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COMPUTATION OF POSITRON ANNIHILATION RATES IN DEFORMED METALS

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Abstract

Positron annihilation techniques are established tools for the study of different properties of materials. In this study, positron annihilation rates in deformed metals were computed using the perturbed hypernetted chain approximation in conjunction with the stabilized jellium model. The results obtained revealed that the enhancement factor of deformed metals is higher than that of undeformed metals and increases with increase in deformation or strain. Enhancement factor of deformed metals varies at different rate with strain for different metals. The results further revealed that strain causes a decrease in the positron annihilation rates in deformed metals. The rate of decrease of positron annihilation rates with strain in deformed metals varies depending on the nature of the metal. The alkali metals has the least rate of decrease of positron annihilation rates with strain while Al has the fastest rate of decrease of positron annihilation rates in deformed metals with strain.

Keywords: Positrons, Annihilation rates, strain, metals and stabilized jellium model

INTRODUCTION

Positron annihilation techniques are an established methods for probing defects and microstructural properties of materials (Sabah, 2015). Positrons with energies ranging from few electron volts to giga electron volts are very useful in different areas of physics and applications. When energetic positron from a radioactive source enters condensed matter, it annihilates with an electron from the surrounding medium by emitting two 511 keV gamma quanta. The properties of these gamma quanta; such as their energies, emission direction and time of emission, which can be measured provides useful information about the material in which the positron annihilate (Eldrup, 1995).

During the process of positron annihilation in condensed matter, a variety of phenomena takes place. These phenomena are reflected in the temporal, spatial and energetic distributions of the annihilation radiation. The positrons lose their energies to electron excitations including target atom ionizations and collective Plasmon-like processes. At lower energies, phonon excitations take place leading to positron thermalization. At thermal equilibrium that is achieved in a few picoseconds, positron motion continues as a quantum diffusion process (Niemanien, 2000).

Positron annihilation studies are carried out experimentally and theoretically. Rajesh et al., (2018) studied positron annihilation lifetime in chemically synthesized FeCo alloy. The FeCo alloy has different lifetime components corresponding to annihilating in vacancies and different types of open volume defects as a result of the unique morphology of the synthesized FeCo alloy. Mizuno et al., 2004 used first principle electronic calculation to calculate positron lifetime in bulk and vacancy states in MgO and ZnO. The semiconductor model reproduced the experimental positron lifetime in the two compounds. For cation vacancy, the positron lifetime calculated based on the semiconductor model was shorter than experimental value as a result of inward relaxation occurring around the cation vacancy. Dryzek (2018) carried out experimental and theoretical studies of positron in defects created during compression and dry sliding in bismuth. The results obtained revealed that positron lifetime increases with increase in the size of the defect clusters. The results further revealed that positron lifetime (inverse of annihilation rate) increased with increase in strain. Mitroy and Barbiellini (2002) used the enhancement factors of the one component local density approximation, the Boronski and Nieminen (1986) two component local density approximation and a modified one component local density approximation enhancement factors to calculate positron annihilation rates for valence and core electrons in different positronic systems. They found that the modified one component local density approximation predicts positron annihilation rates that are reliable for some positronic systems.

In this work, positron annihilation enhancement factor and positron annihilation rates for deformed metals were computed using the perturbed hypenetted chain approximation (Stachowiak and Lach, 1993) through the application of the stabilized jellium model. This will enable us test the applicability of the stabilized jellium model in the study of positron annihilation characteristics of deformed metals. The hypernetted chain approximation provides a simple, direct and efficient method of computing positron annihilation characteristics in metal lattices. The approximation also allows for a wide range of annihilation parameter calculation and provides a reasonable description of the screening of a positron for any density of the electron gas.

