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Model calculations of positron interaction in materials for ITER

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There will be conducted model calculations based on the local density approximation model, Kohn and Sham method based on two-component density functional theory. This is studied the defective structure of α-Fe and W, through simulations of the positron lifetime and momentum distribution of electrons in the defects of different sizes, including nano-defects containing hydrogen and helium atoms, produced by irradiation 14 MeV neutrons - a product of the fusion.

Key words: TCDFT, LDA, PLT, CDB, positron states, method of Kohn and Sham, momentum distribution

INTRODUCTION

The experimental apparatus used to determine the positron lifetime is improved significantly and thus exploring angular correlation of the γ-quanta. There is established the influence of temperature on annihilation spectra. Confirmation of anisotropy in the angular distribution of the γ-quanta in many crystals allows studying the Fermi surface forms not only in pure metals, but and in different combinations of alloys. Modern computers and modern methods based on First Principle are opening up new possibilities for determining the microscopic picture, due to the decay processes in fusion materials. Research in this area is developed. Methods for calculating the positron lifetime in the material are able to predict with great accuracy the structural defects. This thesis presents calculating of positron lifetime in Fe and W (and momentum distribution of the electrons), based on the Two Component Density Functional Theory [TCDFT] in conjunction with local density approximation [LDA] used in calculation of the exchange correlation functional. This is a powerful method for studying the properties of thermonuclear materials in atomic order.

METHODOLOGY

Density functional theory, method of Kohn and Sham, local density approximation

Using density functional, we have consideration the dependence of the quantum system from one parameter in which are included the wave functions of all electrons [1]:

$$n(r) \rightarrow \varphi(r_1, r_2, \ldots r_k) \rightarrow V(r). \quad (1)$$

Electron density (the density of the probability distribution of the electrons in the quantum system) is set as a function of the radius vector of an arbitrary electron:

$$n(r) = k \int d^3 r_2 \int d^3 r_3 \ldots \ldots \int d^3 r_k \varphi^*(r, r_2, \ldots r_k) \varphi(r, r_2, \ldots r_k). \quad (2)$$

In view of the theorem of Hohenberg-Kohn [2] the total energy of the ground state of an electronic system of many electrons can be calculated as a functional of the electron density [3]:

$$E[n(r)] = T[n(r)] + U[n(r)] + \int V_{ext}(r) n(r) d^3 r. \quad (3)$$

According to Method of Kohn and Sham [4], for a system of interacting electrons in an external field $V_o(r)$, can be made a comparison with a system of non-interacting electrons with local potential $V_{s,o}(r)$ such that the ground state of the densities for the two systems - $n(r)$ and $n_s(r)$ will be derived from the following equations:

$$\Big(-\frac{\nabla^2}{2} + V_{s,o}(r) \Big) \varphi_i(r) = \varepsilon_i \varphi_i(r), \quad (4)$$

$$\Big(-\frac{\nabla^2}{2} + V_o(r) + \int \frac{n(r')}{r - r'} dr' + \frac{\delta E_{ex}}{\delta n(r)} \Big) \varphi_i(r) = \varepsilon_i \varphi_i(r). \quad (5)$$

where $v = \delta E_{ex} / \delta n(r)$ is the exchange-correlation potential for a one particle and the part $\int \frac{n(r')}{r - r'} dr'$ characterized Coulomb potential. There are undefined parts E_{xc} and E_c^{e-p}, approximations from which

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the results can be highly dependent. Using LDA [4,5] is an opportunity to overcome this problem for Functional of exchange correlation energy E_{xc} should be used approximation of Functional exchange correlation energy of a homogeneous electron gas e_{xc}^{hom} for an electron multiplied by density in of electrons in the integral relation:

$$E_{xc}^{LDA}[n] = \int drn(r)e_{xc}^{hom}n(r). \quad (6)$$

In the inhomogeneous system allows changing the constant density n_0 to local $n(r)$ displayed by quantum Monte Carlo simulations.

