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A Phenomenological Model for Positron Trapping at Dislocations*

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A multi-state trapping model involving positron trapping at dislocations and jogs is proposed, in which effect of positron detrapping can be omitted. According to this model the dislocations with variant jog density have different functions in positron annihilation process. The case that dislocation trapping is predominant and the open-space ratio between dislocation core and single-vacancy is emphatically discussed. Using the data in some literatures, we have estimated the positron annihilated rate at dislocations and the jog interval on the dislocation line. The results obtained seem reasonable.

1. INTRODUCTION

Many experimental results show that all the measured lifetime, S-parameter and ACAR (Angular Correlation of Annihilation Radiation) curve of positron annihilation after trapping at dislocations are close to that of positron annihilated in vacancies [1-6]. The positron lifetimes in the perfect region, at vacancy sites and after trapping at dislocations are listed in Table 1 of Ref. [1]. We can see from this Table that the positron lifetime after trapping at dislocations is close to but a little shorter than that at vacancy sites.To explain this phenomenon, some models and discussions are proposed.

M. Doyama et al [1, 2] thought that a positron is trapped and annihilated at jogs in dislocations where more open space is provided. They proposed that once a positron arrives at the core of a dislocation, it diffuses very quickly (pipe diffusion) until it finds a vacancy attached to the dislocation or a jog of the dislocation, then it is trapped and annihilated there.

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In 1980, L. C. Smedskjaer et al supposed: (1) the positron-dislocation binding energy is low ($E_b \leq 0.1$ eV); (2) the long positron lifetimes observed from samples containing dislocations are due to annihilations which occurred in defects associated with the dislocations (for example jogs). Based on these two assumptions, let $\lambda_d = \lambda_f$ (λ_d, λ_f are the annihilation rates of a positron at a dislocation core and in the perfect lattice, respectively) , they determined that all the changes in the annihilation parameters come from point-defect positrons associated with the dislocations.

We think that it is inadequate to suppose dislocation to be only a line linking the point-defects, because: (1) low binding energy could have high trapping rate [9], and dislocation contains a function which serves as a step to enlarge traps; (2) considering the open-space in expanding zone at edge-dislocation core, λ_d can never be equal to λ_f; as long as positrons annihilation at dislocation core, the measured annihilation parameter cannot be equal to that in the perfect region. The influence of positron annihilation at the dislocation core on an annihilation parameter cannot be neglected, especially for materials having a longer jog interval (such as in H.C.P. system).

In experimental analysis, 2-state trapping model has been used for metals containing lattice defects, multi-state trapping model still remains in the general discussion. This paper attempts to propose a trapping model that not only fully considers the function of dislocation as a step to enlarge traps [1, 2], but also reflects the influence of positron annihilated at dislocation line itself, and thereby to interpret some experimental phenomena.

2. TRAPPING MODEL

For a simple calculation we suppose: (1) the detrapping rate can be neglected; (2) a stronger trap source (jogs) exists on the dislocation lines, the lifetime of positron annihilations at jogs is equal to that at vacancy sites [1]. According to these suppositions, we proposed an annihilation mechanism illustrated in Fig.1. In Fig.1 horizontal lines represent

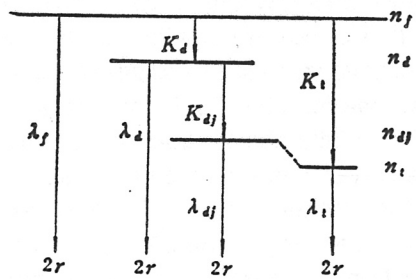

FIG. 1 The sketch shows the annihilation mechanism of positron at dislocation. (The dotted line between n_{dj} and n_t states has such meaning: these two states should be at same level if n_j is a single-vacancy trapping state. Although jogs could trap positrons from free state directly, but its rate is negligible compairing with the trapping rate at jogs in dislocations; furthermore, the former could be counted in trapping rate of n_t state if necessary.)

the possible positron states. The vertical arrows connecting the states represent the trapping rates, while the vertical arrows ending with the symbol 2γ represent the annihilation rates in these states. It can be seen in Fig.1 that the thermalized positrons are divided into 3 groups. The first group moves and annihilates in the perfect region. The second group is trapped at dislocations and moves along the dislocation lines, some of them annihilates in motion with electrons, others are trapped at jogs on the dislocation lines and finally annihilate there. The third group is trapped and annihilates at other vacancy-defect.

