APPLICATION OF FOKKER-PLANCK EQUATION IN POSITRON DIFFUSION TRAPPING MODEL

Iveta Bartošová[1], Peter Ballo[1]

[1] Institute of Nuclear and Physical Engineering, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology in Bratislava, Ilkovičova 3, 812 19 Bratislava, Slovak Republic

E-mail: iveta.bartosova@stuba.sk

Received 11 May 2015; accepted 25 May 2015

1. Abstract

This paper is a theoretical prelude to future work involving positron diffusion in solids for the purpose of positron annihilation lifetime spectroscopy (PALS). PALS is a powerful tool used to study defects present in materials. However, the behavior of positrons in solids is a process hard to describe. Various models have been established to undertake this task. Our preliminary model is based on the Diffusion Trapping Model (DTM) described by partial differential Fokker-Planck equation and is solved via time discretization. Fokker-Planck equation describes the time evolution of the probability density function of velocity of a particle under the influence of various forces.

2. Introduction

The technique of positron annihilation is currently widely used method for detecting defects in solids. The technique operates on the principle that a positron annihilates through interaction with electrons. It is well known that a positron prior the annihilation with an electron in condensed matter spends a finite time 100–300 ps, randomly wandering within the material with thermal energies. The behavior of positrons in molecules or condensed matter is nontrivial due to the strong correlation between electrons and positrons. Even the simplest model that of a single positron imbedded in a homogeneous gas of electrons has proven to be a significant challenge for theory. Positrons attract electrons resulting in increased contact density and hence increased annihilation rate. Furthermore, the momentum density of annihilating electron-positron pairs is increased near the Fermi surface. High sensitivity and good response to the structural defects has destined this technique for use in material engineering. Although it is a promising technology, it remains problematic to process and interpret measured data. For this reason, experimental methods are usually combined with other simulation experiments. With the advent of computers it is possible to realize many refined numerical methods. We can mention the following: Tamm-Dancoff approximation [1], Fermi [2] and perturbed hypernetted chain approximations [3], density functional theory methods [4] and quantum Monte Carlo [5, 6]. Today it is generally accepted as a fact, that a calculation based on the two component density functional theory (TC DFT) is the best what can be offered. However some areas remain in which numerical experiments are unusable, for instance positron annihilation in strongly inhomogeneous materials. In this case it is required to replace purely quantum mechanical approach for something simpler. Simplification based on an approximation of diffusion model has been found as a good idea. This paper is a theoretical prelude to future work involving positron diffusion in solids for the purpose of positron annihilation lifetime spectroscopy. The model is

based on the Diffusion Trapping Model (DTM) described by partial differential equation and is solved via time and space discretization. An important result of the study is that he diffusion model can describe the time evolution of the positron density under the influence of grain boundary in a solid.

3. Diffusion Trapping Model (DTM)

The theoretical description of the positron diffusion comprises two approaches. The simplest approach assumes that during thermalization the positrons are located in two distinct regions of a sample, grain and its boundary, in which they subsequently annihilate [7, 8]. Therefore, only the volume ratio of the two regions is important and the positron diffusion process can be neglected. In the second approach the positron diffusion is taken into account, however at a certain level of calculations approximations are introduced to adjust the resulting solution to fit the well known results obtained using the Standard Trapping Model where diffusion is neglected [9]. Nevertheless, several authors have obtained solutions of the positron diffusion equation for particular cases [10, 11]. Also Monte-Carlo simulations of positron diffusion in spherical and ellipsoidal grains were carried out by Hübner et al. [12]. The main assumption of DTM is that the grain boundary is a perfect sink for positrons in which they are localized and annihilate with the rate $\lambda_b = \frac{1}{\tau_b} < \lambda_f$ (Smoluchowski boundary condition) . In the interior of the grains, positrons can randomly move and annihilate with the rate $\lambda_f = \frac{1}{\tau_f}$, where τ_f is the positron lifetime in a free state. The movement of positron looks pretty chaotic. Chaotic movements can be simulated using diffusion which could be mathematically described by the following Fokker-Planck equation,

$$\frac{\partial u(x,t)}{\partial t} = -\Theta \frac{\partial u(x,t)}{\partial x} + \frac{\partial}{\partial x} D_+(x) \frac{\partial u(x,t)}{\partial x} \tag{1}$$

where θ and D_+ are coefficients of diffusion. Note, D_+ depends on space, but in following discussion it will not be considered. The Fokker-Planck equation is a second order differential equation which describes the time evolution of the concentration (well probability distribution) in time and space of the positron. In general the Fokker-Planck equation can be derived from the Chapman-Kolmogorov equation, but also corresponds to the time dependence given by a Langevin equation. To simulate the interaction between positron and electrons which gather at grain boundaries a single equation is not enough. One more equation needs to be added for electrons and a function which describes the interaction between them.

