

Positron Annihilation in Perfect and Defective TiO₂ Rutile Crystal with Single Particle Wave Function: Slater Type Orbital and Modified Jastrow Functions

Trinh Hoa Lang¹, Chau Van Tao¹, Kieu Tien Dung², Le Hoang Chien¹

¹Faculty of Physics and Engineering Physics, University of Science, Ho Chi Minh City, Vietnam

²Swinburne University of Technology, Melbourne, Australia

Email: thlang@hcmus.edu.vn

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ABSTRACT

Positron annihilation in TiO₂ rutile crystal is studied by an assumption that a positron binds with valence electrons of a titanium dioxide to form a pseudo TiO₂-positron molecule before it annihilates with these electrons. The orbital modification consisting of explicit electron-positron and electron-electron correlation in each electronic orbital is used for the electrons and positron wave functions. By these wave functions, the calculation results of the positron lifetimes in unmitigated and defective TiO₂ crystals are about 170 ps, 266 ps and 243 ps, respectively. These results are in good agreement with experimental data of the positron lifetimes in vacancies of TiO₂ from 180 ps to 300 ps.

KEYWORDS

Positron; Annihilation; Jastrow; Lifetime; VQMC; TiO₂

1. Introduction

The structure of material is studied by positron lifetime spectrum, which has many lifetime components depending on a local structure where a positron annihilates with electrons. The problem is how to determine accurately lifetime components of a positron in experiments. It encourages studying deeply the positron annihilation in element-specific structure of materials such as a single atom, a molecule or a unit cell.

In this paper, the study of positron annihilation with valence electrons of a unit structure of a material is assumed that a positron binds with the unit to form a new ground state through these valence electrons before it is destroyed. By this assumption, the orthonormalized Slater type orbital is used to describe electrons and positron wave functions in the irreducible element. Variation Quantum Monte Carlo (VQMC) [1] is then used to find the ground-state wave function for electrons and positron.

When a positron enters the material, it is slowed down

to a thermal energy and then bound with atoms in the unit structure before annihilating with valence electrons of the atoms. In this state, the positron wave function is approximated by a hybrid wave function of valence electrons.

The ground state of many-body problem is determined by minimizing the energy of each particle rather than the total energy. The problem of total wave function, Slater determinant representing for exchange effects, is avoided by solving the individual particle equation with the Hamiltonian of exchange potential. One particle energy is derived by one particle equation, which is constructed from the Kohn-Sham method and a single particle wave function. This wave function consists of an atomic wave function and a correlation function. By choosing a trial single wave function, the VQMC method is used to find the ground state of positron-valence electron of a unit element.

In this scenario, the optimized electron and positron distributions in real space of unit structure of material are determined by the minimal energy. From this distribution,

other quantities will be calculated by Monte Carlo method.

2. Theory

To study the positron annihilation in a unit structure of material, the two-component density-functional theory [2] is used with some modification in single particle wave function and exchange-correlation potential. Beside simple atomic wave function, a single-electron wave function also includes the correlation functions of electron-electron and electron-positron. The set of one-particle Schrodinger equations for electrons and positrons is given by

$$-\frac{1}{2}\nabla^2\Psi_i^-(r)+[V_x(\rho^-)-\phi(r)]\Psi_i^-(r)=\varepsilon_i^-\Psi_i^-(r) \quad (1)$$

$$-\frac{1}{2}\nabla^2\Psi_i^+(r)+[V_x(\rho^+)+\phi(r)]\Psi_i^+(r)=\varepsilon_i^+\Psi_i^+(r) \quad (2)$$

with

$$\Psi_i^\pm(r)=\varphi_i(r)J(r) \quad (3)$$

where φ_i is the atomic wave function for a single electron or positron; $J(r)$ is the correlation function of electron-electron or electron-positron. These functions are parameterized functions. The electron and positron densities are calculated by summing over the occupied states (n_- and n_+ are the number of electrons and positrons respectively).

$$\rho^- = \sum_i^{n_-} |\Psi_i^-(r)|^2; \rho^+ = \sum_i^{n_+} |\Psi_i^+(r)|^2 \quad (4)$$