The rate equations can be written as

$$\begin{aligned} dn_f/dt &= -\lambda_f n_f - K_d n_f - K_t n_f; \\ dn_d/dt &= -\lambda_d n_d + K_d n_f - K_{dj} n_d; \\ dn_{dj}/dt &= -\lambda_{dj} n_{dj} + K_{dj} n_d; \\ dn_t/dt &= -\lambda_t n_t + K_t n_f. \end{aligned} \tag{1}$$

where the subscripts indicate the positron states: f corresponds to the free state; d, the state trapped at dislocations; dj, the state trapped at the jogs on the dislocation lines; t, the other trapping states and n is the probability of occupation of the respective state; λ, the annihilation rate; K, the trapping rate.

Let $t = 0$ correspond to the time when positron is completely thermalized, so the initial condition is

$$n_f(0) = 1;\ n_d(0) = n_{dj}(0) = n_t(0) = 0,\ t = 0$$

the solutions of Eq.(1) are

$$n_f(t) = e^{-\Gamma_f t}, \qquad \Gamma_f = \lambda_f + K_d + K_t; \tag{2}$$

$$n_d(t) = \frac{K_d}{\Gamma_f - \Gamma_d}\left(e^{-\Gamma_d t} - e^{-\Gamma_f t}\right), \qquad \Gamma_d = \lambda_d + K_{dj}; \tag{3}$$

$$n_{dj}(t) = \frac{K_d}{\Gamma_f - \Gamma_d}\left[\frac{K_{dj}}{\Gamma_d - \lambda_{dj}}\left(e^{-\lambda_{dj} t} - e^{-\Gamma_d t}\right) - \frac{K_{dj}}{\Gamma_f - \lambda_{dj}}\left(e^{-\lambda_{dj} t} - e^{-\Gamma_f t}\right)\right]; \tag{4}$$

$$n_t(t) = \frac{K_t}{\Gamma_f - \lambda_t}\left(e^{-\lambda_t t} - e^{-\Gamma_f t}\right). \tag{5}$$

The respective intensities of annihilation at the various states are

$$I_f = \int_0^\infty \lambda_f n_f(t)dt = \lambda_f/\Gamma_f; \tag{6}$$

$$I_d = \int_0^\infty \lambda_d n_d(t)dt = K_d \cdot \lambda_d/(\Gamma_f \cdot \Gamma_d); \tag{7}$$

$$I_{dj} = \int_0^\infty \lambda_{dj} \cdot n_{dj}(t)dt = K_d \cdot K_{dj}/(\Gamma_f \cdot \Gamma_d); \tag{8}$$

$$I_t = \int_0^\infty \lambda_t n_t(t)dt = K_t/\Gamma_f. \tag{9}$$

Therefore

$$I_f + I_d + I_{dj} + I_t = 1. \tag{10}$$

Usually, the experimental spectrum is the synthesis of several time spectra

$$S(t) = \lambda_f \cdot n_f(t) + \lambda_{dj} \cdot n_d(t) + \lambda_{dj} \cdot n_{dj}(t) + \lambda_t \cdot n_t(t)$$
$$= \sum_{i=1}^{4} I_i \cdot \frac{1}{\tau_i} \cdot e^{-\left(\frac{1}{\tau_i}\right)\cdot t}. \tag{11}$$

