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Positrons in Solids

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Preface

In condensed matter initially fast positrons annihilate after having reached equilibrium with the surroundings. The interaction of positrons with matter is governed by the laws of ordinary quantum mechanics. Field theory and antiparticle properties enter only in the annihilation process leading to the emergence of energetic photons. The monitoring of annihilation radiation by nuclear spectroscopic methods provides valuable information on the electron-positron system which can directly be related to the electronic structure of the medium. Since the positron is a positive electron its behavior in matter is especially interesting to solid-state and atomic physicists. The small mass quarantees that the positron is really a quantum mechanical particle and completely different from any other particles and atoms. Positron physics started about 25 years ago but discoveries of new features in its interaction with matter have maintained continuous interest and increasing activity in the field. Nowadays it is becoming part of the "stock-in-trade" of experimental physics.

A striking feature is the great diversity of fields in which positron annihilation is applied. In addition to solid-state physics, which is the topic of this book, there are intensive activities in atomic physics, and positronium chemistry is the traditional name for the chemical applications. There exists plenty of earlier reference material in the form of review monographs and conference proceedings. However, the recent development and achievements especially in momentum density and defect studies have rapidly attracted the interest of a wider scientific community outside of the traditional positron physics thus providing justification for the publication of this topical volume.

The first chapter is an introduction devoted to readers who have no former familiarity with positron annihilation. It gives a short account of annihilation processes and of conventional experimental techniques. Also some recent topics of positron studies are very briefly discussed.

Chapter 2 is concerned with electron momentum density studies by means of angular correlation of 2γ-annihilation radiation. It discusses the state-of-the-art in the application of independent-particle theory and describes the recent development of two-dimensional detector geometries which have greatly increased the resolution and efficiency of the positron method. The latest results on metals and alloys are thoroughly reviewed.

The extreme sensitivity of positrons to crystal imperfections in metals is reflected through positron trapping. This makes the positron annihilation method capable of yielding unique information on the concentration, configuration and internal structure of lattice defects in solids. Positrons have within a few years proved to be a new microscopic tool the use of which has produced significant achievements in the physics of lattice defects. The new experimental results and progress in theoretical understanding are reviewed in Chaps.3 and 4, respectively.

Chapter 5 deals with ionic solids and serves as an example of problems in nonmetals. It offers a solution to the origin of the complex annihilation characteristics in alkali halides and reviews the interaction of positrons with various kind of defect centers.

I want to thank the authors who have not only contributed to this book but in fact created it. The very fluent cooperation has kept the editorial work at a minimum. In addition, I am especially indebted to Risto Nieminen for his comments and suggestions which have largely influenced the content of the book.

Helsinki, December 1978 *Pekka Hautojärvi*

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1. Introduction to Positron Annihilation

P. Hautojärvi and A. Vehanen

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Positron physics is concerned with the interaction of low-energy positrons with matter. The existence of the positron was predicted by Dirac and verified by Anderson more than 40 years ago. The birth and the rapid initial development of positron physics occurred in the early 1950s as it was realized that the characteristics of the quantum electrodynamic annihilation process depend almost entirely on the state of the positron-electron system in the matter. During the last decade the field has started to grow and widen strongly, as indicated in Fig.1.1 which shows the number of annually published papers [1.1]. The reason for the rapid growth lies in observations that positrons can provide unique information on a wide variety of problems in condensed matter physics. Also inexpensive experimental equipment which nowadays is commercially available has its own contribution to the popularity of positron studies.

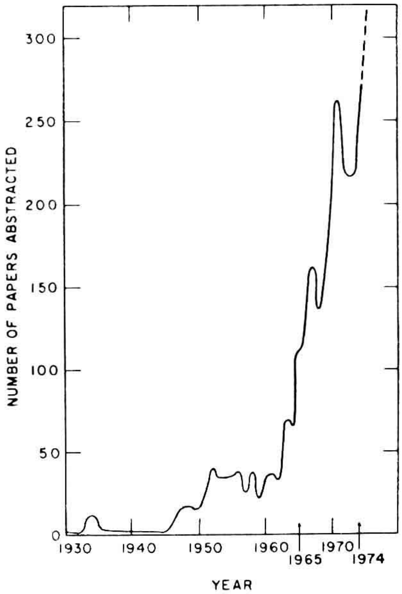

Fig.1.1. The number of annually published papers dealing with the study of low-energy positrons and positronium [1.1]

There have been several international conferences specially devoted to positron annihilation studies. The first was held in Detroit, USA in 1965 [1.2], a European meeting was organized in Saclay, France, in 1969, the second international conference was held in Kingston, Canada, in 1971 [1.3], the third in Otaniemi, Finland, in 1973 [1.4] and the fourth in Helsingør, Denmark, in 1976 [1.5]. The fifth will take place in Lake Yamanata, Japan, in 1979 and even the sixth conference has been scheduled to be held in the USA in 1982.

The positron technique has many advantages in the study of matter. It provides a nondestructive method because the information is carried out of the material by penetrating annihilation radiation. No special sample preparation is necessary and in some applications also in situ studies, e.g., on dynamic phenomena at elevated temperatures are possible. Several reviews and bibliographical surveys on the use of positrons to the study of condensed matter have been published [1.1-9].

This chapter consists of tutorial material for readers having no former familiarity with positron annihilation. The first section describes the principles of the positron method. Section 1.2 deals with the annihilation process of free positrons. The conventional measurement systems for the positron lifetime, the angular correlation of the 2γ-annihilation radiation and the annihilation line shape are discussed together with some examples in Sect.1.3. Positronium formation and its consequences in annihilation characteristics are treated in Sect.1.4. Some recent topics of positron studies are briefly discussed in Sect.1.5 and a short summary is given in Sect.1.6.