Two-component density functional theory, annihilation rate and contact density, effect of the electron-positron correlation on the annihilation rate of the positron

In order to interpreted participate in the system of two types of particles (electrons and positrons) density functional theory should be complete its two component extension. Functional of the total energy $E[n_-,n_+]$ electron-positron system in an external potential V_{ext} is the sum of functional of positrons and functional electrons in distinct and functionally of the Coulomb interaction of these two systems (MIKA-DOPPLER) [4,6]:

$$E[n_-,n_+] = F[n_-]+F[n_+] + \int drV_{ext}(r)[n_-(r)-n_+(r)] - \int dr\int dr'\,\frac{n_-(r)\,n_+(r')}{|r-r'|}+E_c^{e-p}[n_+,n_-] \quad (7)$$

with the following significance of the one-component density functional corresponding to a particular type of particle:

$$F[n] = T[n]+\frac{1}{2}\int dr\int dr'\frac{n_-(r)\,n_+(r')}{|r-r'|}+E_{xc}[n], \quad (8)$$

where T[n] is the functional of the kinetic energy of interacting electrons or positrons E_{xc} corresponds to part exchange correlation energy and $E_c^{e-p}[n_+,n_-]$ is a functional of the electron-positron correlation energy.

The main characteristic of positron annihilation, providing information about the structural features of the environment is the lifetime of positrons τ or annihilation rate λ ($\tau=\frac{1}{\lambda}$). The lifetime of the positron is a function of the positron densities in place of annihilation [7]:

$$\lambda = \frac{1}{\tau} = \pi r_0^2 c\int n_-(r)n_+(r)\gamma(r)d(r), \quad (9)$$

where $\gamma=\gamma[n-(r)]=1+\frac{\Delta n_-}{n_-}$ is a correlation function describing the increase in electron density due to the Coulomb attraction between the electron and the positron. This effect is called a enhancement [4] r_0 is the radius of the electron in its classical sense.In the LDA, annihilation rate is calculated in the form:

$$\lambda = \pi r_0 c\sum_i\int dr\ \gamma_i^{LDA}|\varphi_+(r)|^2|\varphi_i(r)|^2, \quad (10)$$

where φ_+ is the wave function of the positron and $\gamma_i(r)$ is the enhancement factor for the i^{th} electronic state.There is can be made approximation of a physical meaning of two particles, electron-positron wave function:

$$\varphi_i^{e-p}(r) = \varphi_+(r)\varphi_i(r)\sqrt{\gamma_i(r)}, \quad (11)$$

where you can make a comparison of annihilation rate to each electron orbital:

$$\lambda_i = \pi r_0 c\int dr\ \gamma_i|\varphi_+(r)|^2|\varphi_i(r)|^2. \quad (12)$$

The correlating movement strongly depends on the initial condition i (without the presence of a positron). Should be the core and the localized d and f valence electrons to be a less affected by the positron than valence orbitals. The correlating the movement strongly depends on the initial condition of electron i (without the presence of a positron). The positron annihilation rate as a function of the momentum p of the annihilating pair - electron-positron, is determined by the following integral form:

$$\rho(p) = \pi r_0 c\sum_i|\int e^{ip.r}dr\ \varphi_+(r)\varphi_i(r)\sqrt{\gamma_i(r)}dr|^2. \quad (13)$$

With momentum distribution for density picture of the annihilation rate in LDA have the following recording:

$$\rho(p) = \pi r_0 c\sum_i\int e^{ip.r}dr\gamma_i^{LDA}|\varphi_+(r)|^2|\varphi_i(r)|^2. \quad (14)$$

