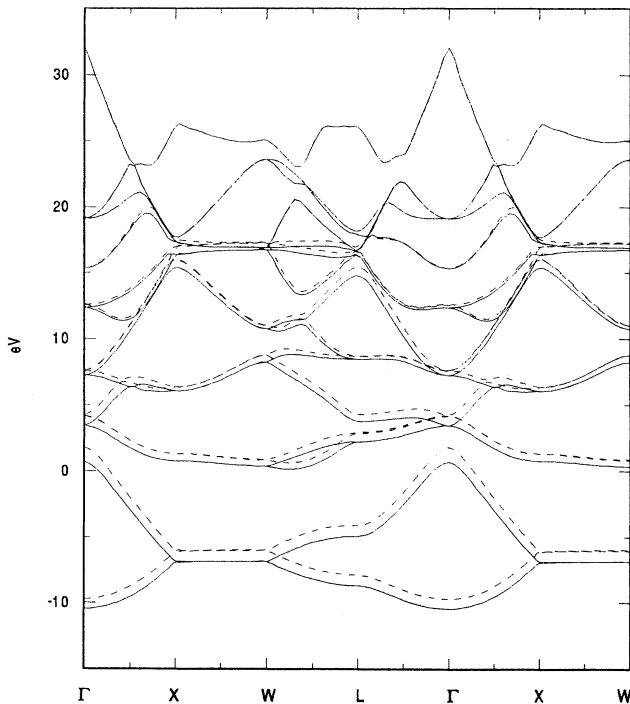


FIG. 1. Positron band structure of Si in the frozen-core approximation, without correlation potential (—) and with correlation potential (---).

culations. The present calculation has quantitative disagreement with both Aourag *et al.* and Pennetta and Baldereschi. Our calculation is seen to be qualitatively similar to the calculation of Aourag *et al.* The difference between the two calculations arises from the fact that they used the point-core approximation to express the positron ionic potential while we have used the frozen-core approximation. It is surprising to observe that our data are different from those of Pennetta and Baldereschi although we have adopted their method in the present calculation. The effect of the electron-positron correlation potential is to raise the positions of the bands without affecting the symmetry significantly. This suggests that the electron-positron correlation potential is isotropic in Si. The effect of the correlation potential seems to systematically decrease with higher band levels. Interestingly it is found that the low lying positron band structure is quite similar to the electron band structure although the positron potential is opposite in sign to the electron potential. This similarity has been explained by Aourag *et al.* as arising from the nearly-free-electron behavior of the electron and positron in Si.

In Fig. 2 we have compared the positron wave function along the [111] direction with and without correlation effects. The present data agree well with those calculated earlier.²⁹ The positron localizes in the tetragonal sites more than in the hexagonal sites. This results from the positron experiencing a more repulsive interaction due to the nuclei at the hexagonal site than at the tetragonal site. With the inclusion of the correlation potential the repulsive potential is reduced and the positron wave function changes. The positron effective masses calculated (neglecting correlation potential) along the [100], [110], and [111] directions are $1.360m$, $1.362m$, and $1.361m$, respectively. This shows that the mass is very close to being isotropic and unlike in metals deviates significantly from the bare mass value. The effective mass becomes slightly lighter along the [100] direction because the positron is under less repulsive interaction. Recently it has been shown that the correlation potential changes the positron wave function quite significantly along certain directions in high T_c materials.^{30,31} The positron effective masses with correlation potential included along the [100], [110], and [111] directions are $1.326m$, $1.333m$, and $1.332m$, respectively. Once again little anisotropy is observed but the effective mass is lowered because the positron experiences a less repulsive field than when it is without the correlation potential.

We have used Eq. (2.11) to calculate the positron band mass. The calculated r_c value is 0.65 a.u. in the present case. The effective mass calculated from this formula is $1.30m$ which is quite close to that calculated using the band structure method described above.

