Model Calculations of Edge Dislocation Defects and Vacancies in α-Iron Lattice

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Abstract. Two models of defects in perfect α-iron lattice were discussed. In the perfect bcc iron lattice $42 \times 42 \times 42 \ a_0$ ($a_0 = 2.87 \ \text{Å}$) an edge dislocation was created, moving the second half of the bulk on one $a_0$ distance. This action generates a little volume in the middle of the bulk which increases of the positron lifetime (PLT) calculated using the superimposed-atom method of Puska and Nieminen [1]. The result of 118 ps PLT in simple edge dislocation's model is in a good concurrence with earlier publications and experimental data [2]. Through the dislocation line one, two and three vacancies were localized. These models give the results for PLT of 146, 157 and 167 ps respectively. The computer simulations were performed using Finnis–Sinclair (FS) N-body potential.

1. Introduction
The knowledge of the behaviour of the basic metals as iron, chromium, beryllium and so on used in different scientific and industry branches like nuclear physics investigations and nuclear reactors through the process of exploitation is very important. There are very well known papers [1–2] that examine theoretical models of defects in metal lattices. This paper continues the consideration of models closer to the practice [3].

The basic theory of model calculating of defects in perfect lattices was given in [1,4,5]. Positron spectroscopy is capable of monitoring of micro-voids even at the earliest stages of their creation. The method is based on positron trapping at open volume defects and it was also used for the characterization of mono-vacancies and vacancy clusters [3,6].

In a perfect α-iron lattice matrix with dimension $42 \times 42 \times 42$ (total 18,522 atoms) a perfect edge dislocation was made by the next procedure. The coordinates $x_{i,j,k}$ and $z_{i,j,k}$ of the atoms are translated according to elasticity theory of dislocations before calculating the total energy of the model crystal:

$$x_{i,j,k} = x_{i,j,k} + U(x,z) \quad z_{i,j,k} = z_{i,j,k} + V(x,z)$$

(1)

where $U(x,z)$ and $V(x,z)$ depend on the parameters of bcc iron lattice.

Modeling the vacancies in the lattice and relaxation of the transformed matrix are made according to the procedures described in [3].
2. Calculation method

The PLT in defects is calculated according to the method of Puska and Nieminen [1]. The electron density distribution $n(r)$ is approximated by superimposing the spherical averaged charge densities $n_{at}(r)$ ($r$ is the distance from the atomic center) of an isolated atom:

$$n(r) = \sum_i n_{at}(r - R_i)$$

where $R_i$ is the position of the $i^{th}$ atom.

The Coulomb potential $V_C(r)$ is represented by superimposing the function $V_{at}(r)$ of distance $r$ from given atom:

$$V_C(r) = \sum_i V_{at}(r - R_i)$$

The correlation potential $V_{corr}(n(r))$ practically was determined by Boroński and Nieminen [4]. The total potential felt by a positron is:

$$V_{tot}(r) = V_C(r) + V_{corr}(n(r))$$

The Kimball–Shortly method is used for obtaining the positron wave function $\psi(r)$ by numeric solution of the Schrödinger equation. The energy eigenvalue is obtained in the every interaction while a saturated minimum value is reached.

The positron annihilation rate is expressed by:

$$\lambda = \pi r_o^2 c \int dr n_v(r) \left[ n_v(r) + n_c(r) + n_d(r) \right]$$

where $n_v = \psi_v^2$ is the density of positron, and $n_v$, $n_c$ and $n_d$ represents the density of valence, core and d-electrons respectively; $r_o$ is the classical electron radius and $c$ is the speed of light. $\Gamma_v$, $\Gamma_c$ and $\Gamma_d$ are the corresponding enhancement factors due to the correlation between positrons and electrons. For core electrons $\Gamma_c = 1.5$. According [7]:

$$\Gamma_v(n_v) = 8/3 + 1/6 r_v^3$$

where $r_v = (3/4\pi n_v)^{1/3}$ is the density parameter of the valence electrons. The value of $\Gamma_d = 2.42$ corresponding to PLT = 108 ps in the perfect bcc iron lattice was obtained (nearer to experimental data).

PLT [$\tau$] is given by:

$$\tau = 1/\lambda$$

3. Results and discussions

In Table 1 are given the main results of the model calculations made in this work. In figure 1 are shown graphically the same data.
Table 1: Main results of calculations

| No | Lattice state                                      | Calculated PLT [ps] | PLT according to earlier lit. data in [3] [ps] |
|----|---------------------------------------------------|---------------------|-----------------------------------------------|
|    |                                                   |                     | Theoretical | Experimental |
| 1  | Perfect lattice                                   | 108                 | 110         | 110          |
| 2  | One vacancy in the middle of bulk                 | 179                 | 181         | 175          |
| 3  | Edge dislocation                                  | 118                 | 117         |              |
| 4  | Edge dislocation + 1 vac. in the dislocation line | 146                 | 140         | 150          |
| 5  | Edge dislocation + 2 vac. in the dislocation line | 157                 |             |              |
| 6  | Edge dislocation + 3 vac. in the dislocation line | 167                 |             |              |

Figure 1. Comparison of the PLT from model calculating and the experimental data.

In figures 2, 3 are shown the positron wave functions in simple vacancy in the perfect lattice, edge dislocation.
4. Conclusions
The PLT of 118 ps for pure edge dislocation in $\alpha$-iron has been obtained. For the model with edge dislocation and vacancies in the dislocation line PLTs of 146, 157 and 167 ps respectively have been calculated. Our calculated results show deviations of about 20 % from the PLT in pure vacancies. However, the vacancy and vacancy clusters contribute to the PLT much more than the pure dislocation. Our results give information about the type of defects in $\alpha$-iron lattice in good agreement with the experiment. There are differences in the PLT for various vacancy localizations outside the dislocation and along the dislocation line. The PLT in the case of compact three-vacancy cluster is about 10 ps higher than the three-vacancy nano-void along the dislocation line.

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