Positron states

The correlating movement strongly depends on the initial condition i (without the presence of a positron). Should be the core and the localized d and f valence electrons to be a less affected by the

positron than valence orbitals. The correlating the movement strongly depends on the initial condition of electron i (without the presence of a positron). A approximation for examination of positron conditions in condensed matter is an estimate of the density of the positrons and that the electronic gas, in which takes place the annihilation. Addition to functional energy of the system is electron-positron correlation potential $E_c^{e-p}[n_+,n_-]$. The outer potential is in function depending on both – by the electronic and by the positron densities:

$$n_-(r) = \sum_{\xi_i \le \xi_f} |\varphi_i(r)|^2, \qquad n_+(r) = \sum_i^N |\varphi_i^+(r)|^2. \tag{15}$$

Using the self-consistent procedure of Kohn-Sham [2, 8] are obtained in the ground state electronic and positron densities, which requires calculation of one-particle Schrödinger equation for positron wave functions. For the positron is the same in the form:

$$-\frac{1}{2}\bigtriangledown^2 \psi_i^+(r) + V_{eff}(r)\psi_i^+ = \xi\,\psi_i^+(r), \tag{16}$$

effective potential is written as:

$$V_{eff}(r) = \phi(r) + \frac{\delta E_{xc}[n_+]}{\delta n_+(r)} + \frac{\delta E_{xc}^{e-p}[n_+,n_-]}{\delta n_+(r)}. \tag{17}$$

The last two parts are included in the so-called correlation potential - V_{corr}, and Coulomb potential has the following form:

$$\phi(r) = \int dr' \frac{-n_-(r') + n_+(r') + n_0(r')}{|r-r'|}, \tag{18}$$

where n_0 is the charge density of the outer potential involved in the complete functionality of the system [2].

RESULTS

Positron state is calculated taking into account the reduction in the exchange-correlation energy E_{ex}, which decrease with given coordinates depends only on the electron density at the corresponding point. The rate of annihilation (and the positrons lifetime - PLT, in a given environment) is calculated as the integral of the local annihilation rates.

PLT

Fig. 1 (a) and (b) shows the change of the lifetime of positrons in the tungsten in increasing vacancy cluster 1 to 30 vacancies filling successively with atoms of hydrogen and helium [10–12]. There is observed reduction in the value of the lifetime of a positron with an increase in the impurity atoms in the vacancy cluster. Increasing the concentration of impurity atoms in the vacancy clusters leads to saturation of the lifetime of the positron and the values at the same has approximate perfect lattice without defects. The conclusions from results of Figure 2 (a) and (b) for iron are similar to findings from the results for the positron lifetime in tungsten.

