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Model Calculations of Positron Lifetime and Momentum Distribution of Electrons in Tungsten Carbide

E. Popov, B. Kolev, T. Troev, L. Petrov

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

Abstract. Vacancy clustering in the two sublattices of hexagonal tungsten carbide was calculated by means of model calculations of positron annihilation. The Density Functional Theory and its Two-Component extension (TCDFT) had been implemented in the Local Density Approximation (LDA) method. The preliminary result of positron lifetime calculation in tungsten carbide (WC) lattice without defects has a value equal to 98.41 ps. The results from calculations of WC lattice containing one vacancy is equal to 127.02 ps. for WC-$1V_C$ and for WC-$1V_W$ is equal to 172.01 ps., respectively. Comprehensive analysis for WC vacation cluster, containing hydrogen and helium atoms have done. We established correlation between the lifetime of the positron and momentum distribution of the electrons and the electron density in the defects.