The Slater type wave functions are used for the single electron wave function and the linear combination of them is used for the single positron wave function. The correlation function has the form $J(r)=e^{-u(r)}$ and $u(r)$ is the Jastrow function. This function is suggested in the new modified Jastrow function which is a combination of long correlation Padé [1] and short correlation Yukawa [3]. The Jastrow function for the electron-electron correlation is given by

$$u^{ee}(r)=\frac{\beta_e}{1+\alpha_e r}+\frac{A_e(1-e^{-F_e r})}{r} \quad (5)$$

and for the electron-positron correlation is given by

$$u^{ep}(r)=\frac{\beta_{ep} r}{1+\alpha_{ep} r}+\frac{A_{ep}(1-e^{-F_{ep} r})}{r} \quad (6)$$

where $\beta_e, \alpha_e, A_e, F_e, \beta_{ep}, \alpha_{ep}, A_{ep}$, and F_{ep} are the variation parameters. These parameters depend on the electronic structure of material.

If the exchange-correlation potential is separated into

exchange and correlation potentials, then the correlation potential is hidden in the correlation wave function, and the exchange potential for a uniform degenerate electron gas is adapted in the atomic calculation by using local electron density as given by [4]

$$V_x(\rho)=\varepsilon_x+\frac{d\varepsilon_x}{d\rho} \quad (7)$$

where ε_x is the exchange energy per electron of a uniform electron gas with density ρ .

$$\varepsilon_x=-\frac{3}{4}\left(\frac{3}{\pi}\rho\right)^{1/3} \quad (8)$$

Now ρ is replaced by a local electron density in an atom.

The Equations (1) and (2) are solved with the wave function in Equations (3), (5) and (6) to find the ground state of the unit structure-positron system by VQMC, which minimizes the electron and positron energy to obtain their ground state wave function.

The pair correlation function of electron and positron is built from Monte Carlo simulation in the ground state. The analytical form of pair correlation function is fitted to the Chebyshev polynomial. Then the positron annihilation enhancement is determined by extrapolating the pair correlation function at $r=0$, which is the distance between electron and positron.

Positron annihilation rate, which depends on the overlap of electron and positron densities and the enhancement factor, is directly given by the value of the pair-correlation function at the origin via the relation [5,6]

$$\Gamma=\frac{\pi r_e^2 c}{\Omega}\sum_i^N\int\rho_i^-(r)\rho_i^+(r)g(0;\rho^-, \rho^+)dr \quad (9)$$

where $g(0;\rho^-, \rho^+)$, the value of the pair-correlation function $g(r;\rho^-, \rho^+)$ at $r=0$ for given electron density, is the enhancement factor. the pair-correlation function is fitted to the Chebyshev polynomial [7] as given by

$$g(r;\rho^-, \rho^+)\equiv g(r)=\sum_{i=0}^N c_i T_i\left(\frac{2r-L}{L}\right) \quad (10)$$

where L is the maximum interaction range of the electron and the positron, which is used for determining the electron distribution in the space around the positron.

This model is applied to study the positron annihilation in the unit cell of titanium dioxide of rutile structure consisting of two titaniums and four oxygens as shown in **Figure 1**. The single-particle wave function in TiO_2 is constructed by the Linear Combination of Atomic Orbitals (LCAO) approximation [8] from an atomic wave function of oxygen and titanium.

The single-particle wave functions for the valance electrons of titanium and oxygen atoms in $3d, 4s$ and $2p$

shells are obtained from the Slater Type Orbital [9] and

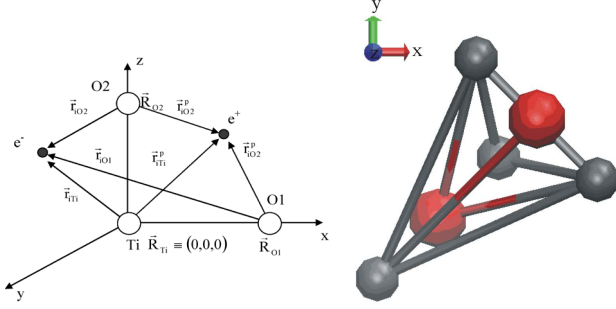


Figure 1. The schematic of the titanium dioxide-positron system and the configuration of the titanium dioxide in a unit cell of rutile crystal structure. The big spheres are titaniums and the smaller spheres are oxygens.

