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The exact solution of the diffusion trapping model of defect profiling with variable energy positrons

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ABSTRACT

We report an exact analytical solution of so-called positron diffusion trapping model. This model have been widely used for the treatment of the experimental data for defect profiling of the adjoin surface layer using the variable energy positron (VEP) beam technique. However, up to now this model could be treated only numerically with so-called VEPFIT program. The explicit form of the solutions is obtained for the realistic cases when defect profile is described by a discreet step-like function and continuous exponential-like function. Our solutions allow to derive the analytical expressions for typical positron annihilation characteristics including the positron lifetime spectrum. Latter quantity could be measured using the pulsed, slow positron beam. Our analytical results are in good coincidence with both the VEPFIT numerics and experimental data. The presented solutions are easily generalizable for defect profiles of other shapes and can be well used for much more precise treatment of above experimental data.

1. Introduction

Defect depth profiling near the surface is an important application of the positron annihilation spectroscopy. For this purpose, the conventional techniques based on the isotope positron source have been successfully applied, in which case the defect distribution extended up to the depth of hundreds micrometers is possible to measure [1]. The detection of the near-surface defect distribution (up to the micrometer or less depths) is also possible, however with a slow positron beam. This technique, in particular, is suitable to study the metals and semiconductors with their surfaces being implanted with different ions, [2,3]. For efficient depth profiling, the positron data analysis should be extended beyond the commonly used simple two-state trapping model. Even in the above conventional techniques positron implantation profile should be taken into account [1]. This is because emitted energetic positrons exhibit the energy distribution which finally leads to a positron implantation profile. It can happen, that the total depth of the defects distribution correlates with that for implantation profile. For the efficient treatment of the data obtained from the slow positron beam measurements, not only the initial implantation profile, but also the thermalized positrons diffusion should be considered. This is taken into account in the positron diffusion trapping model (DTM).

The DTM is an extended version of the trapping model, where only annihilation and trapping rates are introduced. Namely, they are included into the set of rate equations which describe the time evolution of positron populations in different states. No positron dynamics is considered in the trapping model. On the contrary, the DTM accounts for the positrons thermal motions prior to annihilation and after implantation. The epithermal motion is also possible to introduce. These motions are represented in DTM as certain diffusion processes. In this case, the implantation profile is included as an initial condition for the corresponding time-dependent diffusion equation. The solution of the rate equations is necessary to obtain the time evolution of the positron fractions at different states. This permits to deduce the measurable positron annihilation characteristics (PACh) like the lineshape S-parameter of the Doppler-broadened annihilation line, mean positron lifetime and positron lifetime spectrum.

The development of the variable and pulsed slow positron beam techniques, which allows measuring the positron lifetime spectrum nearby and at the surface require the solution of DTM equations. Several approaches have been applied for this purpose. The one-dimensional diffusion equation including both annihilation in the sample interior (the bulk annihilation) and the surface trapping have been considered by Frieze et al. [4]. To solve the corresponding diffusion equation, the authors [4] used Fourier transformation technique. Britton [5], used Green's function method for solution of the diffusion equation assuming the perfect homogeneous defects-free solid. In Ref. [5], the approximate forms for positron populations at the surface and in the bulk have been derived. The final results have been obtained numerically.

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The author [5] have also considered the effects of epithermal positrons reaching the surface as well as internal reflection of thermal positrons. Kögel [6] has elaborated the DTM in a solid with inhomogeneous defects distribution. However, the explicit solutions in Ref. [6] have been obtained only for the standard trapping model with homogeneous defect distribution. The exact solution of the DTM for homogeneous, defect free sample as well as that with uniformly distributed open volume defects was made possible using time domain Laplace transformation and a Green's function method to solve resulting coordinate equation [7]. In this case, the PACh were expressed in the closed analytical form as the functions of the DTM parameters. It is interesting to note, that the solution [7] predicts that the positron lifetime spectrum in a pulsed beam experiment cannot be expressed as a simple sum of exponential functions similar to the standard trapping model. We note also that the pulsed beam technique, which allows to obtain the positron lifetime spectra as the function of its energy, is not completely operational due to the design difficulties.

The beams, where only the positron energy can be varied, i.e., the variable energy positron beam (VEP), are much more popular. In this case, the annihilation lineshape parameter is measured as a function of positron energy. To solve the DTM for that case, only the steady-state diffusion equations solution is necessary. In this solution, the corresponding time dependence is integrated from zero to infinity. This case is much simpler as it does not require the inversion of Laplace transform and allows considering the inhomogeneous case where defect concentration varies with the depth. This situation is the most interesting since it delivers adequate description of many surface physics problems. However, even in that case the DTM has been solved only numerically. Aers et al. [8, 9] proposed a numerical algorithm for defect profiling using variable energy positron where defect concentration can vary with the depth like a step function. The drift of positrons in an external electric field has been included similarly. Van Veen et al. [10] presented the VEPFIT program which realizes the numerical approach to the DTM solution for the materials with layered structure. The program has frequently been used for treatment of the data obtained in the variable energy positron beam. This is because this program contains the procedure which allows to fit the different model parameters to the experimental data. Unfortunately, this program cannot be used for the pulsed beam technique for evaluation of the measured positron lifetime spectra.