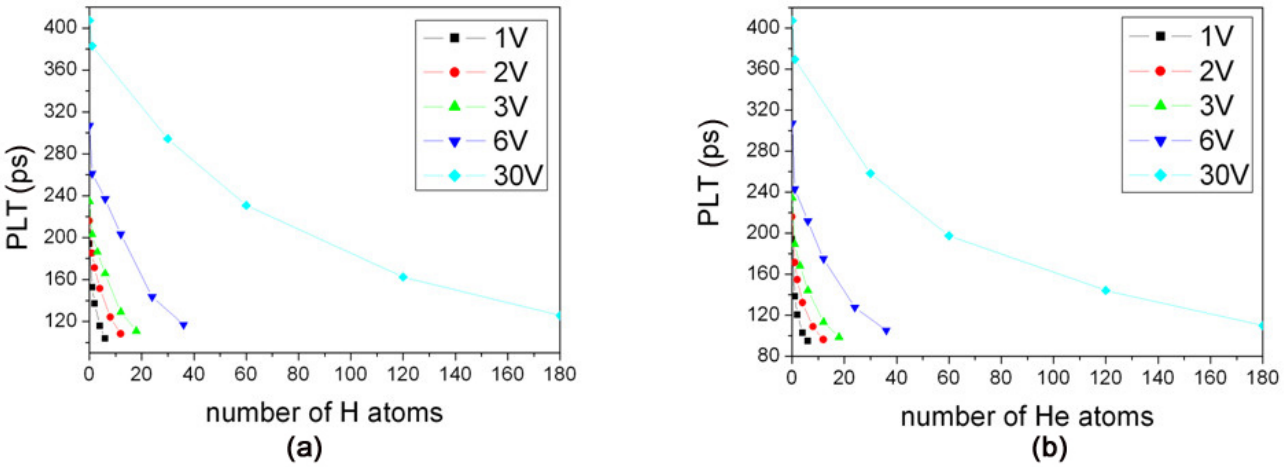

Fig. 1. (a) Comparison of the values of the lifetime of positrons in tungsten with an increase of the impurity hydrogen atoms in 1, 2, 3, 6 and 30 vacations [9]. (b) Comparison of the values of the lifetime of positrons in tungsten with an increase of the impurity helium atoms in 1, 2, 3, 6 and 30 vacations [9].

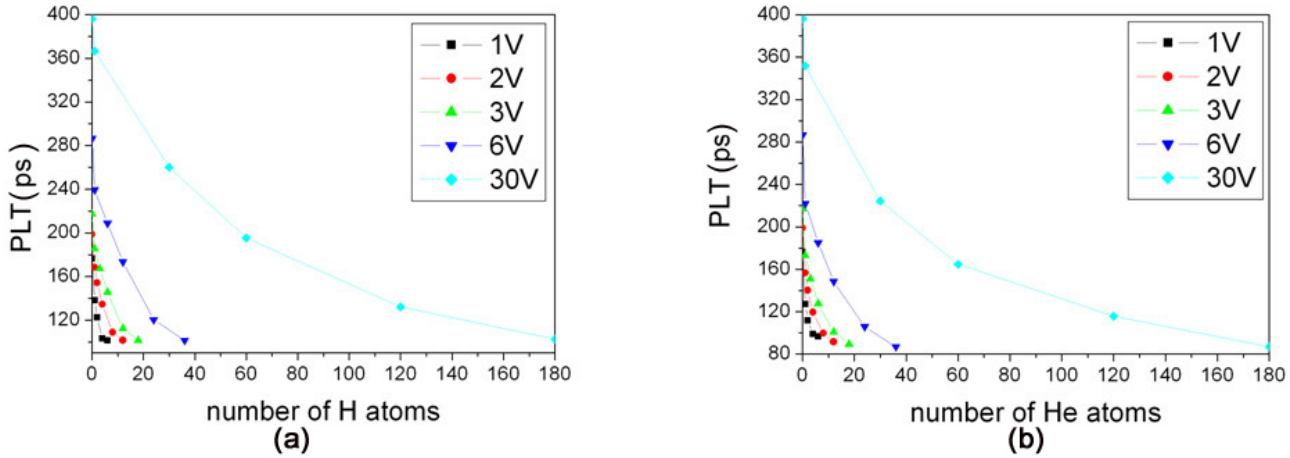

Fig. 2. (a) Comparison of the values of the lifetime of positrons in iron with an increase of the impurity hydrogen atoms in 1, 2, 3, 6 and 30 vacations [9]. (b) Comparison of the values of the lifetime of positrons in iron with an increase of the impurity helium atoms in 1, 2, 3, 6 and 30 vacations [9].

CDB

Coincidence Doppler Broadening (CDB) is interpretation of the momentum distribution for electrons witch is projected with the S (shape) and W (wing) parameters, where S parameter is corresponded of the annihilation with a valance electrons and W parameter corresponded of the annihilation with a core electrons.With an increasing number of vacancies in the cluster are visible expressed extreme values (maximum at S parameter and minimum at W parameter) at saturation with hydrogen atoms. It follows that at a given electron density, relative contributions of the valence electrons to the annihilation is maximum, and for a core electrons is minimum. Where the density is changed is observed increasing in the contribution of core electrons and the reduction from the valence electrons.

There are considered this parameters in case when the impurity atoms are helium Fig. 4 (a) and (b). Maxima for the S parameter and minima for the W parameter as in saturation with hydrogen were not observed. The explanation for this fact may be associated with the specificity of hydrogen and helium electronic structures.