The calculated effective mass is found to be lower than $1.5m$ extracted from the positron mobility data obtained by several groups.^{2,10,32} This suggests that the contribution of the positron-phonon and positron-plasmon interactions is not negligible in Si. Thermal motion of the positron is well represented by the Maxwell-Boltzmann distribution. In the presence of the positron-phonon scattering the width of this Gaussian is broadened and a tail

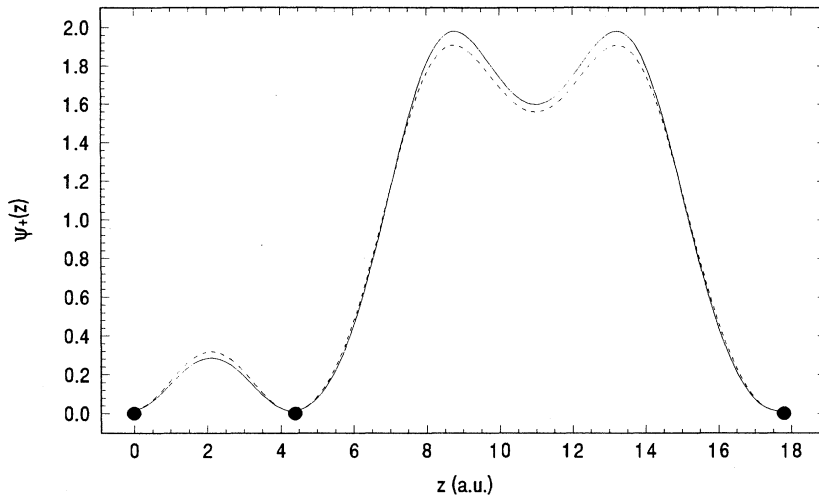


FIG. 2. Positron wave function (one positron in a unit cell) along [111] without the correlation potential (—) and with the correlation potential (---).

appears which smears the Fermi momentum cutoff in angular correlation data.¹³ In order to obtain the contribution of this effect, high precision and high resolution angular correlation data are required. Unfortunately no such data exist for Si from which the positron-phonon contribution to the effective mass can be derived.

Ishii has considered the soliton state of the positron coupled by a plasmon to calculate the positron effective mass in solids.¹⁴ In this calculation the quasiparticle, referred to as a *wakeon*, moves with a velocity such that its energy consists of the bare positron energy, the bare plasmon energy, and an interaction term. Ishii showed that the effective mass just depends on a single parameter r_s , and is given by

$$m^* = \frac{m_b}{\left[1 - \frac{5}{3}\alpha^4(m/m_b)^2 r_s/a_0\right]}, \quad (3.1)$$

where $\alpha^3 = 4/9\pi$ and a_0 is the Bohr radius. With this plasmon-phonon factor included in our calculation the effective mass becomes $1.46m$ in good agreement with that obtained from experimental data. This result suggests the contribution to the effective mass from the positron-phonon interaction is negligible. Further studies are clearly required to confirm this.

IV. CONCLUSION

The band effective mass of the positron in Si has been calculated using two first-principles methods in this paper. The first method which employs the pseudopotential scheme yields a positron band structure with positron band masses of almost equal values in the different lattice directions. The second perturbation analysis has yielded an isotropic band mass in good agreement with that obtained from the pseudopotential method, a fact which may make the simplified scheme easily extendable to other semiconductors. These calculations also have shown the effect of positron-electron correlation is not negligible as regards the band structure and band masses. Work is in progress to extend these calculations to other elemental and compound semiconductors.

In addition to the positron band mass the contributions of the positron-phonon and positron-plasmon interactions must be included to get meaningful agreement with the experiment. The fact that our calculated band masses are lower than the observed positron effective mass indicates that the sum of these effects cannot be ignored. An estimate of the positron-plasmon contribution indicates that this interaction is capable of explaining the observed discrepancy between experimental effective mass and theoretical band mass, a fact that could suggest the positron self-interaction with the phonon field is negligible.

¹ M. A. Shullman, G. M. Beardsley, and S. Berko, *Appl. Phys.* **5**, 367 (1975).

² J. Mäkinen, *Mater. Sci. Forum* **105–110**, 369 (1992).

³ *Semiconductors: Physics of Group IV Elements and III-V Compounds*, edited by O. Madelung, Landolt-Börnstein, New Series, Group III, Vol. 17, Pt. a (Springer-Verlag, Berlin, 1991).

⁴ J. Bardeen and W. Shockley, *Phys. Rev.* **80**, 72 (1950).

⁵ E. M. Gullikson and A. P. Mills, *Phys. Rev. B* **35**, 8759

(1987).