$$\frac{\partial u_+(x,t)}{\partial t} = D_+ \frac{\partial^2 u_+(x,t)}{\partial x^2} + f(u_+(x,t), u_-(x,t)) \tag{2}$$

$$\frac{\partial u_-(x,t)}{\partial t} = D_- \frac{\partial^2 u_-(x,t)}{\partial x^2} - f(u_+(x,t), u_-(x,t)) \tag{3}$$

where: D_- is coefficient of diffusion for electrons. If the electrons are well localized the coefficient D_- is set to zero. In our case it was necessary to set this coefficient to the value close to zero ($D_- > 0$) because of numerical speculation. Such systems have incredible susceptibility to instability, but there are methods that miraculously eliminate this problem.

4. Numerical methodology

The goal is to construct a numerical method that allows us to approximate the unknown analytic solution u(x,t) reasonably well in discrete grid points. Then the simplified diffusion equation looks like this:

$$\frac{1}{\Delta t}(u_{i,j}-u_{i,j-1})=\frac{\Theta}{\Delta x^2}(u_{i-1,j}-2u_{i,j}+u_{i+1,j})+\frac{1-\Theta}{\Delta x^2}(u_{i+1,j-1}-2u_{i,j-1}+u_{i-1,j-1}) \quad (4)$$

Previous equation can be simplified by incorporating variable α, which is expressed as $\frac{\Delta t}{\Delta x^2}$

Using the definition of α, the equation can be rewritten as:

$$-\alpha u_{i-1,j}+(2+2\alpha)u_{i,j}-\alpha u_{i+1,j}=\alpha u_{i-1,j-1}+(2-2\alpha)u_{i,j-1}+\alpha u_{i+1,j-1} \quad (5)$$

or in "compressed" matrix format as:

$$(2\hat{I}+\alpha\hat{B})V_j=(2\hat{I}-\alpha\hat{B})V_{j-1}/nonumber \quad (6)$$

Using this matrix we can rewrite the numerical scheme to a simple set of equations:

$$V_j=(2\hat{I}+\alpha\hat{B})^{-1}(2\hat{I}-\alpha\hat{B})V_{j-1} \quad (7)$$

which form in fact a time discretization scheme. An important advantage of this scheme is that the numerical stability is guaranteed for all possible combinations of time (Δt) and space (Δx^2) and is named after its inventors, Crank and Nicolson. Computational grid for the Crank- Nicolson scheme is shown in Fig. 1.

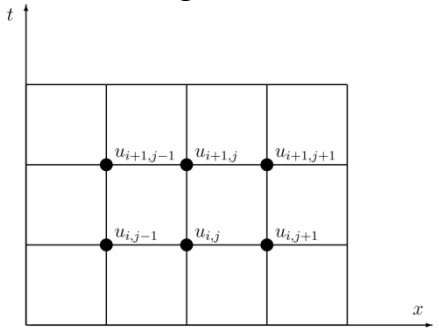

Fig.1: *Calculation grid for the Crank-Nicolson scheme. The scheme combines backward and forward Euler schemes, respectively. The scheme yields a truncation in time which goes from $O(\Delta t^2)$ and it is stable for all possible combinations of (Δt) and (Δx^2).*

The last step is to split the solution into two parts (positron and electrons) and add a function $f(u_+(x, t), u_-(x, t))$ that describes the reaction between positrons and electrons. In a compressed matrix form it can be written as:

$$A^{(1)}V^{(+)}_{j+1\ j}=A^{(2)}V^{(+)}_{j}+f_j \quad (8)$$

$$A^{(1)}V^{(-)}_{j+1\ j}=A^{(2)}V^{(-)}_{j}-f_j \quad (9)$$

Where $A^{(1)}=2\hat{I}+\alpha\hat{B}$ and $A^{(2)}=2\hat{I}-\alpha\hat{B}$ refers to positron and $V^{(-)}$ to electrons. Time and space discretization was carried out as shown in Fig. 2.