1.1 Positron Method

When energetic positrons from a radioactive source are injected into a condensed medium they first slow down to thermal energies in a very short time of the order of 1 ps. The mean implantation range varying from 10 to 1000 μm guarantees that the positrons reach the bulk of the sample material. Finally, after living in thermal equilibrium, the positron annihilates with an electron from the surrounding medium dominantly into two 511 keV gamma quanta. The average lifetime of positrons is characteristic of each material and varies from 100 to 500 ps. The picture above is distorted in molecular media, where positronium formation may occur during the slowing down process. This phenomenon, however, is treated separately in Sect.1.4.

Figure 1.2 shows schematically the positron annihilation experiment, where the most commonly used radioisotope ^{22}Na is implied. Within a few picoseconds after the positron emission the nucleus emits an energetic 1.28 MeV photon which serves as a birth signal. The lifetime of the positron can thus be measured as the time delay between the birth and annihilation gammas. The momentum of the annihilating

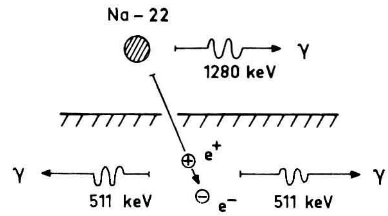

Fig.1.2. The positron experiment. Positrons from a radioactive isotope like ^{22}Na annihilate in the sample material. Positron lifetime is determined from the time delay between the birth gamma (1.28 MeV) and the two annihilation quanta. The momentum of the electron-positron pair is measured as an angle deviation between the two 511 keV quanta or as a Doppler shift in the energy of the annihilation radiation

electron-positron pair is transmitted to the annihilation quanta and it can be detected as a small angle deviation from collinearity between the two 511 keV photons. The motion of the pair also produces a Doppler shift to the annihilation radiation and this is seen in an accurate energy measurement of one of the photons.

1.2 Annihilation of Free Positrons

The positron-electron annihilation is a relativistic process where the particle masses are converted into electromagnetic energy, the annihilation photons. From the invariance properties of quantum electrodynamics several selection rules can be derived. One-gamma annihilation is possible only in the presence of a third body absorbing the recoil momentum and its relative probability is negligible. The main process is the two-gamma annihilation, since the spin-averaged cross section for the three-gamma annihilation is 0.27% of that for the two-gamma annihilation. The three-gamma annihilation is important only in a spin-correlated state like ortho-positronium, where the selection rules forbid the two-quantum process. This situation is treated in Sect.1.4.

From the nonrelativistic limit of the 2γ-annihilation cross section derived by DIRAC [1.10] one obtains the annihilation probability per unit time or the annihilation rate

$$\lambda = \pi r_0^2 c n_e \quad , \tag{1.1}$$

which is independent of the positron velocity. Here r_0 is the classical electron radius, c the velocity of light and n_e is the electron density at the site of the positron. By measuring the annihilation rate λ, the inverse of which is the mean lifetime τ, one directly obtains the electron density n_e encountered by the positron. Thus a positron can serve as a test particle for the electron density of the medium. However, because of the opposite charges, a strong Coulomb attraction exists between the positron and electrons. Consequently, the electron density n_e is enhanced from the equilibrium value in matter due to the Coulomb screening of the positron. Calculation of these positron-electron correlations is a complicated many-body problem which is well understood only in the case of electron gas.

The kinetic energy of the annihilating pair is typically a few electron volts. In their center-of-mass frame the photon energy is exactly m_0c^2 = 511 keV and the photons are moving strictly into opposite directions. Because of the nonzero momentum of the pair the photons deviate from collinearity in the laboratory frame. As illustrated in Fig.1.3 the momentum conservation yields a result

$$\theta \simeq p_T/m_0c \quad , \tag{1.2}$$

where $180^\circ-\theta$ is the angle between the two photons in the laboratory frame and P_T is the momentum component of the electron-positron pair transverse to the photon emission direction. Usually θ is very small($\theta < 1^\circ$) and (1.2) is valid. Because the momentum of the thermalized positrons is almost zero, the measured angular correlation curves describe the momentum distribution of annihilated electrons in matter.

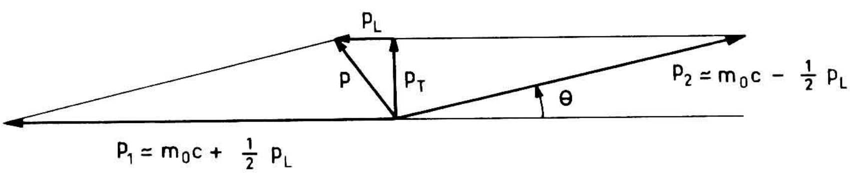

Fig.1.3. The vector diagram of the momentum conservation in the 2γ-annihilation process. The momentum of the annihilating pair is denoted by p, subscripts L and T refer to longitudinal and transverse components, respectively

The motion of the pair also causes a Doppler shift in the energy of the annihilation photons measured in the laboratory system. The frequency shift is $\Delta\nu/\nu = v_L/c$, where the longitudinal center-of-mass velocity v_L of the pair equals $p_L/2m_0$. Since the energy of a photon is proportional to its frequency, we get for the Doppler shift at the energy m_0c^2

$$\Delta E = (v_L/c)E = cp_L/2 \quad . \tag{1.3}$$

Thus also the line shape of the annihilation radiation reflects the momentum distribution of electrons in matter.