**Positron annihilation on FeB complex: the searching estimations**

The difference in both the size of atoms and their electron structure in FeB complex is the source of forming the strains and deformations in the crystal lattice of silicon. The thermalized positron has the excursion length [1] equal, approximately, to ~ 1000 Å over the temperature range ~25 to 300 K and thus may form a many-body electron-positron localized state at the FeB complex in case its concentration is not very much lower than ~ 1015 – 1014 cm−3. The rate of this localization (k) with the consequent emission of annihilation gamma-quanta out of the volume of FeB complex is determined by measuring the positron annihilation characteristics. The latter are known to be determined by both the open volume and chemical nature of atoms involved in a defect [1]. The positron probing of defects becomes indispensible when other methods (e. g., such as EPR and IR spectroscopy), are not informative ones. In addition, also one may point out to the NMR and acoustic nuclear magnetic resonance that are not used for studying nuclei having zero nuclear spin.

**Positron Trapping.** To detect acoustic loading on a defect by positron annihilation one needs to have positron states related to it. A propensity of the thermalized positron to be localized in the region of negative effective charge related to the impurity atoms of different nature together with the open volume of a defect is generally accepted to describe by the trapping model [2]:

(1)

where the resulting probability of 2–gamma annihilation is measured assuming that the positron trapping rate k allows one to determine conditional probability ηof the event of 2–gamma annihilation of e+e− pair in the centers studied [2, 3]:

. (2)

The averaged positron lifetime τav is expected to depend on the acoustic loading, and τ0 is a positron lifetime out of a defect; this value is not measured. As τ0 magnitude it is generally accepted to use so-called τbulk value which is, e.g., determined experimentally for a defect-“free” material. The cross-section of positron localization with the subsequent 2–gamma annihilation *σ*+ determines the value of k:

(3)

where C is the coefficient of localization of positron pair at the center [1]; C = N(FeB)×v+ (v+ is the velocity of positron on its excursion length ~ (4τD+)0.5 where τ and D+ are the positron lifetime and the positron diffusion coefficient, respectively [1, 2]. Over the range of concentrations N(FeB) from 2·1013 cm−3 to ~1014 cm−3 the *k* value k{N(FeB); *σ*+ = 10−12 cm2} increases from ~0.5 to ~ 1 ns−1. In the case of increase of the positron trapping cross section up to 10−11 cm2 for the same range of concentrations of defects the value of the positron trapping rate increases from ~2 to ~10 ns−1. This range of the k magnitudes is well detected using both the spectroscopy of positron annihilation lifetime (PALS) and coincidence Doppler broadening (CDB) of the annihilation radiation.

The k value may turn out to be more pronounced due to yet much larger values of cross-sections. It should be noted in this connection that large cross sections ~ 3.32 ×10–11 cm2 and ~ 10–10 cm2 related to excitonic Auger capture of holes and multiphonon emission capture, respectively, have been reported for the FeB complex [4, 5].

Thus, one can expect observing the emission of annihilation radiation modulated by ultra-sound (US) loading on FeB centers whose association was shown to be accelerated in the solar cells [6]. Special interest in this connection is a paradoxical divergence in the frequency dependency of reduced energy barrier for Fe ion migration when using longitudinal and transverse waves. This intriguing dependency observed suggests forming the anisotropic deformation field ambient FeB complex which consists of the atoms of Si, Fe, B and others, such as oxygen and carbon in Cz-grown silicon.

 **Elementally-Specific Annihilaton Radiation.** The ion cores of different chemical nature in the atomic environment of the positron makes the emission of the high-momentum annihilation gamma-quanta to be elementally specific one inasmuch as the wave functions of the ion core electrons *retain to a great extent their atomic character in solids*. The data obtained for these electron-positron states by the angular correlation of annihilation radiation (ACAR) of high resolution for the poly-crystaline metallic Fe (in its γ-phase), as well as for so-called β-B and dislocation-free n–type FZ–Si [111] single crystal (grown by the floating-zone technique) are shown in Fig. 1. The electron-positron ion radii rm obtained by these data are close to the values of ionic radii: for different coordination numbers ri(Fe2+; Fe3+) and ri(Si4+) values range 0.63 to 0.92 ×10−8 cm and 0.4 to 0.54×10−8 cm, respectively; the ionic radius of boron ri(B3+) is equal to ≈0.27×10−8 cm [10, 11]. The rm (B) value is larger than the length of ionic radius ri(B3+) as the maximum overlapping of the ion core electrons and positron wave functions [12] is shifted outwards the ion core of B atom more effectively than it takes place for ion cores of Fe and Si atoms.

Fig.1. The high-momentum component of the elementally-specific angular correlation of annihilation radiation (ACAR) spectra obtained by the spectrometer of high geometrical angular resolution Δ ≈ 0.48×10−3 m0c (m0 and c are the electron mass and the light velocity, respectively). The measurements were performed at room temperature and their results are given for boron (dots), silicon (squares), and iron (triangles). The electron-positron ionic radii rm were restored (see [7, 8, 9] for more detail). The lines are the results of fitting, the slopes of the linear functions are obtained with the accuracy which is characterized by the standard deviation / the Pearson’s coefficient, respectively: 0.042/0.998 (Fe), ≈ 0.114/0.956 (B) and 0.101/0.99 (Si).

The many-body electron positron state at FeB complex modulated by US loading must generate similar *spectrum* of high-momentum components of 2–gamma annihilation radiation.

The resulting emission of 2–gamma annihilation radiation out of Fe, Si, and B subvalent and ion core electron states to be probed with positrons follows the squares under the lines in Fig.1. Similar trend should be observed for the many-body electron-positron state at FeB pair including its complexes with common impurities in Cz-Si. The relative contributions of these elementally-specific channels of annihilation radiation depend on the both configuration and symmetry of FeB complex, thus manifesting themselves in the mutually interrelated both the average positron lifetime, τav, and conditional probabilities, η; see Eq.1 and Eq. 2. The numeral values of these parameters will be changed under US loading, thus allowing one to observe the acoustic-positron annihilation phenomena. Instead of a high-precision ACAR measurements, the coincidence Doppler broadening (CDB) of the annihilation radiation (CDB) may be used for detecting the electron-positron annihilation in the ion cores of atoms involved in the microstructure of defects, with the subsequent analysis of S-W-parameters of CDB spectra [1].

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