Equation (11) is the sum of four exponential decay terms, which can be denoted as 4 components. The τ_i and I_i (i = 1, 2, 3, 4) in Eq. (11) are the lifetimes and intensities of the components:

$$\tau_1 = \frac{1}{\Gamma_f} = \frac{1}{\lambda_f + K_d + K_t}, \tag{12}$$

$$I_1 = \frac{1}{\Gamma_f} \cdot \left(\lambda_f - \lambda_d \cdot \frac{K_d}{\Gamma_f - \Gamma_d} + \lambda_{dj} \cdot \frac{K_d}{\Gamma_f - \Gamma_d} \cdot \frac{K_{dj}}{\Gamma_f - \lambda_{dj}} - \lambda_t \frac{K_t}{\Gamma_f - \lambda_t}\right); \tag{12'}$$

$$\tau_2 = \frac{1}{\Gamma_d} = \frac{1}{\lambda_d + K_{dj}}, \tag{13}$$

$$I_2 = \frac{K_d}{\Gamma_f - \Gamma_d} \cdot \frac{\lambda_d - \lambda_{dj}}{\Gamma_d - \lambda_{dj}}; \tag{13'}$$

$$\tau_3 = \frac{1}{\lambda_{dj}}, \tag{14}$$

$$I_3 = \frac{K_d}{\Gamma_f - \lambda_{dj}} \cdot \frac{K_{dj}}{\Gamma_d - \lambda_{dj}}; \tag{14'}$$

$$\tau_4 = \frac{1}{\lambda_t}, \tag{15}$$

$$I_4 = \frac{K_t}{\Gamma_f - \lambda_t}. \tag{15'}$$

From (12) to (15) we have

$$I_1 + I_2 + I_3 + I_4 = 1. \tag{16}$$

Sometimes, we only use a mean lifetime to express this spectrum

$$\tau_M = (\tau_1 \cdot I_1 + \tau_2 \cdot I_2 + \tau_3 \cdot I_3 + \tau_4 \cdot I_4)/(I_1 + I_2 + I_3 + I_4)$$
$$= \frac{1}{\Gamma_f}\left[1 + \frac{K_d}{\Gamma_d}\left(1 + \frac{K_{dj}}{\lambda_{dj}}\right) + \frac{K_t}{\lambda_t}\right]. \tag{17}$$

3. DISCUSSIONS

3.1 Trapping Model Corresponding to the Dislocations in Four Different Cases

Case 1. Dislocation lines have no jog. In this case $K_{dj} = 0$. Therefore $I_{dj} = 0$, $I_3 = 0$

and $\tau_M = (1 + K_d/\lambda_d + K_t/\lambda_t)/\Gamma_f$. This is the result of the common 3-state trapping model [10, 11] and dislocation lines play a simple trapping role like other vacancy-defects do.

Case 2. Dislocation lines have a very high jog density. In this case the dislocation line should be described as a continuous strong bound state at jogs [8]. We have $K_{dj} \to \infty$. Therefore $I_d = 0$; $I_2 = 0$; and $\tau_M = (1 + K_d/\lambda_{dj} + K_t/\lambda_t)/\Gamma_f$, where all the positron trapping at dislocations are trapped and annihilate at jog's sites, and dislocation lines are only a step to enlarge trapping.

Case 3. In general cases. The dislocations in an actual metal sample always contain certain jogs, which is between the two extreme cases mentioned above. In order to underline the function of dislocation line as a step to enlarge trapping, Eq.(17) can be rewritten as follows

$$\tau_M = \frac{1}{\Gamma_f}\left[1 + \frac{K_d}{\lambda_{dj}}(1 - \varepsilon) + \frac{K_t}{\lambda_t}\right], \tag{18}$$

where

$$\varepsilon = (\lambda_d - \lambda_{dj})/(\lambda_d + K_{dj}). \tag{19}$$

ε decreases with increasing K_{dj} when λ_d, λ_{dj} are constant. In case 2 ($K_{dj} \to \infty$), one gets the minimum of ε; $\varepsilon_{min} = 0$; in case 1 ($K_{dj} = 0$) one gets the maximum of ε; $\varepsilon_{max} = (\lambda_d - \lambda_{dj})/\lambda_d$. In general case $\varepsilon_{min} < \varepsilon < \varepsilon_{max}$ and $\varepsilon/\varepsilon_{max} = \lambda_d/(\lambda_d + K_{dj})$ is the measure of the fraction of positrons annihilated at dislocation line in all positrons trapped at dislocations.

