# WHY DOES EVERYONE TALK ABOUT POSITRON ANNIHILATION ? ALL WE KNOW COMES FROM EXPERIENCE

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## Introduction

Visits to certain physical workplace resembles to story about wife lieutenant Columbo. Everybody talk about her, but nobody yet seen her. We mean wife of lieutenant Colombo not positron annihilation. Speaking about positron annihilation spectroscopy (PAS) [1] is the situation even more complex. Sending question to Google about the positron annihilation spectroscopy one will receive around 190,000 references. This may not seem like much, but it is still ten times more than gives question about recipes for pangalactic gargle blaster. Everyone claims to understand it, but describes it differently. We mean PAS not pangalactic gargle blaster. When we look at PAS seriously, we must say that annihilation is an experimental method with wide use and it is a well established tool for study of the defects properties in metals and semiconductors. The fact that defects can attract positrons gives a unique chance to distinguish between a perfect sample and a sample containing imperfections. Whereas is the average electron density at the vacancy lower than in the bulk the lifetime of the trapped positron is increased compared to the value in the perfect bulk lattice. In the case of semiconductors gives PAS good possibility to distinguish different charge states of the same vacancy. Result is not unambiguous because extra charge usual invokes adjacent ionic relaxations. This in fact can remarkably change the positron lifetime. It looks great but as it is usual in life, things are not as simple as seem at first sight. Before we could commend with the first amazing result, we need to think and to do many things. The aim of this article is to describe some aspects of PAS technique including theoretical, numerical as well as technical details but also perspectives which the technique could offer in the future. We believe that it can help to remove superstitions and myths that accompany this technique.

## Positron Annihilation Spectroscopy technology

In a real experiment, the geometry is organised so that a flux of positrons generated from a $^{22}$Na source is allowed to strike a thin piece of material. The kinetic energy of the positrons, which is initially in the range of 0 $\approx$0.544 MeV, is rapidly lost to electrostatic interactions as the positrons move about in the solid. During this slowing down process, which is similar to what would be experienced by any charged particle, annihilation of the positron is unlikely. When a positron has become "thermalized" at the thermal energy level of the lattice (about 0.025 eV at room temperature). Typically, within a few hundred picoseconds, the positron (propagating in its own Bloch state) will then annihilate with one of the electrons in the sample being studied. The result is the creation of two annihilation photons, which are moving along a straight line in approximate opposite direction (please see Fig.1). In fact, the deviation from anticolinearity between the photons can be directly related to the momentum of the electron-positron pair

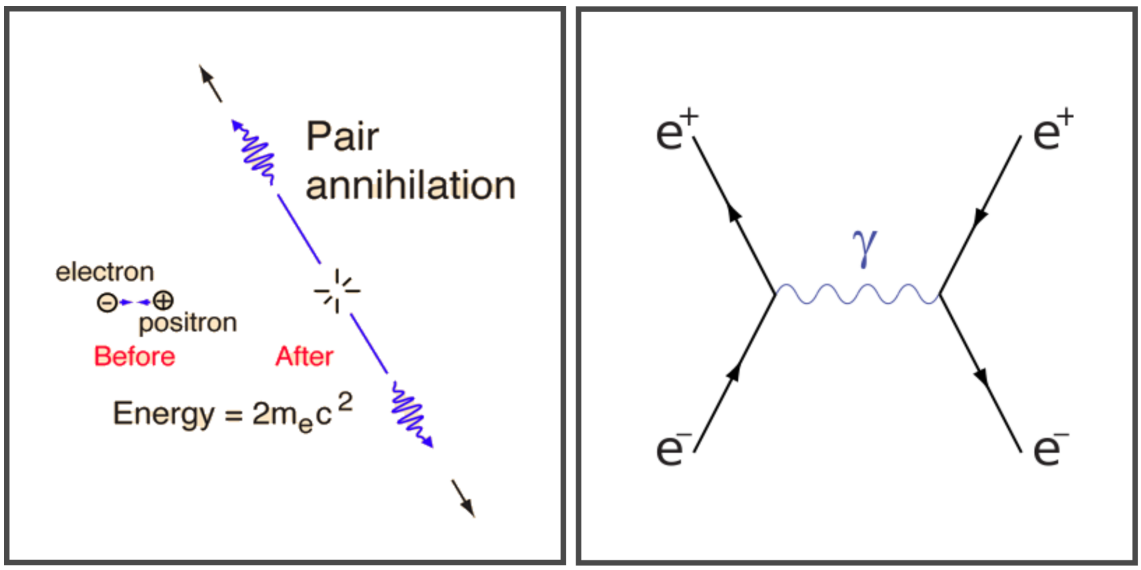


Fig. 1: *Annihilation: when electron and positron collide 2 photons are released. In general when a charged fermion collides with its anti-fermion the total energy – the energy contained in the rest masses of these fermions and their kinetic energies – is converted into 2 photons, which are moving along a straight line in approximate opposite direction (left panel). Schematic representation of Electron-Positron Annihilation - Feynman Diagram (right panel).*

immediately prior to annihilation. Since the positron is thermal with a Maxwell-Boltzmann momentum distribution (at normal experimental source activities, it is only one positron in the sample) the angular deviation is simply proportional to the electron momentum. Since the distribution of these angular deviations, the so-called two-photon momentum density (TPMD), is itself a sum over occupied momentum states, it contains information about the occupation number within the Brillouin zone and hence about the Fermi surface. This information may be important in the case of semiconductors.