are constructed by the LCAO approximation as shown.

$$\begin{aligned} \varphi_i^{3dz^2}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{3dz^2}(Z_{Ti}, r - R_{Ti}) \\ &+ C_2 \varphi_i^{3dz^2}(Z_{O1}, r - R_{O1}) + C_3 \varphi_i^{3dz^2}(Z_{O2}, r - R_{O2}) \end{aligned} \quad (11)$$

$$\begin{aligned} \varphi_i^{3dxz}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{3dxz}(Z_{Ti}, r - R_{Ti}) \\ &+ C_2 \varphi_i^{3dxz}(Z_{O1}, r - R_{O1}) + C_3 \varphi_i^{3dxz}(Z_{O2}, r - R_{O2}) \end{aligned} \quad (12)$$

$$\begin{aligned} \varphi_i^{3dyz}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{3dyz}(Z_{Ti}, r - R_{Ti}) \\ &+ C_2 \varphi_i^{3dyz}(Z_{O1}, r - R_{O1}) + C_3 \varphi_i^{3dyz}(Z_{O2}, r - R_{O2}) \end{aligned} \quad (13)$$

$$\begin{aligned} \varphi_i^{3dxy}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{3dxy}(Z_{Ti}, r - R_{Ti}) \\ &+ C_2 \varphi_i^{3dxy}(Z_{O1}, r - R_{O1}) + C_3 \varphi_i^{3dxy}(Z_{O2}, r - R_{O2}) \end{aligned} \quad (14)$$

$$\begin{aligned} \varphi_i^{3dx^2-y^2}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{3dx^2-y^2}(Z_{Ti}, r - R_{Ti}) \\ &+ C_2 \varphi_i^{3dx^2-y^2}(Z_{O1}, r - R_{O1}) \\ &+ C_3 \varphi_i^{3dx^2-y^2}(Z_{O2}, r - R_{O2}) \end{aligned} \quad (15)$$

$$\begin{aligned} \varphi_i^{4s}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{4s}(Z_{Ti}, r - R_{Ti}) \\ &+ C_2 \varphi_i^{4s}(Z_{O1}, r - R_{O1}) + C_3 \varphi_i^{4s}(Z_{O2}, r - R_{O2}) \end{aligned} \quad (16)$$

$$\begin{aligned} \varphi_i^{2px}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{2px}(Z_{O1}, r - R_{O1}) \\ &+ C_2 \varphi_i^{2px}(Z_{O2}, r - R_{O2}) + C_3 \varphi_i^{2px}(Z_{Ti}, r - R_{Ti}) \end{aligned} \quad (17)$$

$$\begin{aligned} \varphi_i^{2py}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{2py}(Z_{O1}, r - R_{O1}) \\ &+ C_2 \varphi_i^{2py}(Z_{O2}, r - R_{O2}) + C_3 \varphi_i^{2py}(Z_{Ti}, r - R_{Ti}) \end{aligned} \quad (18)$$

$$\begin{aligned} \varphi_i^{2pz}(Z_{Ti}, Z_{O1}, Z_{O2}; r) &= C_1 \varphi_i^{2pz}(Z_{O1}, r - R_{O1}) \\ &+ C_2 \varphi_i^{2pz}(Z_{O2}, r - R_{O2}) + C_3 \varphi_i^{2pz}(Z_{Ti}, r - R_{Ti}) \end{aligned} \quad (19)$$

where $\varphi_i^{3dz^2}(Z, r)$, $\varphi_i^{3dyz}(Z, r)$, $\varphi_i^{3dxz}(Z, r)$, $\varphi_i^{3dxy}(Z, r)$, $\varphi_i^{3dx^2-y^2}(Z, r)$, $\varphi_i^{4s}(Z, r)$, $\varphi_i^{2px}(Z, r)$, $\varphi_i^{2py}(Z, r)$, and $\varphi_i^{2pz}(Z, r)$ are Slater-type orbitals of atomic wave functions. $r - R_{Ti}$, $r - R_{O1}$, and $r - R_{O2}$ are distances of i th electron from titanium and from oxygens, respectively.