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3.0 Theoretical Consideration

3.1 Electron gas parameter of deformed metals

In order to obtain the electron gas parameter of a deformed metal, we consider a hypothetical crystal having the shape of a parallelepiped of equivalent faces. The deformation is assumed to be a measured quantity and the metallic crystal is assumed to be made up of simple crystallites. Consider a cubic cell of side length a_o and volume given as (Keiegna and Pogosor, 1999).

$$\Omega_o = a_o^3 = \frac{4}{3}\pi r_o^3 \quad (1)$$

where r_o is the radius of the Winer-Seitz cell given as $r_o = Z^{\frac{1}{3}} r_s$, where r_s is the electron gas parameter of undeformed metal defined as the radius of the sphere containing one electron on average and a measure of inter electronic spacing in the metal. r_s is defined as

$$r_s = \left[\pi \frac{4}{3} n\right]^{\frac{1}{3}} \quad (2)$$

where n is the density of the undeformed metal.

If an elongative force is applied along the x-axis of a cube that causes it to deform, the volume of the unit cell is

$$\Omega_0 = a_x\ a_y^2 = \frac{4}{3}\ \pi\ ab^2 \quad (3)$$

where a_x, a_y and a_z are the sides of the deformed cubic cell. If the unaxial strain is U_{xx}, then

$$a_x = a_0\left[1 + u_{xx}\right]$$

$$a_z = a_0[1 + U_{zz}] = a_0\left[1 - \upsilon\, U_{xx}\right] \quad (4)$$

where υ is the polycrystalline Poisson ratio that relates the transverse compression to the elongation in the direction of the applied deformation that is $U_{xx} = U_{yy} = -\upsilon\, U_{zz}$. The ratio of the unit volume of the deformed cubic cell to that of the undeformed cell is

$$\frac{\Omega_d}{\Omega_o} = \frac{a_o\,[1+U_{xx}][1+U_{yy}]a_o[1+U_{zz}]a_o}{a_0^3} \quad (5)$$

$$\frac{\Omega_d}{\Omega_o} = [1 + U_{xx}]\left[1 + U_{yy} + U_{zz}U_{yy}\right] \quad (6)$$

Neglecting higher order terms of uniaxial strain, then (Kiejna and Pogosor, 1999)

$$\frac{\Omega_d}{\Omega_o} = 1 + U_{xx} + U_{yy} + U_{zz} \quad (7)$$

The average electron density of the deformed metal is

$$n_{av} = \frac{n_o\Omega_o}{\Omega} = \frac{n_o a^3}{a_o[1 + U_{xx}]a_0\left[1 - \upsilon\, U_{xx}\right]^2} \quad (8)$$

$$n_{av} = n_o\left[1 - \left(1 - 2\upsilon\right)U_{xx}\right] + 0 \quad (9)$$

The electron gas parameter of the deformed metal is obtain from its volume as

$$\frac{4}{3}\pi r_{su}^3 = \frac{4}{3}\pi ab^2$$

$$r_{su}^3 =$$

$$r_{su} = r_s^3\left[1 + U_{xx} - \upsilon\, U_{xx} + \upsilon\, U^2{}_{xx} - \upsilon\, U_{xx} - \upsilon\, U^2{}_{xx}\right] \quad (10)$$

Neglecting higher order terms in the strain or deformation we have (kiejna and Posogo, 1999).

$$r_{su} = r_s\left[1 + U_{xx}\left(1 - 2\upsilon\right)\right]^{\frac{1}{3}} \quad (11)$$

Equation (11) gives the expression for the electron gas parameter of deformed metal, r_{su}, which is a measure of the inter-electroniC distance in a deformed metal.