In Figures 5 (a) and (b) are considered the parameters S and W as a function of the increasing number

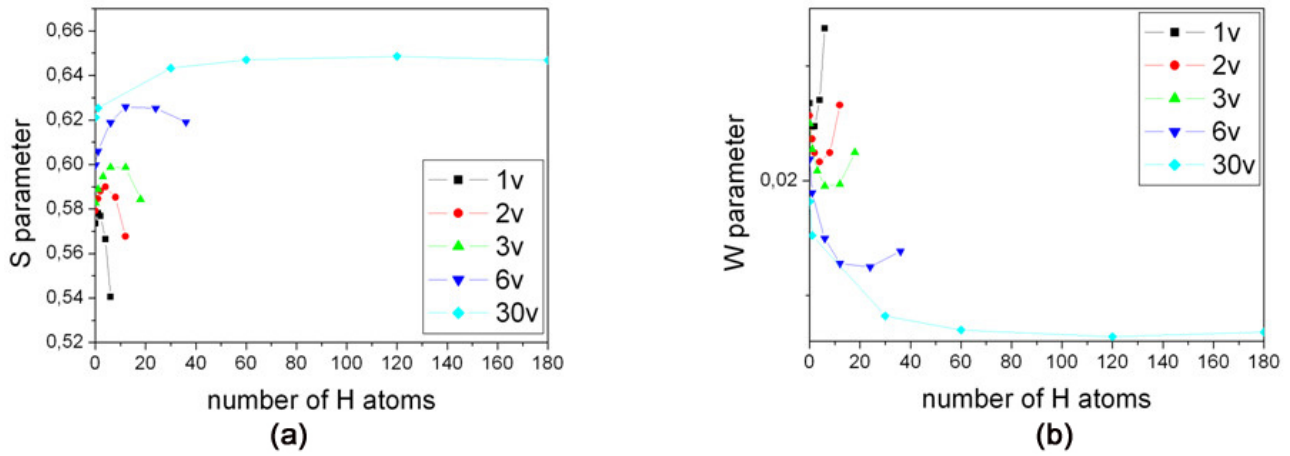

Fig. 3. (a) Comparison of the values of S parameters in the tungsten with increased number of addition hydrogen atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v). (b) Comparison of the values of W parameters in the tungsten with increased number of addition hydrogen atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v).

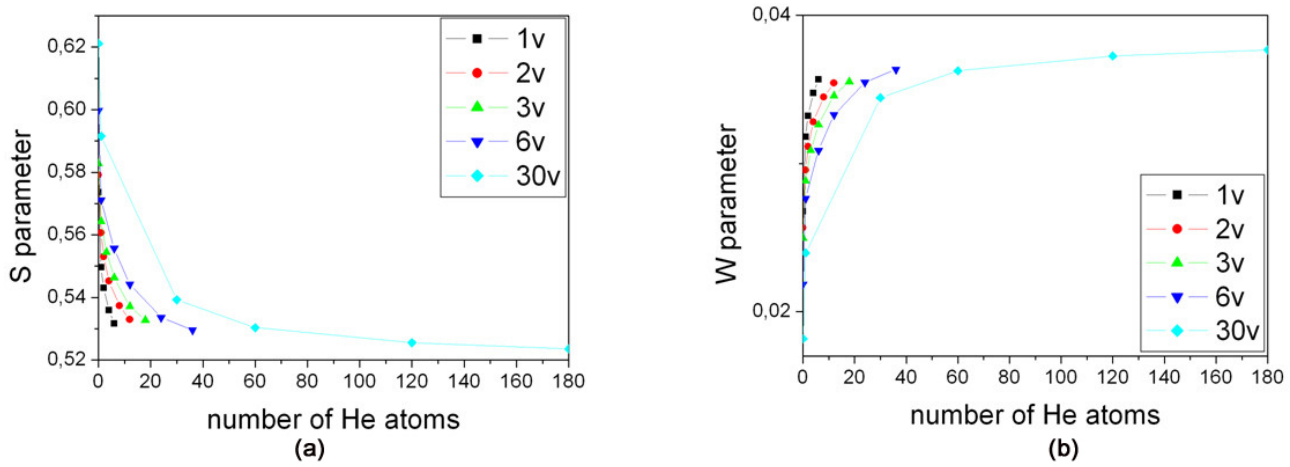

Fig. 4. (a) Comparison of the values of S parameters in the tungsten with increased number of addition helium atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v). (b) Comparison of the values of W parameters in the tungsten with increased number of addition helium atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v).