⁶ I. J. Rosenberg, R. H. Howell, and M. J. Fluss, *Phys. Rev. B* **35**, 2083 (1987).

⁷ B. K. Panda, C. D. Beling, and S. Fung, *Phys. Rev. B* **50**, 5695 (1994).

⁸ M. J. Puska, P. Lanki, and R. M. Nieminen, *J. Phys. Condens. Matter* **1**, 6081 (1989).

⁹ M. Sayed, K. O. Jensen, and A. B. Walker, *Mater. Sci. Forum* **105–110**, 811 (1992).

- ¹⁰ C. D. Beling, R. I. Simpson, M. G. Stewart, Y. Y. Wang, S. Fung, J. C. H. Wai, and T. N. Sun, *Phys. Status Solidi A* **102**, 443 (1987).
- ¹¹ H. L. Au, C. C. Ling, B. K. Panda, T. C. Lee, S. Fung, and C. D. Beling, *Phys. Rev. Lett.* **73**, 2732 (1994).
- ¹² M. J. Stott and P. Kubica, *Phys. Rev. B* **11**, 1 (1975).
- ¹³ T. Hyodo, T. McMullen, and A. T. Stewart, *Phys. Rev. B* **33**, 3050 (1986).
- ¹⁴ A. Ishii, *Prog. Theor. Phys.* **70**, 644 (1983).
- ¹⁵ M. J. Puska and R. M. Nieminen, *Rev. Mod. Phys.* **66**, 841 (1994).
- ¹⁶ G. B. Bachelet, D. R. Hamann, and M. Schlüter, *Phys. Rev. B* **26**, 4199 (1982).
- ¹⁷ D. M. Ceperly and B. L. Alder, *Phys. Rev. Lett.* **45**, 566 (1980).
- ¹⁸ J. P. Perdew and A. Zunger, *Phys. Rev. B* **23**, 5044 (1981).
- ¹⁹ J. Arponen and E. Pajanne, *Ann. Phys. (N.Y.)* **121**, 343 (1979); *J. Phys. F* **9**, 2359 (1979); as parametrized by E. Boronski and R. M. Nieminen, *Phys. Rev. B* **34**, 3820 (1986).
- ²⁰ W. Brandt and J. Reinheimer, *Phys. Lett.* **35A**, 109 (1971).
- ²¹ M. J. Puska and C. Corbel, *Phys. Rev. B* **38**, 9874 (1988); M. J. Puska, S. Mäkinen, M. Manninen, and R. M. Nieminen, *ibid.* **39**, 7666 (1989).
- ²² C. Pennetta and A. Baldereschi, in *Positron Annihilation*, edited by L. Dorikens-Vanpraet, M. Dorikens, and D. Segers (World Scientific, Singapore, 1989), p. 693.
- ²³ E. Clementi and C. Roetti, *At. Data Nucl. Data Tables* **14**, 177 (1974).
- ²⁴ P. Kubica and M. J. Stott, *J. Phys. C* **4**, 1969 (1974).
- ²⁵ B. Chakraborty and R. W. Siegel, *Phys. Rev. B* **27**, 4535 (1983).
- ²⁶ J. A. Appelbaum and D. R. Hamann, *Phys. Rev. B* **8**, 1777 (1973).
- ²⁷ L. Gilgien, G. Galli, F. Gygi, and R. Car, *Phys. Rev. Lett.* **72**, 3214 (1994).
- ²⁸ H. Aourag, A. Belaidi, T. Kobayasi, R. N. West, and B. Khelifa, *Phys. Status Solidi B* **156**, 497 (1989).
- ²⁹ H. Rojas, B. Barbiellini, and T. Jarlborg, *Mater. Sci. Forum* **105–110**, 799 (1992).
- ³⁰ E. C. von Stetten, S. Berko, X. S. Li, R. R. Lee, J. Brynestad, D. Singh, H. Krakauer, W. E. Pickett, and R. E. Cohen, *Phys. Rev. Lett.* **60**, 2198 (1988).
- ³¹ S. Ishibashi, *J. Phys. Condens. Matter* **6**, L71 (1994).
- ³² R. Blank, L. Schimmele, and A. Seeger, *Mater. Sci. Forum* **105–110**, 603 (1992).