3.2 Positron annihilation rate in deformed metals

The ground state electron and positron densities in metals can be calculated using the generalized Kohn-Sham method. This method requires the solving of the following set of one particle Schrondinger equation for electrons and positrons respectively (Puska and Niemanien, 1994).

$$-\frac{1}{2}\nabla^2\varphi_i(r) + \left[\frac{\partial E_{xc}(n_+)}{\partial n_{+(r)}} - \emptyset(r) + \frac{\partial E_c^{e-p}(n_+n_-)}{\partial n_-(r)}\right]\varphi_i(r) = E_i\varphi_i(r) \quad (12)$$

$$-\frac{1}{2}\nabla^2\varphi_i^+(r) + \left[\frac{\partial E_{xc}(n_+)}{\partial n_{+(r)}} - \emptyset(r) + \frac{\partial E_c^{e-p}(n_+n_-)}{\partial n_-(r)}\right]\varphi_i^+(r) = E_i^+\varphi_i^+(r) \quad (13)$$

where Ø(r) is the Coulomb potential defined as

$$\emptyset(r) = \int \frac{dr^I\, n_-(r^I)n_+(r^I)n_o(r^I)}{/r - r^I/} \quad (14)$$

n_0 (r) is the positive charge density providing the external potential, $V_{ext,}$ n_- (r) and n_+ (r) are the electron positron densities respectively given as

$$n_- = \sum_{E_i \leq E_F} |\psi_i(r)|^2 \quad (15)$$

and

$$n_+(r) = \sum_{i=1}^{N} |\psi_i^+(r)|^2 \quad (16)$$

The potential experienced by the positron in a perfect crystal is the sum of the coulomb potential and the correlation potential $V_{corr}^{(n_-(r))}$

$$V(r) = \emptyset(r) + V_{corr}^{(n_-(r))} \quad (17)$$

The total annihilation rate can be obtained from the overlap of the electron and positron densities which results in the enhancement of the electron density at the positron site;

$$\lambda = \frac{\int dr\, \varphi_+(r)^2}{\tau(n_-(r))} \quad (18)$$

In the local density approximation, the positron annihilation rate λ is given as;

$$\lambda = \int dr\, n_+(r)\tau(n_-(r)) \quad (19)$$

where $\tau(n(r))$ *is* the positron annihilation rate in an electron gas, $\tau(n_-(r))$ is expressed as

$$\tau(n_-(r)) = \pi r_0^2 cng(r_s) \quad (20)$$

where r_o is the classified electron radius, c is the speed of light in vacuum and n is electron density, $g(r_s)$ is the enhancement factor, which takes into consideration the electron-positron correlation.

The enhancement factor can be expressed as (Stachowiak and Lach, 1993);

$$g(r_s) = 1 + 1.23 r_{su} + higher\ terms \quad (21)$$

In the perturbed hypernetted chain approximation the enhancement factor is given as (Shachowiak, 1990);

$$g(r_s) = 1 + 1.23 r_s - 0.1375 r_s^2 + \frac{r_s^3}{6} \quad (22)$$

The modified perturbed hyper netted chain approximation for deformed metals is

$$g(r_{su}) = 1 + 1.23 r_{su} - 0.1375 r_{su}^2 + \frac{r_{su}^3}{6} \quad (23)$$

where r_{su} is the electron gas parameter of the deformed metal.

$$r_{su} = r_s\left[1 + U_{xx}(1 - 2\upsilon)\right]^{\frac{1}{3}}$$

4. Results and Discussion

Figures 1, 2, 3 and 4 shows the variation of enhancement factor with strain for deformed metals calculated using the perturbed hypernetted chain approximation. As shown in figures, strain (or deformation) causes an increase in the enhancement factors of the metals. In Fig. 1, potassium has the highest enhancement factor compared to the other metals whose enhancement factors are shown in the figure. This may be due to its low density. Alkali metals have large enhancement factor as a result of their low densities (Puska and Nieminen, 1994). The strain causes an increase in the enhancement factor of the metals. This shows that the strain causes more distortion of the positron wave function as the enhancement factor or correlation function describes both the distortion of the positron wave function from its initial state and the enhancement of the densities of the individual electronic states on the positron site. This may also be due to the increase in the inter-particle spacing in the metals caused by the strain. As revealed in the figures, the enhancement factor of all the metals follows the same pattern but all do not increase with strain at the same rate. Generally, the enhancement factor of the deformed metals are higher than that of the undeformed metals as the enhancement factor of undeformed metals varies between two and eight (Puska and Nieminen, 1994).