The single-particle wave function for the positron in the bound state with valance electrons of oxygen and titanium is a hybrid wave function of these electron wave

functions. According to the principle of linear superposition, the single-particle wave function for positron is supposed to take the form

$$\begin{aligned} \varphi_i^p(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) &= c_1 \varphi_i^{3dz^2}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) \\ &+ c_2 \varphi_i^{3dxz}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) + c_3 \varphi_i^{3dyz}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) \\ &+ c_4 \varphi_i^{3dx^2-y^2}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) \\ &+ c_5 \varphi_i^{3dxy}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) + c_6 \varphi_i^{4s}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) \\ &+ c_7 \varphi_i^{2px}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) + c_8 \varphi_i^{2py}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) \\ &+ c_9 \varphi_i^{2pz}(Z_{Ti}^p, Z_{O1}^p, Z_{O2}^p; r) \end{aligned} \quad (20)$$

where Z_{Ti} , Z_{O1} , Z_{O2} , Z_{Ti}^p , Z_{O1}^p and Z_{O2}^p are the variation parameters in the atomic wave function of electron and positron in TiO_2 ; C_1 , C_2 and C_3 are the weighted coefficients of the electron wave function with

$C_1 = C_2 = C_3 = 1/\sqrt{3}$; and $c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8$ and c_9 are the weighted coefficients of the positron wave function with $c_1 = c_2 = c_3 = c_4 = c_5 = c_6 = c_7 = c_8 = c_9 = 1/3$.

Using equations from (11) to (20) and (1) to (8), the minimized energy is calculated by VQMC to obtain the ground-state wave function of this system. Assuming that the ground-state wave function is valid for TiO_2 rutile, the properties of electron-positron annihilation in TiO_2 rutile, therefore, are determined.

3. Results and Discussion

To calculate the ground-state wave function of electrons and a positron in TiO_2 molecule, fourteen sets of energy data corresponding to the variation of fourteen parameters Z_{Ti} , Z_{O1} , Z_{O2} , β_e , α_e , A_e , F_e , Z_{Ti}^p , Z_{O1}^p , Z_{O2}^p , β_{ep} , α_{ep} , A_{ep} , and F_{ep} are generated. Each result is calculated by varying one of the parameters, and the other thirteen parameters are kept as constants. The set of optimized parameters, which make the trial wave function well approach to the exact wave function, is determined by minimizing energy of the system. These optimized parameters are given in **Table 1**.

The enhancement factor and positron lifetime in a perfect TiO_2 rutile crystal are determined from these parameters. The electron-positron pair correlation distribution in the perfect rutile crystal of TiO_2 is determined by Monte Carlo simulation as shown in **Figure 2(a)**. The enhancement factor is extrapolated by a pair correlation function which is fitted to the Chebyshev polynomial in Equation (10). The number of coefficients, N , in Equation (10) is determined by minimizing the chi square of fitting goodness of the pair correlation function as shown in **Figure 2(b)**. The minimal chi square corresponds to $N = 41$ with the value of chi square χ^2 of

0.255448 and the values of the coefficients are given in the **Table 2**. After fitting analytical form of pair correlation function of electron-positron $g(r=0, \rho^-, \rho^+)$ is constructed, the enhancement factor is calculated with $g(r=0, \rho^-, \rho^+)=1938.54$ as shown in **Figures 2(c)** and **(d)**. This enhancement factor can be considered as an effective number of electrons [10]. So the value of the enhancement factor is reasonable in compare with the results in the Reference [10]. From Equation (9) and the enhancement factor, annihilation rate is estimated by an overlap of electron and positron densities. The calculation annihilation rate is $\Gamma = (5.858 \pm 0.007) \times 10^9 \text{ (s}^{-1}\text{)}$. The positron lifetime is the inverse of the annihilation rate $\tau = (170 \pm 2) \text{ ps}$. The fitting parameters of the Chebyshev polynomial are shown on **Table 2**.

