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Evaluation of point-core approximation effect on the positron energy levels in diamond structure solids

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ABSTRACT

Positron work function, positron affinity, positron energy band, deformation potential and some other important positron-related parameters are studied in the elemental semiconductors which have the diamond structure, using the first-principle norm-conserving pseudopotential method. While both the local density approximation (LDA) and the generalized gradient approximation (GGA) are employed in the positron structure theoretical research, to deal with the positron-electron exchange-correlation (EC) energy, only the GGA framework is adopted in electron total energy calculation. The nonlinear core correction is included in the positron-electron EC potential and the core electrons are considered within the frozen-core model. Point-core approximation is used to model the positron-ion interact potential. The calculation results agree well with the reference data. However, the positron band effective mass which has a dominate part of the total effective mass is systematic lower than the result which is obtained from other approaches. Because of the sensibility of the positron diffusion constant to the total effective mass, it is found that the point-core approximation could not provide an accurate forecast for the diffusion parameter.

1. Introduction

Many experimental methods based on positron annihilation have been applied to material science since it had been discovered in the last century. They give much valuable information on the electronic structures of condensed media, especially defects in solids [1,2], and belong to one of the few methods which could detect the electron Fermi surfaces directly [3,4]. These positron related experimental results are usually, however, complicated in the form of the positron or data related to the momentum content of the annihilating electron-positron pair in a specific environment. So, the interpretation of these data calls for theoretical methods with quantitative predicting power [5]. Much as in the case of other methods, the theory of positron annihilation has developed from some models which describes the positron-solid interaction to "first-principle" methods predicting the annihilation characteristics for different environments and conditions [6], each method has unique features. One of the most popular first-principle methods is the pseudopotential framework, because that it can be used to treat large defect systems without miss much precision under the present computing conditions, and therefore it is used in this paper to study the positron levels and related parameters.

Although it is well known that surface effect is complicate, the positron affinity, which is defined as the sum of the positron and electron chemical potential, is independent of the surface properties. That is to say, the standard first-principle methods can be used to calculate it. This positron parameter can be understood generally in two different physical pictures. The first one is that it can be defined as the energy gained by taking a thermalized positron from the vacuum level to the lowest bulk energy level [7,8]. The other definition which is first established in metals by Puska et al. [9] is related to the Fermi level in two different conductors. In this picture, the positron affinity is often labeled as A_+ ($A_+ = \mu_- + mu_+$, μ_- and μ_+ represent the electron and positron chemical potential respectively), and is much more widely used in positron related calculation. In this paper, the second definition is also used. The positron work function is expressed as $\varphi_+ = -\varphi_- - A_+$, where φ_- and φ_+ represent the electron and positron work function respectively. In this definition, the electron work function is the vacuum energy level minus the Fermi energy level.

The positrons may experience many processes such as thermalization, diffusion, trapping and so on after they implanted into a

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solid. In the thermalization process, when positron energy is lower than ~1 eV, interaction between positron and longitudinal acoustic phonons becomes much more important than the inelastic scattering effect in solids, and this gives rise to the longer positron lifetime especially at low temperature. So, the deformation potential theory which is used to theoretical research the positron-phonon interaction plays an important role in the low temperature positron lifetime spectroscopy experiment. In this theory scheme, the positron diffusion constant mainly concerns with the positron effective mass and the deformation potential at a temperature. As a consequence, the two parameters are calculated.

During the past decades, due to the convenient of selecting the so-called crystal zero, many researchers focused on the linear muffin tin orbital approach within the atomic sphere approximation (LMTO-ASA) when they studied the positron energy level [9–12]. In the year about 1999, Panda et al. gave a reliable result within the first-principle norm-conserving pseudopotential (NCPP) framework [8]. After that, few researchers focus on it in the field of positron energy level research, and hence, it is needed to prove the reliability of this approach further. In the present work, this method is used to study the positron affinity. To move forward a single step, the other related parameters such as positron effective mass, work function et al. are obtained.

Here, the elemental semiconductors diamond (C), silicon (Si) and germanium (Ge) are taken as examples. The paper is organized as follows: in Section 2, the calculation model and theoretical background are briefly introduced. Section 3 gives the calculation results and some discussions. At last, it is concluded in Section 4.

2. Calculation model and method

All of C, Si and Ge belong to space group of Fd3m, each primitive cell has two atoms. The input lattice constants for geometry optimization of them are 3.58 Å, 5.43 Å and 5.66 Å respectively [8,13]. Since the LDA and GGA corrections for electron energy level calculations are not very important in positron related parameters computations [8], only the GGA in the scheme of Perdew-Burke-Ernzerhof (PBE) is used at the present work for correcting the electron-electron exchange–correlation (XC) potential [14,15]. The pseudo atomic calculation is performed for C $2s^2 2p^2$, Si $3s^2 3p^2$ and Ge $4s^2 4p^2$. The electronic wave functions are expanded in a plane wave basis set with energy cut off 680 eV for C, 350 eV for Si and 400 eV for Ge. The $8 \times 8 \times 8$, $6 \times 6 \times 6$ and $4 \times 4 \times 4$ Monkhorst-Pack meshes are used to sample the Brillouin zones of C, Si and Ge respectively. The convergence tolerance of maximum energy change, the maximum force, the maximum stress and the maximum displacement for all the researched semiconductors are set to 1.0×10^{-5} eV/atom, 0.03 eV/Å, 0.05 GPa, 0.001 Å, respectively. In the electron work function calculation, the self-consistent dipole correction which was supposed by Neugebauer and Scheffler is considered [16].