Figure 5, 6, 7 and 8 shows the variation of positron annihilation rates in deformed alkali, simple, transition and inner transition metals with strain. The figures reveals that generally as the strain increases, positron annihilation rates in the deformed metals decrease but the rate of decrease varies from one metal to another. Aluminum, Al has the fastest rate of decrease followed by Beryllium, Be while Potassium, K has the least rate of decrease of all the metals used in the work. Positron annihilation rates vary least with strain for low density metals. This may be due to the small change in the electron density as a result of the applied strain or deformation. The variation of positron annihilation rates in deformed metals with strain further shows that the rate of decrease of positron annihilation rate with deformation (or strain) in deformed metals depends on the nature of the metal.

The results obtained in this work is in good agreement with the experimental work of Dryzek, (2018), who found that mean positron life time (inverse of positron annihilation rate) in bismuth increases with increase in strain. As strain increases, there is increase in plastic deformation leading to the creation of point defects. These defects act as traps for the positrons in the deformed metals.

5. Conclusion

Positron enhancement factor and annihilation rates in deformed metals have been studied using the the perturbed hypernetted chain approximation in conjunction with stabiized jellium model. Strain or deformation causes an increase in the enhancement factor of deformed

metals. The enhancement factor of deformed metals is higher than that of undeformed metals. Low density deformed metals have high enhancement factor unlike high density deformed metals. Strain causes a decrease in positron annihilation rates in deformed metals. Positron annihilation rates in deformed metals depend also on the nature of the metal.

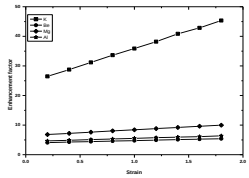

Fig. 1: Variation of enhancement factor computed using the perturbed hypernetted chain approximation with strain for some deformed simple metals.

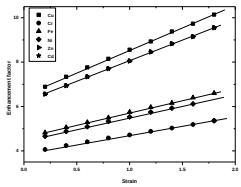

Fig. 2: Variation of enhancement factor computed using the perturbed hypernetted chain approximation with strain for some deformed transition metals.

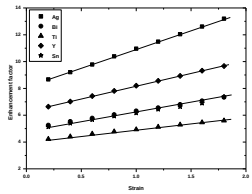

Fig. 3: Variation of enhancement factor computed using the perturbed hypernetted chain approximation with strain for some deformed inner transition metals.

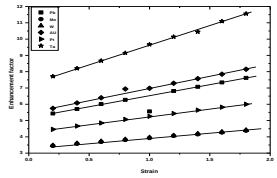

Fig. 4: Variation of enhancement factor computed using the perturbed hypernetted chain approximation with strain for some deformed inner transition metals.

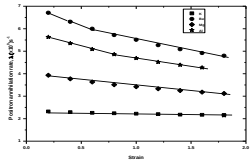

Fig. 5: Variation of positron annihilate rate in deformed simple metals with electron gas parameter.

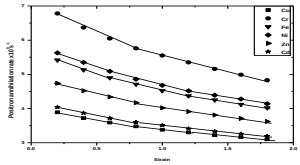

Fig. 6: Variation of positron annihilate rate in some deformed transition metals with electron gas parameter.

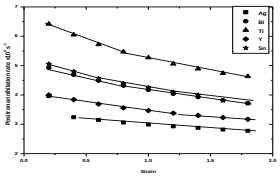

Fig. 7: Variation of positron annihilate rate in some deformed inner transition metals with electron gas parameter.

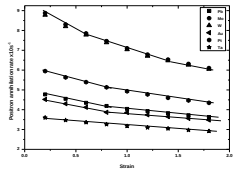

Figure 8: Variation of positron annihilate rate in some deformed inner transition metals with electron gas parameter.

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