In the present Letter, we report an exact analytical solution of the DTM for the case when a sample contains defects with inhomogeneous distribution. Applying the Laplace transformation in time domain, we construct the Green's function of the time-dependent diffusion equation assuming that the defect depth profile is expressed by either the step function or a selected continuous function. Our formalism permits to deduce the time evolution of positron fractions at different states and from this to obtain the PACh, including the positron lifetime spectrum. This was not possible until now with previously known DTM solutions.

2. The formalism

2.1. Statement of the problem

In our consideration, a sample is a semi-infinite medium situated at positive semi-axis $0 \leqslant x < \infty$, Fig. 1. Point $x = 0$ plays a role of the medium surface, where the energetic positrons enter a sample. After a few picoseconds they thermalize and begin to diffuse. The time of diffusion beginning is considered as the initial time instant $t = 0$. The penetration depth dependence of the initial positron concentration is called the positron implantation profile [12]; we denote it as $u(x, t = 0) \equiv P(x)$. $P(x)$ is also a function of the incident positrons energy. In our consideration, the total number of implanted positrons is normalized to unity:

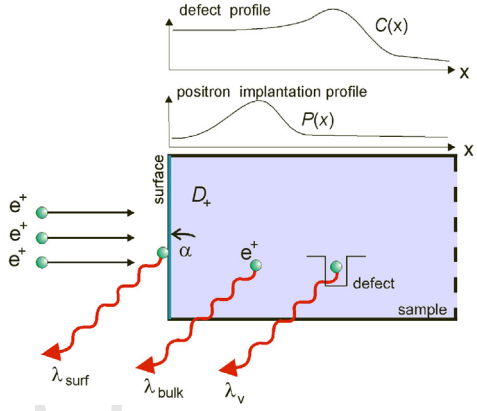

Fig. 1. Sample irradiated by slow positrons and three states (considered in the Letter) which can be occupied by them after thermalization (main lower panel). The positron annihilation occurs and the annihilation radiation is emitted from these states. The initial positron concentration or positron implantation profile $P(x)$ is presented in the middle panel. The defect depth profile, described by the $C(x)$ function and proportional to the trapping rate profile $k(x) = \mu C(x)$, is reported in the upper panel.

$$\int_0^\infty P(x)\,dx = 1. \tag{1}$$

Generally speaking, a sample can contain defects with certain profile $C(x)$ close to its surface. The defect, like vacancy or their cluster can trap a positron with a specific trapping rate μ. Thus the whole defect profile traps positrons at a rate $k(x) = \mu C(x)$, Fig. 1. We denote the positron (which can freely diffuse) concentration in a bulk as $u(x, t)$. We denote the part of the above positrons trapped at the defects (vacancies) as $n_v(t)$. Certain positron fraction $n_{sur}(t)$ can diffuse back to the surface, which is a sink for thermalized positrons. We assume that the entering positrons cannot be trapped by the defects and the surface, i.e., $n_v(t = 0) = n_{surf}(t = 0) = 0$.

In the DTM model, the concentration $u(x, t)$, obeys the diffusion equation which incorporates the annihilation rate in the free state λ_{bulk} and spatially dependent trapping rate $k(x)$. This yields

$$\frac{\partial u(x,t)}{\partial t} = D_+ \frac{\partial^2 u(x,t)}{\partial x^2} - \big[\lambda_{bulk} + k(x)\big]u(x,t), \tag{2}$$

where D_+ is a bulk positron diffusion coefficient, $0 \leqslant x < \infty$. As the thermalized positrons can be trapped at the surface with the absorption coefficient α, the solution of Eq. (2) should obey the radiative boundary condition at the surface:

$$-D_+ \frac{\partial u(x,t)}{\partial x}\bigg|_{x=0} + \alpha u(x = 0, t) = 0. \tag{3}$$

Positrons trapped at the surface can also annihilate with the rate λ_{sur}. This generates one more rate equation for the surface positron fraction $n_{sur}(t)$:

$$\frac{dn_{surf}(t)}{dt} = \alpha u(x = 0, t) - \lambda_{surf} n_{surf}(t). \tag{4}$$

Finally, the positrons fraction, trapped at the defects in a sample, obeys the equation:

$$\frac{dn_v(t)}{dt} = \int_0^\infty k(x)u(x,t)\,dx - \lambda_v n_v(t), \tag{5}$$