

"Physico-Chemical nanomaterials science"

Parameterization algorithms for mixed positron-electron interaction in nanostructured substances

A. Ingram^{1,2}

¹ *Opole University of Technology, 75, Ozimska str., 45370 Opole, Poland*

² *Scientific Research Company "Carat", 202, Stryjska str., Lviv, 79031, Ukraine*
E-mail: a.ingram@po.opole.pl

At the present, the phenomenon of electron interaction with its antiparticle (positron) known as positron-electron annihilation in lifetime (PAL) measuring mode has been employed in a number of important practical applications like those probing free-volume nanostructuring in solids [1]. Under nanostructuring, the reconstruction route of PAL spectrum involves mixed positron (e^+) and positronium Ps (bound positron-electron state) channels resulting in three-term decomposed PAL spectra. The parametrization of these channels using simple trapping models (STM) [1] has a vital consequence for nanomaterials engineering.

In this report, this problem is reconsidered for different nanostructured solids with a help of available mathematical parameterization algorithms, such as:

- (i) two-term STM fully ignoring third component in the PAL spectrum,
- (ii) three-term STM accepting third component as common e^+ -trapping input,
- (iii) two-term STM with third component inserted in a source contribution,
- (iiii) two-term STM for generalized three-to-two component transition.

It is shown that intrinsic nanoscale structural inhomogeneities due to *guest* nanoparticles embedded in *host* substances can be described in terms of substitution trapping in e^+ -related and Ps-related sites (e^+ -to-Ps trapping conversion), allowing parameterization of interfacial free-volume voids responsible for e^+ -trapping and defect-free bulk lifetime of nanostructured matrix [2,3].

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