The enhancement factor and positron lifetime in TiO_2 rutile crystal of an oxygen defect, created by removing one oxygen atom from a unit cell of TiO_2 perfect rutile crystal, are also calculated from these parameters, which is assumed that they is still valid for the electron and positron wave functions in the TiO_2 rutile crystal of an oxygen defect. The distribution of electron-positron pair correlation in the TiO_2 of an oxygen defect is obtained from Monte Carlo simulation as shown in **Figure 3(a)**. The number of coefficients, N , in this case is identified by the minimization of the chi square corresponding to $N = 42$ with the value of chi square χ^2 of 0.0542912 as shown in **Figure 3(b)** and the values of the coefficients are given in the **Table 3**. The enhancement factor in TiO_2

of an oxygen defect is obtained by the extrapolation of the pair correlation function at $r = 0$ with $g(r=0, \rho^-, \rho^+)=725.99$ as shown in **Figures 3(c)** and **(d)**. The annihilation rate and lifetime of positron, which are determined from this enhancement factor and the overlap of electron and positron densities, are $\Gamma = (3.756 \pm 0.006) \times 10^9 \text{ (s}^{-1}\text{)}$ and $\tau = (266 \pm 3) \text{ ps}$, respectively. This positron lifetime is greater than the value in the perfect crystal of TiO_2 . It shows that this result is suitable to predict the positron lifetime in a monovacancy defect.

The enhancement factor and the positron lifetime in TiO_2 rutile crystal of a titanium defect, created by removing one titanium atom from a unit cell of TiO_2 perfect rutile crystal, are determined similarly. The wave function parameters of electron and positron in the TiO_2 rutile crystal of a titanium defect is still valid, and the distribution of electron-positron pair correlation is obtained from Monte Carlo simulation as shown in **Figure 4(a)**. The number of coefficients, N , is determined by the

Table 1. The values of optimized parameters of electron and positron wave function.

Z_{Ti}	Z_{O1}	Z_{O2}	α_e	β_e	A_e	F_e
9.3	21.3	5.0	1.0	11.7	1.7	7.0
Z_{pTi}	Z_{pO1}	Z_{pO2}	α_{ep}	β_{ep}	A_{ep}	F_{ep}
0.4	0.2	0.09	0.9	0.6	1.8	0.6

