On positrons irradiation in the defects of vacancy type

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Abstract. It was predicted the radiation of low energy positrons at their interaction with the defects of the vacancy type. Models of positron traps have been proposed. The energy transitions of positrons in the defects were calculated.

Introduction
It is known that a change in the physical properties of the irradiated and deformed metals, alloys and other materials is not only due to a change in the crystal structure of a solid, but also the electronic structure of defects. Investigation of the influence of defects on the electronic properties of materials allows to identify common patterns of electrons kinetic properties in imperfect crystals (using the method of positron annihilation) and to obtain information about the electronic structure of the defects. This is primarily due to the unique ability of positron to localize in areas with excess electronic charge in crystals, which are usually inherent to the defects in the crystal structure allowing to solve link issues of electronic and atomic structures [1 – 3]. The impact of defects on the parameters of positron annihilation in metals was first discovered by I.Y. Dekhtyar et al. [4, 5] for nickel and its alloys with iron. It is shown that plastic deformation Narrows the angular correlation curves, and count rate increases at the maximum. This is due to the presence of excess negative charge in the defect area during the formation of stress field around the dislocations. The resulting local dipoles cause the polarization of S- and d-bands and positrons are captured effectively by dislocation cores, which was confirmed by experimental data on the angular correlation and positron lifetime [6, 7]. The best capture occurs on polymers [8]. In this case, the energy spectrum of electrons in the defect is undergoing significant changes, the probability of positrons annihilation with conductivity electrons increases by reducing their annihilation in the atomic core and due to the high lifetime of positrons in these areas. Various models of positron capture are currently used to obtain quantitative results on the change in electronic structure of metals and alloys, as well as analytical relations between the intensity of photons annihilation and pulsed electron spectrum [9, 10]. We propose a model of positrons capture by vacancy traps and model of positron emission in the defects.

1. Physical models
Probability of positrons capture by trap can be provided when positron falling to defect area. Corresponding expressions for the probability can be obtained from quantum-mechanical calculations. Here are some model calculations.
1.1. One-dimensional potential hole

In the case of one-dimensional hole, the probability of positron escape from the defect can be represented as follows (Figure 1 a)

\[ \beta_i(E) = \begin{cases} 0, & \text{if } E > U_0, \\ 1, & \text{if } E < U_0. \end{cases} \]

where \( U_0 \) is depth of the potential hole of the trap.

1.2. Rectangular potential barrier model

In the first approximation, the probability of positrons escape from the traps is determined by Wentzel-Kramers-Brillouin method. For rectangular potential barrier required probability is represented in the form of (Figure 1 b):

\[ \beta_i(E) = \begin{cases} 1, & \text{if } E \geq V_0, \\ \exp \left\{ -\frac{2m_0}{\hbar} \sqrt{V_0 - E} (r_2 - r_1) \right\}, & \text{if } E < V_0. \end{cases} \] (1)

The probability for other models can be found similarly.

1.3. Model of positrons emission in vacancy defects

Considering the simplest Schrödinger equation it can be assumed that a positron-vacancy (cluster) system is characterized by certain values of the positron energy. In this case, transition of the positron from one state to another is carried out with a discrete loss of energy by emission. In the defects, positron emits low-energy photons, wavelength of which can be determined from the following relationship:

\[ \lambda = \frac{\hbar c}{E_\gamma}. \]
Setting the values of $E_\gamma$ energy in the range of $0.001 - 10$ eV, and assuming that $h = 6.62 \times 10^{-34}$ J/s, and $c = 3 \times 10^8$ m/s, $1 \leq \lambda \leq 10^4$ nm range can be obtained. Thus, the photon spectrum is above the visible region (by energy).

Positrons motion in rectangular potential hole with $U_0$ depth and a width can be considered as follows. It is obvious that the spectrum of doubly degenerate levels is continuous when $E > U_0$, and is discrete when $E < U_0$. Schrödinger equation in the range of $0 < x < a$ is written as:

$$\varphi + \frac{2m}{h^2} (E - U_0) \varphi = 0.$$

Solution of this equation has the following form:

$$\varphi = A_2 \sin(hx + \gamma), K = \sqrt{\frac{2m}{h^2} (E - U_0)}.$$

It is easy to find graphically and results in at least one discrete energy level $E_1$. The number of levels increases with the size of the hole and its depth.

2. Results and Discussion

$\beta_1(E)$ probability for various values of $U_0$ and $r_2 - r_1$ was calculated using the formula (1) in relation to the difference of the potential barrier height and positron energy $E$ (Figure 2). It can be seen that the probability is characterized as follows: the higher positron energy or the lower potential barrier height, the higher probability of positron escape from the trap. With increasing width of the potential barrier $\beta_1(E)$ value is reduced. The target probability behaves similarly for other capture models.

![Figure 2](image)

1–10; 2 – 9.3; 3 – 8.4; 4 – 7.0; 5 – 6.0; 6 – 5.0; 7 – 4; 8 – 3.0; 9 – 2.0; 10 – 1.5; 11 – 1.0; 12 – 0.75; 13 – 0.53

**Figure 2.** Dependence of the escape probability for positrons on the $(U_0 - E)$ value for various values of the potential barrier width $(r_2 - r_1) \times 10^{-10}$ m.

As can be seen from the calculations, the interaction potentials of positrons with vacancies, divacancies and vacancy complexes have the value of a few electron volts. In the first approximation, the positron-vacancy interaction or a complex can be represented in the form of the potential hole (or
the potential hole with a barrier). The vacancy estimate for molybdenum at a \( a \approx 0.32 \) nm and \( U_0 = 1.2 \) eV gives \( E_1 = 0.72 \) eV; for the vacancy of \( a \approx 0.64 \) nm there are two levels: \( E_1 = 0.37 \) eV; \( E_2 = 1.13 \) eV. From (2) it can be seen that the positron emission is the most possible for large vacancy complexes, the \( R \) size of which is several interatomic distances. For the energy of \( 10^{-3} - 10 \) eV the range is \( 2\AA \leq R \leq 200\AA \). Consequently, using the positron (by emissions) it is possible to study the defects by the above energy range and approximate size and concentration. In real crystals, the interaction of positrons will essentially vary from the model, although the physical nature of the process is not changed.

Conclusion
1. The models of the potential barriers of the positron traps is proposed, as well as the model of positrons emission in vacancy defects. The probability of positrons escape from the traps is calculated and it is shown that the higher positron energy or the lower potential barrier height, the higher probability of positron escape from the trap. With increasing width of the potential barrier \( \beta_i (E) \) value is reduced.

2. From the results obtained it follows that the positron emission is the most possible for large vacancy complexes, the \( R \) size of which is several interatomic distances. For the energy of \( 10^{-3} - 10 \) eV the range is \( 2\AA \leq R \leq 200\AA \). Using the positron (by emissions) it is possible to study the defects (its size and concentration).

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