Calculations of Positron Annihilation Parameters in Fe-0.3%wtC Structure

B. Kolev, **E. Popov, T. Troev, S. Peneva**

Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 72 Tzarigradsko shaussee Blvd., BG-1784 Sofia, Bulgaria

Abstract. Hierarchical vacancy clustering in the sample of two components (iron and carbon) was calculated by the methods of the positron annihilation. We present the results of positron lifetime (PLT) for the Fe-0.3%wtC. The calculated value of PLT for a perfect matrix without defects is equal to 216.9 ps. The values of PLT calculated for one vacancy in Fe-0.3%wtC – 246.61 ps. It was established a dependence between the PLT and the increasing vacancy cluster. Analysis has been done for samples with increasing impurity atoms of helium and hydrogen in the vacation clusters. The calculations are based on the Two-Component Density Functional Theory (TCDFT), using the Local Density Approximation (LDA) method. In addition, information from the momentum distribution of electrons in the sample is extracted and synthesized.