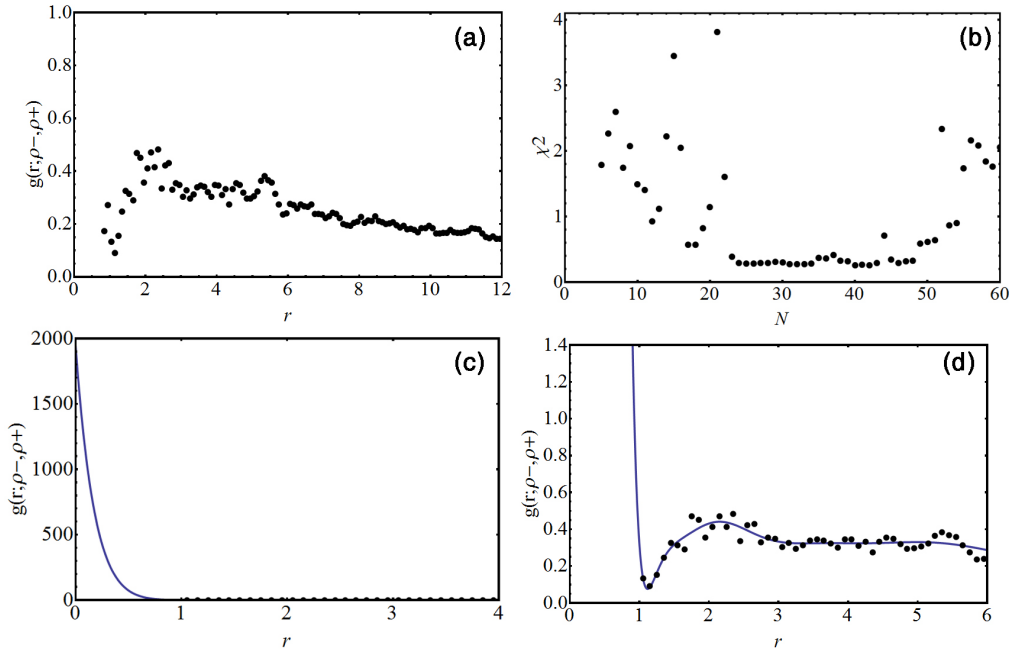


Figure 2. (a) The electron-positron pair distribution obtained by Monte Carlo simulation with the optimized wave function of electron and positron in TiO_2 perfect rutile crystal; (b) The chi square of goodness of fit in the term of the number of Chebyshev coefficients; (c), (d) The fitted pair correlation function of electron-positron in TiO_2 perfect rutile crystal. The black dot is Monte Carlo simulation and the solid line is its fitting curve.

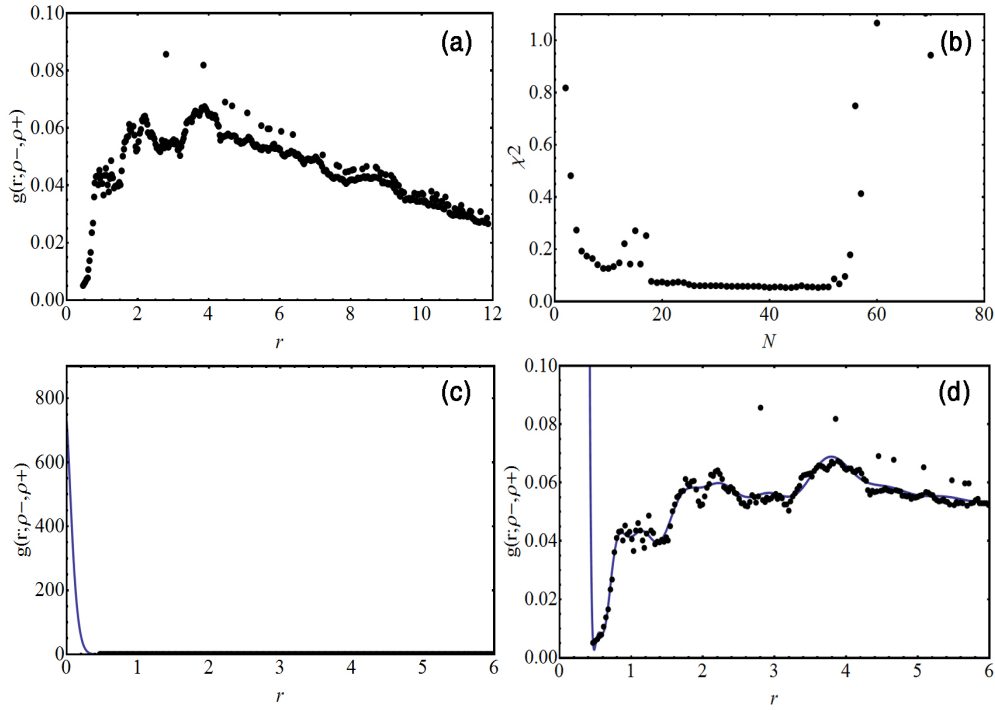


Figure 3. (a) The electron-positron pair distribution obtained by Monte Carlo simulation with the optimized wavefunction of electron and positron in TiO₂ rutile crystal of an oxygen defect; (b) The chi square of goodness of fit in the term of the number of Chebyshev coefficients; (c), (d) The fitted pair correlation function of electron-positron in TiO₂ rutile crystal of an oxygen defect. The black dot is Monte Carlo simulation and the solid line is its fitting curve.