Case 4. When dislocation density is very high in material so that all positrons implanted are trapped at dislocations. In this case the measured positron lifetimes are always regarded as a single lifetime in some literatures [3-7], but there still exist two positron-annihilating-states in our trapping model, which are n_d and n_{dj}. This lifetime should be the mean lifetime of 2-state (n_d and n_{dj}) and is marked by τ_M^d (superscript d indicates that all positrons are trapped at dislocations). According to the 2-state trapping model [10, 11] we have

$$\tau_M^d = \frac{1}{\Gamma_d}\left[1 + \frac{K_{dj}}{\lambda_{dj}}\right] = \tau_v(1 - \varepsilon), \tag{20}$$

where it is assumed $1/\lambda_{dj} = \tau_v$. In order to estimate ε, we obtain from (20)

$$\varepsilon = (\tau_v - \tau_M^d)/\tau_v. \tag{21}$$

The values of ε from this estimation are listed in Table 1.

3.2 The Estimation of Open-Space Ratio between Dislocation Core and Single-Vacancy:

At first, we assume: (1) the screening effect of electron on positron can be neglected; (2) the electron density is homogeneous in a very small volume element which positrons

TABLE 1
ε values

	τ_v(ps)	τ_M^d (ps)	$\varepsilon = \frac{\tau_V - \tau_M^d}{\tau_V}$
Cu	180	176	0.022
Au	215	192	0.107
Al	240	228	0.050
Fe	175	169	0.034
Mo	200	175	0.125
Cd	232	211	0.091

have seen. Let V_0, V_d and V_v be the volume elements where the same amount of electrons is involved, in perfect region, in dislocation core and in single vacancy respectively. Generally, V_d and V_v are larger than V_0, and we can write $V_d = V_0 + \Delta V_d = V_0(1 + \Delta V_d/V_0)$ and $V_v = V_0 + \Delta V_v = V_0(1 + \Delta V_v/V_0)$; so the electron density in V_d and in V_v is $\rho_d \approx \rho_f (1 - \Delta V_d / V_0)$ and $\rho_v \approx \rho_f (1 - \Delta V_v/V_0)$ respectively, where ρ_f is the electron density in V_0. From $\lambda = \pi r_0^2 C \iiint \rho^-(r_+) \cdot \rho^+(r_+) d^3 r_+$ [12] we have

$$\lambda_d \sim \lambda_f [1 - \Delta V_d / V_0]; \tag{22}$$

$$\lambda_v \sim \lambda_f [1 - \Delta V_v / V_0]. \tag{23}$$

We define γ as the open-space ratio between a dislocation core and a single vacancy:

$$\gamma \equiv \Delta V_d / \Delta V_v = (\lambda_f - \lambda_d)/(\lambda_f - \lambda_v). \tag{24}$$

Examples listed in Table 2 can give us some quantitative ideas about the parameter γ.

3.3 The Calculation of λ_d, K_{dj} and L (Jog Interval)

Generally, the samples in which dislocation trapping is predominant are mainly prepared by plastic deformation, the jog density on dislocation line and K_{dj} are very large.

TABLE 2
The Estimation of the Open-Space Ratio γ.

Crystals	τ_f (ps)	λ_f(ns)$^{-1}$	τ_d (ps)	λ_d(ns)$^{-1}$	τ_v(ps)	λ_v(ns)$^{-1}$	$\gamma = \frac{\lambda_f - \lambda_d}{\lambda_f - \lambda_v}$
Al_2O_3[13]	149	6.71	166	6.02	223	4.48	0.31
Al	163[11]	6.14	183[9]	5.46	240[11]	4.17	0.34