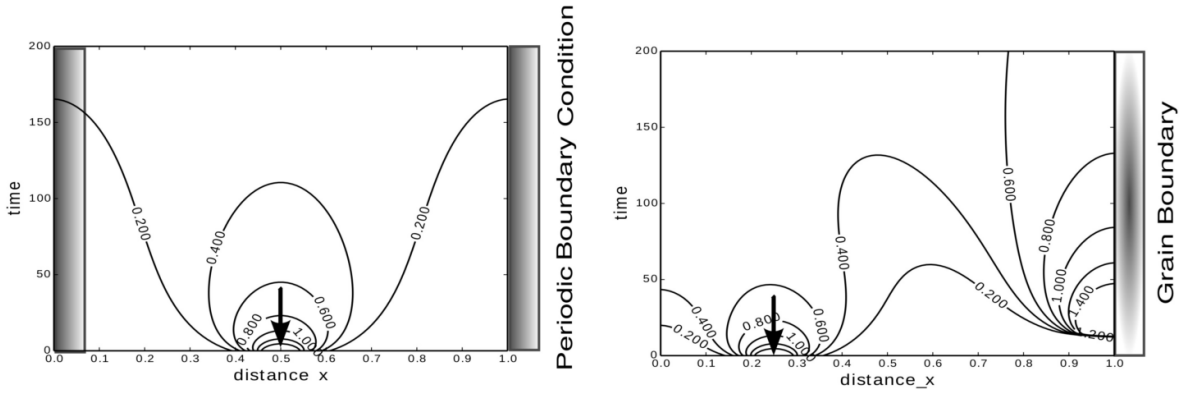

Fig. 2: *Time and space evolution of positron distribution of concentration with periodical border conditions and uniform distributed electron- upper panel and with a grain boundary which is populated by extra electrons- lower panel. In both cases, the arrow points to the location where the positron was generated. In cases where the positron was generated in the vicinity of a grain boundary it is clearly visible, that the positron aims towards the grain boundary which is populated by electrons.*

5. Numerical methodology

As has been mentioned it the beginning, that this article is an introduction how to explore further the possibilities of numerical simulation of positron diffusion in a crystal lattice. Despite of many difficulties it has been shown that the Crank - Nicolson method is sufficiently stable also in long time simulations and independent on the time and space discretization. Also the diffu- sion model in conjunction with the scheme, which describes the interaction between electrons and positrons, can say many in the future. We have concluded that the model and method of calculation may be used to simulate the behavior of positrons in inhomogeneous environment and certainly we will consider this problem in the future.

Acknowledgement

Financial support from the National Science Foundation (DMR 1359523 grant) as well as from Slovak scientific agencies VEGA 1/0204/2013 and APVV AK48 are highly acknowledged.

References:

[1] J. Arponen, E. Pajanne: *Annals of Physics*, **121**, 343 (1979).
[2] L. J. Lantto: *Physical Review B*, **36**, 5160 (1987).
[3] E. Boronski, H. Stachowiak: *Physical Review B*, **57**, 6215, (1998).
[4] N. D. Drummond, P. Lopez Rios, C. J. Pickard, R. J. Needs: *Physical Review B*, **82**, 035107 (2010).
[5] E. Boronski: *Europhysics Letters*, **75**, 457 (2006).
[6] N. D. Drummond, P. Lopez Rios, R. J. Needs, C. J. Pickard: *Physical Review Letters* **107**, 207402 (2011).
[7] C. Hidalgo, N. de Diego: *Appl. Phys. A*, **27**, 149 (1982).
[8] Y. Dong, L.Y. Xiong, C.W. Lung: *J.Phys. Condens. Mater*, **3**, 3155 (1991).
[9] W.Brandt, R. Paulin: *Phys.Rev. B*, **5**, 2430 (1972).
[10] R.Nieminen, J.Laakkonen, J.Hautojärvi, A. Vehanen: *Phys. Rev. B*, **19**, 1397 (1979).
[11] A.Dupasquier, R.Romero, A. Somoza: *Phys.Rev. B*, **48**, 9235 (1993).
[12] C.Hübner, T.Staab, R. Krause-Rehberg: *Appl. Phys. A*, **61**, 203 (1994).