Table 2. The fitting parameters of the Chebyshev polynomial of electron-positron correlation function in TiO₂ perfect rutile crystal.

c_0	c_1	c_2	c_3	c_4	c_5	c_6
70.4145	-140.217	138.477	-135.738	132.067	-127.506	122.129
c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}
-116.039	109.36	-102.218	94.7435	-87.0644	79.3092	-71.6018
c_{14}	c_{15}	c_{16}	c_{17}	c_{18}	c_{19}	c_{20}
64.0554	-56.768	49.8222	-43.2871	37.2192	-31.6572	26.6246
c_{21}	c_{22}	c_{23}	c_{24}	c_{25}	c_{26}	c_{27}
-22.1309	18.1715	-14.7288	11.7764	-9.27894	7.19698	-5.48736
c_{28}	c_{29}	c_{30}	c_{31}	c_{32}	c_{33}	c_{34}
4.10671	-3.011	2.15877	-1.50904	1.02616	-0.674875	0.426965
c_{35}	c_{36}	c_{37}	c_{38}	c_{39}	c_{40}	c_{41}
-0.256795	0.145687	-0.0764166	0.0367376	-0.0155249	0.00567258	-0.00118012

minimization of chi square of fitting goodness of the pair correlation function as shown in **Figure 4(b)**. The minimal chi square corresponds to $N = 42$ with the value of chi square χ^2 of 4.80132. The values of the coefficients are given in the **Table 4**. From this pair correlation function, the enhancement factor is calculated with $g(r=0, \rho^-, \rho^+) = 1385.38$ as shown in the **Figures 4(c)**

and **(d)**. The results of the annihilation rate and the positron lifetime are $\Gamma = (4.109 \pm 0.003) \times 10^9 \text{ (s}^{-1}\text{)}$ and $\tau = (243 \pm 2) \text{ ps}$, respectively. This lifetime is as well greater than the positron lifetime in the perfect TiO₂ crystal but it is smaller than the positron lifetime in the TiO₂ of oxygen defect. The results of the positron lifetime in oxygen and titanium defects in TiO₂ rutile crystal are still in

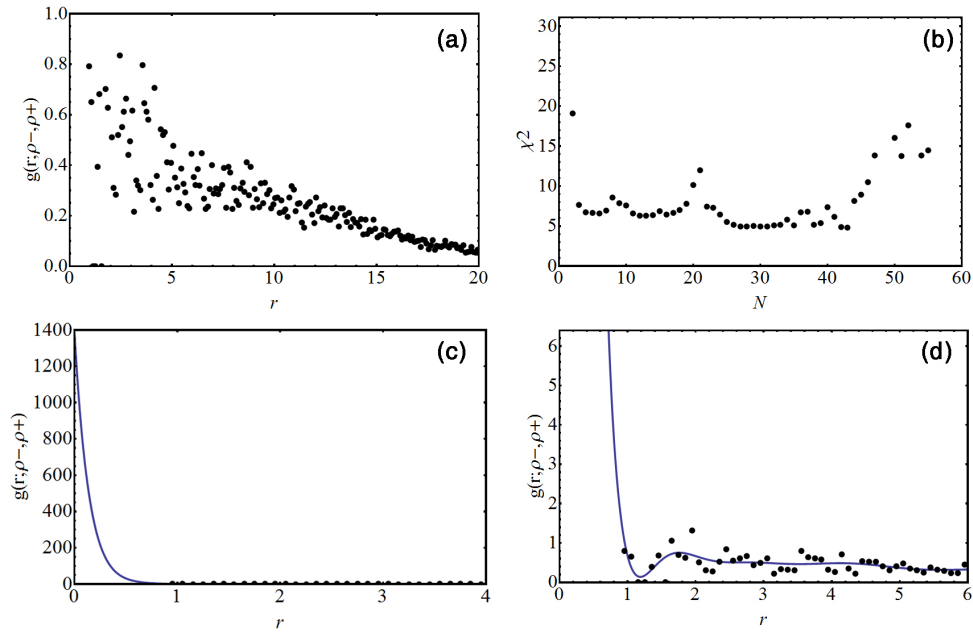


Figure 4. (a) The electron-positron pair distribution obtained by Monte Carlo simulation with the optimized wavefunction of electron and positron in TiO_2 rutile crystal of a titanium defect; (b) The chi square of goodness of fit in the number of the Chebyshev coefficients; (c), (d) The fitted pair correlation function of electron-positron in TiO_2 rutile crystal of a titanium defect. The black dot is Monte Carlo simulation and the solid line is its fitting curve.