of hydrogen atoms, in clusters of vacations, containing 1, 2, 3, 6 and 30 vacations.

There is seen that the extremum in iron has more steepen compared with the extremum in tungsten. This effect is due to the electronic structure of the iron, tungsten and hydrogen, and the annihilation of the positron with electrons from various orbitals. Annihilation occurs mainly with electrons of s and d orbitals. Since iron has 2 more electrons from tungsten in its valence d orbital, it is reasonable to expect an increase in the probability of annihilation in this orbital Fig. 6 compared with the same in tungsten, and higher values for the S parameter. For the same reason, in case of defects, it is expected annihilation generally to be higher in the iron. Behavior and values of the annihilation of the hydrogen electrons are similar in both cases. In consideration figures Fig 6 (a) and (b) is presents the relative contribution to the annihilation, ie higher rate of annihilation in iron (in the presence of defects).

At Figure 7 (a) and (b) is shown the dependency of the S and W parameters with the increasing number of helium atoms. In a comparison between the

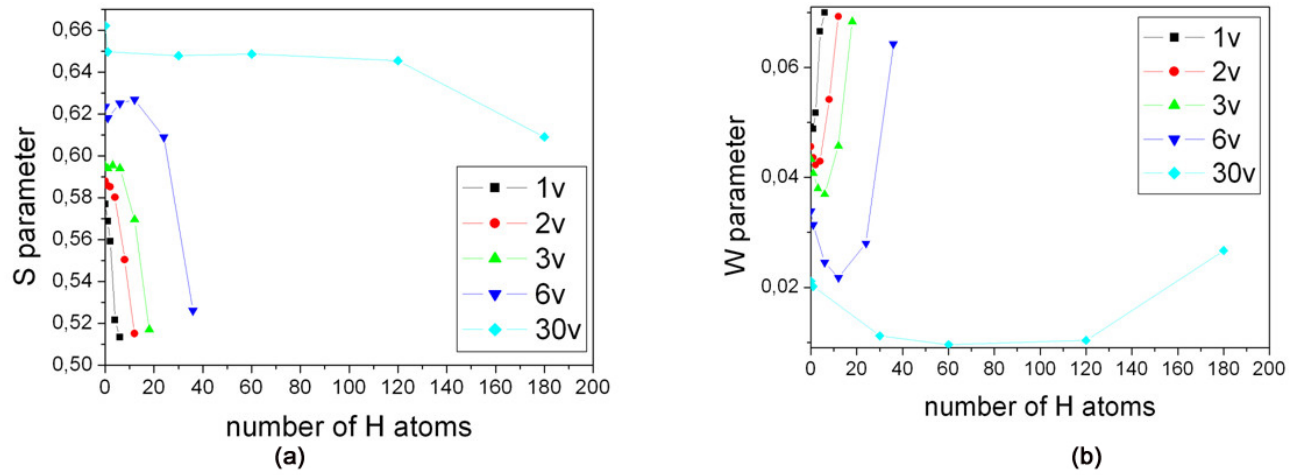

Fig. 5. (a) Comparison of the values of S parameters in the tungsten with increased number of addition hidrogen atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v). (b) Comparison of the values of W parameters in the tungsten with increased number of addition hidrogen atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v).