**Numerical simulation**

For a thorough understanding and interpretation of experimental results is needed accompanying theory. With the advent of full blown computers we can afford things we could not even dream about it yesterday. Speaking about the possibilities which are made possible by supercomputers - we can manipulate with single electrons and positrons. Of course with many compromises and in simulation space only but we can. One of them is density functional theory (famous DFT) [2]. Based on DFT, there are two main approaches: the conventional scheme and the full two-component scheme (TC DFT) [3]. The conventional scheme is more convenient and produces consistent results for physical observables compared with the full two-component scheme, and has been employed in most applications for positron states so far. On the other hand TC DFT is more compact and could give a result faster in comparison with classical DFT. Also, before we begin to look forward to the possibilities of super-computers do we have to solve one important thing. It is about how to properly set the electronic structure that is present in every bit of matter and greatly affect the outcome of PAS experiment. The formalism can be used with either the Green's-function or supercell method for calculating defect characteristics. With the use of this formalism and the self-consistent pseudopotential scheme within a super-

cell, the electronic structure and positron states and annihilation characteristics associated with the defects in both metal and semiconductor could be studied. The sensitivity of the calculated electronic structure and formation energy to the type of pseudopotential and electronic structure is very intensive examined. A formalism for self-consistently calculating, the correct method of setting pseudopotentials (it's difficult - you believe us) the response of electrons and positrons to atomic defects in solids (you need a lot of time and effort at least to understand it) are explained in the following articles.

**Model based on the diffusion**

Previous considerations based on a straightforward calculation, brings excellent results, but are still limited to a small (up to a hundred) number of atoms. In cases where such a small number of atoms is not enough are numerical experiments based on single positron manipulation unusable. A situation can occur when we try to simulate the positron annihilation in a 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 (though it's still damn complicated) has been found as a good idea. The model is based on the Diffusion Trapping Model (DTM) [4] described by partial differential equation and is solved via time and space discretization. An important result of the study is that diffusion model can correct describe the time evolution of the positron density under the influence of grain boundary in a solid.

At this point should be discussed some facts. The diffusion equation has energy dissipation built into the high order terms. There are special nonlinear forms of diffusion equation that can describe traveling wave solutions but for the simplest linear diffusion equation, any initial pulse shape (positron initial distribution) is rapidly smeared out, and the pulse maximum doesn't move in a way that could be described as traveling. The peak may shift a bit as it spreads out. The distribution of concentration has only one characteristic direction, parallel to the x-axis in the (x,t) plane. Discontinuities cannot propagate forward in time, and are immediately smoothed. In contrast with wave equation, there is no theoretical limit to the speed with which disturbances propagate. A positron will in theory start to move distant places immediately. This is obviously not possible in view of the limit speed of light. This physical fact must be compensated with other members in the diffusion equation. In our case, as we will see in the next paper, it this is the right setting of response function.

Another big problem which must be addressed is the susceptibility to numerical instability. The problem could be satisfactorily solved using Crank - Nicolson [5] numerical schemes. It will be shown that this technique enables to simulate the positron diffusion during long time. We will talk about it later, and believe us, it looks very promising.

**Diffusion Quantum Monte Carlo**

As we have shown simulations using diffusion brings quite good results. On the other hand, methods derived from quantum theory, brings more credible information. At least at first glance. This has led some researchers to combine these two methods with the aim to create Diffusion Quantum Monte Carlo (DQMC). In essence, this technique is based on the property that in the asymptotic imaginary time limit ($t \to \infty$) the Euclidean evolution operator acting on a trial state $\psi_T$ projects out the ground state $\psi$ with a component in $\psi_T$. Translated into normal parlance it means that the group (quantum) walkers after a sufficiently long (imaginary) time arrives at the right place. It should be noted that this technique is tied with the quantum properties of positron, which is ,in the fact, a fermion. The problem is usual referred as the "minus sign problem". In

quantum simulation it refers to the fact that the amplitude of probability is not positive-definite which leads to numerical instability when summing over path of quantum walkers since large amplitudes of one phase can completely negate other large contributions but with the reverse phase. The solution is hidden in the sampling of alternative configurations and has to be extremely dense, at least for situations where interference is expected to be important. When you have enough computing power, enough patience and especially will be lucky QMC will bring great results. Given the tremendous requirements for computing power we are limited to small systems of atoms. Benefits of this method is to identify trends and calculation rules. One of great result is that inclusion of electron-positron correlation is crucial in the investigation of bound states of the positron in negative (charged)and neutral atomic systems. This method will not be presented at this conference, but for sure we will use it in the future with the aim to recognize some computational aspects.

**Conclusion**

This article is an essay about the principles and application of PAS technology. It was demonstrated many times that this technique is very versatile with a big future in many areas. In particular, the technique could be used in metallic materials as well as in semiconductors. The many advantage is high sensitivity and relative simplicity of the experiment. It must be noted (and this must be constantly kept in the mind) that proper use is based on good experiment (we wrote about this a little) and especially on proper evaluation of the collected data (we wrote about this a much). For valid data we need a good model which comes from experiences. Details that are not discussed here will be reported in subsequent articles, and most of them have been collected by the effort of our young colleagues.

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