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Pseudopotential method for description of positron annihilation in spherically symmetric potential

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The radiation resistance is the key issue for the creation of new structural elements for new-generation nuclear reactors and the operation extension of existing nuclear power plants. The study of the mechanisms of formation and dynamics of radiation defects is of considerable scientific interest. The initial stage of the evolution of radiation defects is the production of point-type defects. One of the most effective methods for studying point defects is spectroscopy of positron lifetime, which depends on the electron distribution. Despite the rather simple idea, its practical implementation is associated with both certain technical difficulties, and the development of a general process theory. The method of positron annihilation spectroscopy (PAS) includes measurement of positron lifetime, determination of probabilities of 3γ and 2γ positron annihilation, influence on the main characteristics of annihilation of various external factors [1-3]. The PAS method is used to study the electron structure of the material and the concentrations of point and extended defects. Local formations (defects) are characterized by reduction of electron density compared to defect-free regions, so the lifetime of the positron is longer in this defect. Each defect is corresponded its own lifetime and the intensity of the corresponding component in the total experimental spectrum, which determined by the concentration of such defects [1-3]. The positron annihilation rate is determined by the overlap of the electron and positron densities in the region of the positron localization. It also depends on the cross section of the electron-positron pair annihilation process.
A series of methods have been developed to study the electronic structure of matter. They all have their advantages and disadvantages and differ in the required initial data. For this problem, we considered the pseudopotential method , which allows us to build the potential of the positron-vacancy interaction. The method idea suppose the replacement of the atom potential by a weak potential with the same amplitude of conduction electrons scattering. The method is based on the factorization of the positron wave function into an energy-independent basic function and the smooth envelope (pseudo-wave) function. Thus, the annihilation process of the positron in a spherically symmetric potential can be described.

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Primary authors: VORONA, Marina (Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine); Dr LEBED, Oleksandr (Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine)

Presenter: VORONA, Marina (Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine)

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