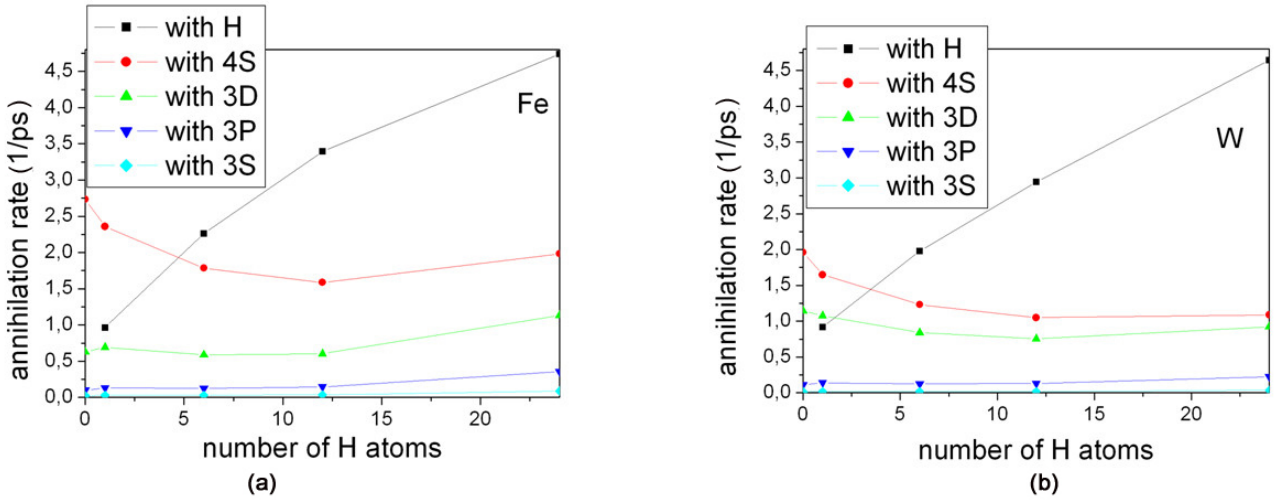

Fig. 6. (a) Speed annihilation in orbitals in vacancy cluster from 6 vacancies in iron with depending of the number of hydrogen atoms in the cluster. (b) Speed annihilation in orbitals in vacancy cluster from 6 vacancies in tungsten with depending of the number of hydrogen atoms in the cluster.

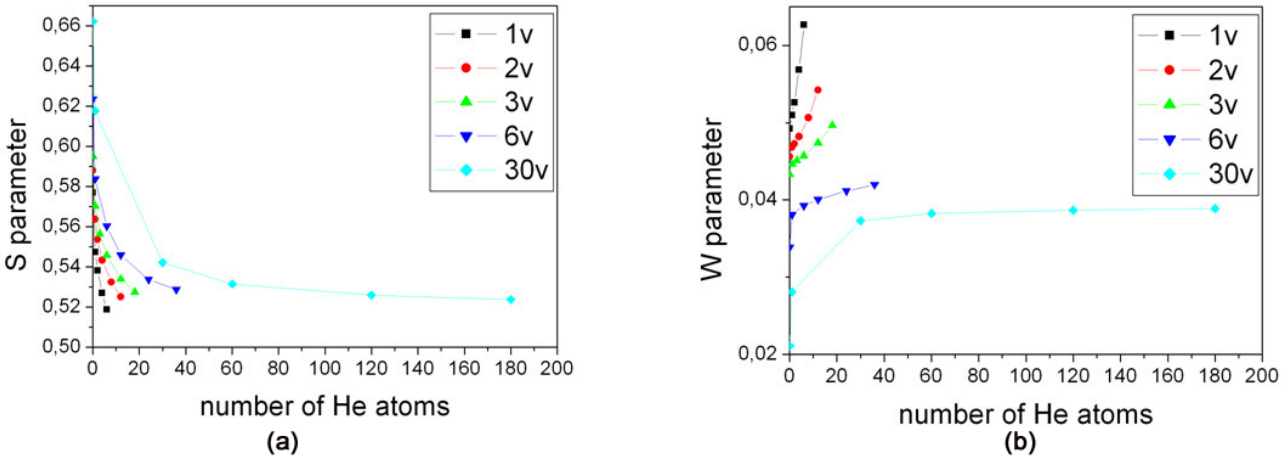

Fig. 7. (a) Comparison of the values of S parameters in the iron with increased number of addition helium atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v). (b) Comparison of the values of W parameters in the iron with increased number of addition helium atoms in different vacancy clusters (1v, 2v, 3v, 6v, 30v).