Table 3. The fitting parameters of the Chebyshev polynomial of electron-positron correlation function in TiO_2 rutile crystal of an oxygen defect.

c_0	c_1	c_2	c_3	c_4	c_5	c_6
37.8892	-75.8345	73.6828	-71.8773	67.9538	-64.4962	59.1933
c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}
-54.5708	48.4607	-43.2659	36.9648	-31.7844	25.8588	-21.1936
c_{14}	c_{15}	c_{16}	c_{17}	c_{18}	c_{19}	c_{20}
16.0801	-12.2772	8.2345	-5.45376	2.55904	-0.798657	-1.03033
c_{21}	c_{22}	c_{23}	c_{24}	c_{25}	c_{26}	c_{27}
1.91072	-2.86718	3.0876	-3.41355	3.20978	-3.14677	2.73426
c_{28}	c_{29}	c_{30}	c_{31}	c_{32}	c_{33}	c_{34}
-2.48459	2.02515	-1.73136	1.32634	-1.0722	0.768341	-0.587157
c_{35}	c_{36}	c_{37}	c_{38}	c_{39}	c_{40}	c_{41}
0.388003	-0.277632	0.164543	-0.109164	0.054657	-0.032698	0.0113866
c_{42}						
-0.00547715						

good agreement with shorter lifetime components of positron in the vacancies of TiO_2 rutile [11].

4. Conclusions

Base on the principle of linear superposition, the Kohn-Sham approximation, the Slater-type orbital, the modification of Jastrow and the VQMC method, we derived a

theoretical model to determine the positron lifetime for some element-specific structure of materials.

In the scenario of purely theoretical calculations, we use real space electron and positron distributions to estimate the value of the positron lifetime in TiO_2 rutile crystal structure. The calculation results show that the lifetime of a positron in the perfect crystal, $\tau = 170$ ps, is shorter than in the oxygen defect crystal, $\tau = 266$ ps, and

Table 4. The fitting parameters of the Chebyshev polynomial of electron-positron correlation function in TiO₂ rutile crystal of a titanium defect.

c_0	c_1	c_2	c_3	c_4	c_5	c_6
6.07754×10^7	1.20559×10^8	1.17631×10^8	1.12902×10^8	1.06587×10^8	9.89649×10^7	9.03585×10^7
c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}
8.11122×10^7	7.15712×10^7	6.20594×10^7	5.28646×10^7	4.42233×10^7	3.63156×10^7	2.92604×10^7
c_{14}	c_{15}	c_{16}	c_{17}	c_{18}	c_{19}	c_{20}
2.31199×10^7	1.79034×10^7	1.35778×10^7	1.00766×10^7	7.31121×10^6	5.18058×10^6	3.58056×10^6
c_{21}	c_{22}	c_{23}	c_{24}	c_{25}	c_{26}	c_{27}
2.41016×10^6	1.57734×10^6	1.00146×10^6	615300.0	364584.0	207501.0	112760.0
c_{28}	c_{29}	c_{30}	c_{31}	c_{32}	c_{33}	c_{34}
58065.6	27972.7	12369.2	4816.32	1501.99	228.485	-140.146
c_{35}	c_{36}	c_{37}	c_{38}	c_{39}	c_{40}	c_{41}
-178.757	-122.485	-67.26	-29.8891	-11.66	-3.41396	-0.867937
c_{42}						
-0.0781081						

the titanium defect crystal, $\tau = 243$ ps. In comparison with the experimental results, the positron lifetime of this calculation in the perfect crystal is also shorter than the short lifetime component of the positron in the vacancies of TiO₂ rutile. However, the positron lifetimes of this calculation in the crystal of oxygen and titanium defects are still in good agreement with the positron lifetimes in the vacancies of TiO₂ rutile. Therefore, the results can be used to predict lifetime components of positron in the perfect and defective TiO₂ rutile crystal.

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