Therefore τ_2 in Eq. (13) is only of the order of a few ten picoseconds, so it is hard to resolve into τ_1 and τ_2 from the shorter lifetime components and to get λd. Using the data in Table 2 and the model of edge dislocation core[9],and taking the open-space ratio γ to be 0.32 for crystals in Table 1, λ_d can be obtained from (24)

$$\lambda_d = \lambda_f - \gamma(\lambda_f - \lambda_v), \tag{25}$$

Then from Eq.(19) we have

$$K_{dj} = \frac{1}{\varepsilon}(\lambda_d - \lambda_{dj}) - \lambda_d. \tag{26}$$

The results estimated for λ_d and K_{dj} from (25), (26) are listed in Table 3. In order to estimate the jog interval, let $K_{dj} = f\bar{v}c_{dj}$, where C_{dj} is the number of jogs at unit length of dislocation line, $\bar{v}$ is the average speed of the positron during its movement along dislocation line, and f is the trapping efficiency when a positron passes a jog. As the jog interval L is defined as the distance between two jogs, we have

$$\bar{L} = 1/c_{dj} = f\bar{v}/K_{dj}. \tag{27}$$

Taking f = 0.1–1, $\bar{v} \approx 10^7$ cm/s [14] the values of $\bar{L}$ for different crystals can be obtained from their K_{dj}, and are listed in Table 3. Table 3 shows: (1) for cubic system L is about 10^3–10^4 Å, which seems to be a reasonable order of magnitude; (2) for hexagonal system (Cd), L is about 10^5–10^6 Å. It seems that the main slip plane of Cd is (0001) (base plane in H.C.P. crystals) and jogs may not be increased greatly in plastic deformation. When positrons are trapped at dislocation in hexagonal system like Cd, they annihilate mainly at dislocation core rather than at jogs (This case is contrary to that in cubic crystal). Therefore, the experimental studies of positron annihilation at dislocation core should be depend on the investigation in hexagonal system.

TABLE 3
The Estimative Value of λ_d, K_{dj} and $\bar{L}$

	τ_f(ps)	τ_v(ps)	λ_d(ns)$^{-1}$	ε	K_{dj}(ns)$^{-1}$	$\bar{L}$(Å)
Au	139	215	6.92	0.107	21.2	4.7×10^3—4.7×10^4
Cu	122	180	7.35	0.022	74.3	1.3×10^3—1.3×10^4
Al	163	240	5.51	0.050	21.3	4.7×10^3—4.7×10^4
Fe	117	175	7.64	0.034	74.9	1.3×10^3—1.3×10^4
Mo	117	200	7.41	0.125	11.9	8.4×10^3—8.4×10^4
Cd	199	232	4.80	0.091	0.55	1.8×10^5—1.8×10^6

Note: 1. The data of τ_f and τ_v are quoted from Ref.[1] except for τ_v of Fe [7]. 2. The values of ϵ are taken from Table 1.

Jogs play an important role in deformation dynamics, yet very few studies have been conducted so far. The above discussion shows that there is a close relationship between jog density and positron parameter. For this reason, it is possible to continue a further study for jogs using positron annihilation technique. The dispersion of data in deformation sample may have connections with the different concentration of jogs on dislocation line.

Besides, E. Kuramato et al [15] have measured the positron lifetime of plastically deformed single crystals of iron and applied the common 3-state trapping model (jogs and vacancy clusters are the sources of traps) to estimating the jog interval L, L = 36–360 Å. They thought that this is definitely too short, (probably one order of magnitude shorter). It may be due to the neglect of the function of screw-dislocation as a step to enlarge trapping. If applying the trapping model suggested above to estimate L using E. Kuramoto et al's data, the same order of jog interval $\bar{L}$ as that of iron in Table 3 can be obtained.

4. SUMMARY

This paper proposes a model of positron trapping at dislocation in which the detrapping can be omitted. This model not only fully considers the function of dislocation as the step to enlarge trapping, but also reflects the influence of positron annihilation at dislocation line itself.

Based on this model, the open-space ratio between dislocation core and single-vacancy has been discussed, and the annihilation rates of positron at dislocation core have been estimated. Using the data in some literature, we inferred the jog interval on the dislocation line. The results obtained seem reasonable. Therefore, it is possible to study the jog concentration by using positron annihilation technique.

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