graphics of Fig. 3 and Figure 7 we can see a wider range of variation of the values for the different S and W parameters in iron than tungsten. The explanation of this fact, again is in the specificity of the electronic structure on the two elements.

CONCLUSIONS

Since iron has two electrons more from tungsten in its free d orbital, it is logical to expect increased annihilation in this orbital, and higher values for the S parameter. For the same reason, in case of defects, it is expected annihilation generally is higher in the iron. In some electron density the relative contribution of valence electrons to annihilation is maximum, while the same relative contribution from the core electrons is minimum. Where the density is changed the relative contribution of the core electrons is increased while from the valence is decreased.

By increasing the number of impurity atoms in the small vacancy clusters (1, 2 and 3 vacancies), the positron lifetime in iron and tungsten approach, which is a consequence of a changing in the condi-

tions in which is flow annihilation. The overlap of the wave functions of the positron with those of electrons from the material that study becomes less and the basic process is determined by the electrons from cover of the impurity atoms.

When clusters are small enough can be expected the interacting electrons on the boundary of the defect to have a relatively larger contribution to the annihilation. The functional of the density of the exchange-correlation energy is expected to have higher values in a small volume of the defects. The influence of the exchange-correlation energy over to the general functional after a certain size of defect is changed the trend on the S and W parameters in the saturation of the same defect with impurity hydrogen atoms.

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МОДЕЛНИ ПРЕСМЯТАНИЯ НА ПОЗИТРОННОТО ВЗАИМОДЕЙСТВИЕ В МАТЕРИАЛИ ЗА ИТЕР

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(Резюме)

Пресметнати са позитронната и електронната вълнови функции във волфрам и желязо, чрез локалния функционал на плътността на базата на TCDFT. Установено е съществуването на корелация между времето на живот на позитроните, импулсното разпределение на електроните (S и W параметрите) и концентрацията на образуваните дефекти.

Тъй като желязото притежава 2 електрона повече от волфрама в своята свободна d орбитала, то е логично да очакваме увеличена анихилация в тази орбитала, спрямо същата при волфрам, както и по-високи стойности за S параметъра. По същата причина, при наличие на дефекти, се очаква анихилацията като цяло да е по-висока при желязото. При определена електронна плътност относителния принос на валентните електрони, към анихилацията, е максимален, докато същият от свързаните е в своя минимум. При промяна на тази плътност се отчита покачване на относителния принос на свързаните електрони и намаляването му от валентните. Измерванията в стойностите за S и W параметрите са по-големи при желязо отколкото при волфрам. Обяснението е в спецификата на електронната структура на двата елемента.

С увеличаване на броя примесни атоми в малките ваканционни клъстери (1, 2 и 3 ваканции), времето на живот на позитрона при желязо и волфрам се доближава, което е следствие от промяната на условията в които протича анихилацията. Препокриването на вълновите функции на позитрона с тези на електроните от съответния материал, който изследваме става все по-малко и основно процесът се определя от електроните от обвивката на примесните атоми.

Когато клъстерите са достатъчно малки може да се очаква взаимодействащите си електрони на границата на дефекта да имат относително по-голям принос към анихилацията. Функционалът на плътността на обменно-корелационната енергия се очаква да има по-високи стойности в по-малки обеми на дефектите. Влиянието на обменно-корелационната енергия върху общия функционал след определен обем на дефекта променя тенденцията на S и W параметрите в насищането на същия дефект с примесни водородни атоми.