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Positron Annihilation in Condensed Matter

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The positron as the antiparticle of the electron was predicted by Dirac in 1928 [9]. First experimental indications of an unknown particle were found in cloud-chamber photographs of cosmic rays [1]. This particle was identified later as the positron, which was thus the first antiparticle in physics. The annihilation of the positron with electrons in matter was first studied in the 1940s. It was discovered early that the energy and momentum conservation during the annihilation process could be utilized to study properties of solids. The bound state of a positron and an electron, as the lightest known atom to be formed, is analogous to a hydrogen atom, where the proton is replaced by the positron. This e^+–e^- state is called positronium (Ps). It was predicted by Mohorovicic in 1934 [19] and discovered by Deutsch in 1951 [8].

The early experiments with positrons were dedicated to the study of the electronic structure, e. g., the Fermi surface in metals and alloys [2, 5]. The various experimental techniques of positron annihilation based upon the equipment of nuclear spectroscopy were developed strongly in the two decades after 1945. In addition to the angular correlation of annihilation γ-quanta, Doppler-broadening of the annihilation line and positron-lifetime spectroscopy were established as independent methods. It was realized by the end of the 1960s that the annihilation parameters are sensitive to lattice imperfections. It was discovered that the positron may be trapped in crystal defects, i. e., the wave function of the positron is localized at the defect site until annihilation. This behavior of positrons was demonstrated by several authors, e. g., MacKenzie *et al.* [18] for thermal vacancies in metals, Brandt *et al.* [3] in ionic crystals, and Dekhtyar *et al.* [7] after plastic deformation of semiconductors. The investigation of crystal defects has become the dominant issue of positron annihilation studies. Up to the mid-1980s, defect studies in solids were mainly carried out in metals and alloys. The experience obtained in this field was applied to elemental and compound semiconductors (for a review, see [16]).

The trapping of the positron in defects is based on the formation of an attractive potential at open-volume defects, such as vacancies, vacancy agglomerates, and dislocations. The main reason for this potential is the lack of a repulsive positively charged nucleus in such a lattice defect. The sensitivity range for the vacancy detection in metals starts at about one vacancy per 10^7 atoms. This enormous sensitivity is caused by the fact that the positron diffuses about 100 nm through the lattice and probes a high number of atoms until annihilation. When the positron is trapped in an open-volume defect, the annihilation parameters are changed in a characteristic way. The positron lifetime increases in an open-volume defect due to the lower electron density. Momentum conservation during 2γ annihilation leads to a small angular spread of the collinear γ quanta or a Doppler shift of the annihilation energy. Both properties, the density and the momentum distribution of electrons participating in the annihilation, result in observables to be detected in a positron experiment. The analysis of the annihilation radiation thus gives the possibility to detect defects. Clustering of vacancies as a typical defect reaction may be observed as the increase in the defect-related lifetime due to the further decrease in the electron density. In addition, a higher affinity of the positron to atoms of one element in a binary metallic alloy may also lead to the confinement of the positron wave function, i. e., the positron may get trapped there until the annihilation. This was first observed for Guinier–Preston zones in Al–Zn alloys [10].

The positron-trapping behavior in semiconductors is more complex compared with metals. This is mainly due to the fact that the positron as a charged particle is sensitive to the charge state of defects. The defect identification is more difficult in compound semiconductors since the variety of point defects increases. The improvement of the theoretical understanding of positron trapping (for a review see [20]), the refinement of positron lifetime spectroscopy as the main technique for defect studies, and the increasing amount of data have made it possible to give reliable qualitative and quantitative information on defects in solids and particularly in semiconductors. A large number of investigations have been carried out for differently grown bulk semiconductor crystals. Irradiation with high-energy electrons at low temperature represents an important tool for defined generation of point defects. Many positron studies on the defect structure have been carried out after such irradiation. In comparison with theoretical calculations, the defects can be characterized by their specific positron lifetimes.

In addition to the positron traps known from metals, negatively charged non-open-volume defects, e. g., acceptor-type impurities or negatively charged antisites in a compound, represent positron trapping centers at low temperatures. The Coulomb potential of these defects is responsible for the formation of shallow Rydberg states. Positrons may be bound with a small binding energy to such centers, which are called shallow positron traps [22].

Beside defect studies of metals and semiconductors, the characterization of polymers is a growing field. The free volume appearing in amorphous polymers due to their structural (static or dynamic) disorder is of fundamental importance for several macroscopic properties of these materials, such as viscosity, molecular transport, segmental and local polymer dynamics, and physical aging. Despite a great interest in investigations of free volume in polymers, only limited experimental information about its real structures, the hole dimensions and the size and shape distributions, is available. During the past decade positron annihilation lifetime spectroscopy has been developed to the most important method for studying sub-nanometer sized local free volume (holes) in polymers [11].

Another important field for the application of positron annihilation in materials science of condensed matter is the characterization of nanometer-sized pores [14]. Positronium is formed and gives rise to very long components in the lifetime spectrum (1 ns to more than 100 ns) which can be used to determine the pore size [15]. The filling of pores by the condensation of gases can thus directly be observed [25].

Positrons can also be used to study the surface of solids. Low-energy positron diffraction has been proven to provide additional information over the diffraction with low-energy electrons, LEED [21]. Furthermore, the release of Auger electrons from a solid surface can also by stimulated by the annihilation of positrons with core electrons [24]. For this purpose, the positrons can be implanted into the surface with very low energies of only a few eV, so that the Auger spectrum is essentially free of secondary-electron background which is an important advantage over the conventional Auger electron spectroscopy (AES). The chemical information corresponds almost completely to the outermost atomic surface layer.

The background-reduced measurement of positron annihilation of core electrons by Doppler-broadening coincidence spectroscopy [17] provides chemical information on the surroundings of the annihilation site by comparison of measured and theoretically calculated Doppler spectra in the high-momentum region. The sublattice of a vacancy defect in a compound, eventually the type of impurities stabilizing a defect complexes, and the annihilation in small impurity clusters may be observed.

Modern devices are often based on layered structures, such as epitaxially grown layers, oxides, or implanted layers. The disadvantage of conventional positron techniques directly utilizing positrons from the β^+ decay of a radioactive source is the broad energy distribution and the large penetration depth of positrons in the sample. Consequently, only bulk material can usually be investigated. This drawback has been overcome by the development of the slow-positron-beam technique (for a review see [23]). This is based on the moderation of positrons. Monoenergetic positrons are obtained at surfaces exhibiting a negative positron work function, e. g., tungsten. The emitted positrons are guided as a beam to the sample. The variation of the incident positron energy in an accelerator stage enables the measurement of near-surface defect profiles. The positron beam can be pulsed and thus the positron lifetime can also be measured. The focusing of the positron beam allows the three-dimensional probing of defect structures, i. e., the development of a positron microscope [6, 12]. Currently (2005), large efforts are undertaken to combine these sophisticated instruments to high-intensity positron sources based on pair production produced in a fission reactor [13] or by stopping an electron beam of a LINAC [4].

See also: Antimatter; Fermi Surface; Lattice Defects; Positronium; Radiation Damage in Solids; Microscopy, Optical; Auger Effect.

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Table of Contents

Volume 1

Encyclopedia of Physics, Third Edition. Edited by George L. Trigg and Rita G. Lerner

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Volume 2