In positronic structure calculation, the nonlinear core correction (NLCC) is included to manage the positron-electron XC energy and the core electrons are deal within the frozen-core approximation, which assumes that the core electrons are not polarized by the positron. Louie et al. have shown that the addition of a pseudocore electron density to the pseudovalence electron density gives accurate estimation of the XC potential [17,18]. The point-core approximation (PCA) model is used to construct the positron-ion coulomb interaction potential, and it has been used in the positron annihilation calculation within the pseudopotential framework [19–21]. However, the PCA effect on the positron energy level structure has not been researched systematically. Therefore, there are mainly two purposes to write this paper, one is to further prove the reliability of the NCPP in the field of positron level calculation, and the other is to evaluate the PCA effect on the positron level in solids.

The positronic wavefunctions are usually expanded in the plane wave basis set:

$$\Psi_{nk} = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{K}} C_{nk} \cdot exp(i(\boldsymbol{k} + \boldsymbol{K}) \cdot \boldsymbol{r}) \tag{1}$$

and the positronic schrodinger equation can be written as (in Hartree atomic units):

$$\sum_{\boldsymbol{K}} [A \cdot \delta_{\boldsymbol{K}\boldsymbol{K}'} + V_t(\boldsymbol{G})] \cdot C_{nk}(\boldsymbol{K}) = 0 \tag{2}$$

Table 1
Optimized structural data, and the electron work functions of three different surfaces for C, Si and Ge. The unit of work function is eV.

Host	a_0 (Å)	ε_∞	Electron work function (eV)		
			[1 0 0]	[1 1 0]	[1 1 1]
C	3.579	5.62	6.81	4.96	4.08 3.50 [31]
Si	5.478	11.90	5.13 4.91 [32]	4.47	4.74 4.74 [32]
Ge	5.783	16.00	4.98	4.67	4.63 4.80 [32]

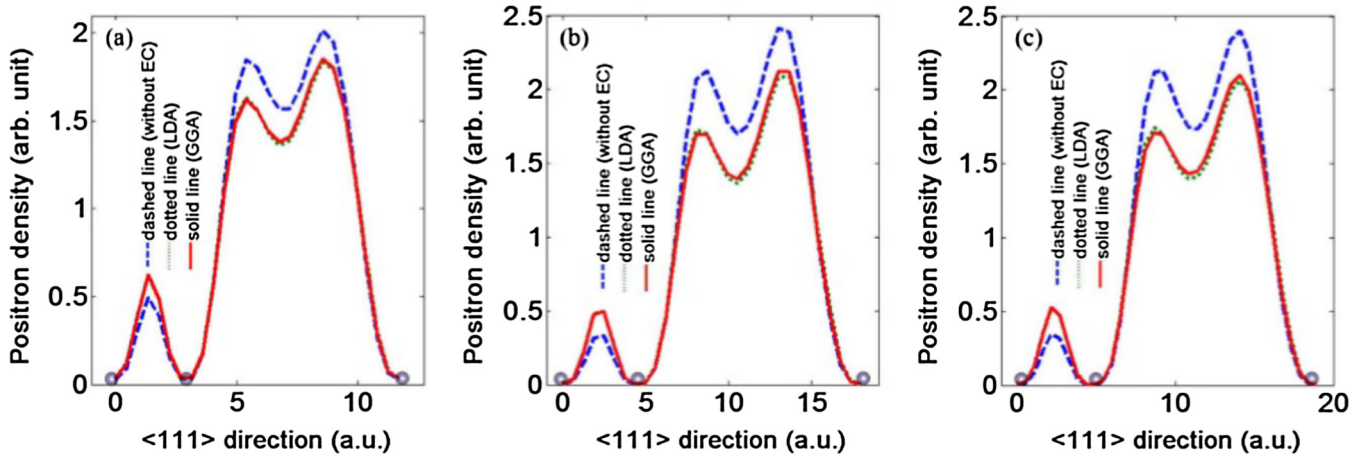

Fig. 1. The thermalized positron density distribution in the unit cell along the ⟨1 1 1⟩ direction within different positron-electron EC potential, the dashed lines represent without the EC effect, the dotted lines and the solid lines express the LDA and GGA schemes respectively, and (a) for C, (b) for Si and (c) for Ge.