Introduction into Positron Annihilation

- **Introduction** (How to get positrons? What is special about positron annihilation?)
- **The methods of positron annihilation** (positron lifetime, Doppler broadening, ACAR ...)
- **Interaction of positrons with solids** (thermalization, diffusion, trapping)
- **The trapping model** (Which defects are detectable? Determination of absolute defect concentrations. The sensitivity limit of defect detection.)
- **Defect investigation - Examples** (vacancies in thermal equilibrium; defects after electron irradiation and plastic deformation; grown-in vacancies in semiconductors)
- **Future developments** (Positron Microscopy in Munich, Livermore and Bonn)

**Literature:**
R. Krause-Rehberg, H.S. Leipner
„Positron Annihilation in Semiconductors“
Springer-Verlag, 1998
ISBN 3-540-64371-0
Positrons are obtained either by:

- $\beta^+ \text{ decay: }^{22}\text{Na} \rightarrow ^{22}\text{Ne} + \beta^+ + \nu_e + \gamma_{(1.27\text{MeV})}$ (half life: 2.6 years, up to $10^6 \text{ e}^+/\text{s}$)

- pair production using a beam of MeV-electrons onto a target (Bremsstrahlung creates positrons; $\approx 10^9 \text{ e}^+/\text{s}$; discontinuous positron beam)

- nuclear reaction: $^{113}\text{Cd}(n,\gamma)^{114}\text{Cd} \rightarrow \text{three } \gamma \text{ rays and pair production; continuous positron beam; } \approx 10^{10} \text{ e}^+/\text{s}$ (Forschungsreaktor München)

Positrons hit the sample:

- “Sandwich geometry” ($^{22}\text{Na}$ source between two identical samples)

- positron beam (source and sample separated)
- Positron wavefunction is localized at vacancy site until annihilation
- Positron annihilation parameters change when annihilating in a defect
- Defects can be detected (identification and quantification)
- Attractive potential mainly due to missing ion (repelling core is absent)
- in semiconductors: additional Coulomb tails ($\propto 1/r \rightarrow$ rather extended)
- no positron trapping by positive vacancies
- Positron lifetime is measured as time difference between 1.27 MeV quantum ($\beta^+$ decay) and 0.511 MeV quanta (annihilation process)

- PM=photomultiplier; SCA=single channel analyzer (constant-fraction type); TAC=time to amplitude converter; MCA= multi channel analyzer
Positron Lifetime Spectra

- lifetime spectra consist of exponential decay components
- positron trapping in open-volume defects leads to long-lived lifetime components
- spectra analysis is performed by non-linear fitting routines after source and background subtraction
- result: lifetimes $\tau_i$ and intensities $I_i$

$$ N(t) = \sum_{i=1}^{k+1} \frac{I_i}{\tau_i} \exp\left(-\frac{t}{\tau_i}\right) $$
The Methods of Positron Annihilation

1. Positron lifetime

Birth $\gamma$-ray
1.27 MeV

$\Delta t$

2. Angular correlation

$\Theta_{x,y} = \frac{P_{x,y}}{m_0 c}$

positron source
22-Na

Sample

100 $\mu$m
diffusion (100 nm)

Thermalization (1 ps)
Angular Correlation of Annihilation Radiation - ACAR

2D-detector array

Sample

2D-detector array

\[
N_c(\Theta_x, \Theta_y) = A_c \int_{-\infty}^{\infty} \sigma(\Theta_x m_0 c, \Theta_y m_0 c, p_z) dp_z
\]

Coincidence counting rate \(N_c\):
2D-ACAR of defect-free GaAs

(Tanigawa et al., 1995) 3D-Fermi surface can be reconstructed from measurements in several directions of a single crystal
2D-ACAR of Copper

Theory

Experiment

Fermi surface

of copper

(Berko, 1979)
Three Methods of Positron Annihilation

1. **Positron lifetime**

   *Birth γ-ray 1.27 MeV*

   \[ \Delta t \]

   *Positron source 22-Na*

   *Sample 100 μm*

   *Diffusion (100 nm)*

   *Thermalization (1 ps)*

2. **Angular correlation**

   \[ \Theta_{x,y} = \frac{p_{x,y}}{m_0 c} \]

3. **Doppler broadening**

   \[ 0.511 \text{ MeV} \pm \Delta E, \quad \Delta E = p_z c / 2 \]
- electron momentum in propagation direction of 511 keV $\gamma$-ray leads to Doppler broadening of annihilation line
- can be detected by conventional energy-dispersive Ge detectors and standard electronics
**Line Shape Parameters**

**S parameter:**

\[ S = \frac{A_S}{A_0} \]

**W parameter:**

\[ W = \frac{A_W}{A_0} \]

W parameter mainly determined by annihilations of core electrons (chemical information)
Doppler Coincidence Spectroscopy

- coincident detection of second annihilation $\gamma$ reduces background
- use of a second Ge detector improves energy resolution of system
Doppler Coincidence Spectra

\[ E_1 + E_2 = 2 \, m_0 \, c^2 = 1022 \, \text{keV} \]
Thermalization in Solids

- broad positron emission spectrum
- deep implantation into solids
- no use for study of defects in thin layers
- moderation necessary

Mean (maximum) implantation depth of unmoderated positrons (1/e 0.999):

Si: 50µm (770µm)    GaAs: 22µm (330µm)    PbS: 15µm (220µm)
Moderation of Positrons

W (110) single crystal foil (negative workfunction)

2 μm

fraction

annihilation ≈ 13%

thermalization
diffusion

monoenergetic positrons
E ≈ 3 eV

fast positrons ≈ 87%
up to several 100 keV

Moderation efficiency: 10^-4
Implantation Profiles of monoenergetic Positrons

- depth resolution is function of implantation depth
- exact implantation profiles are obtained by Monte-Carlo simulations

\[ P(z, E) = \frac{m z^{m-1}}{z_0^m} \exp \left[ -\left( \frac{z}{z_0} \right)^m \right] \]

\[ z = f(E, \rho) \quad z_0 = \text{const.} \quad m = 2 \]

(Makhov, 1961)
The Positron Beam System at Halle University

- spot diameter: 5mm
- time per single Doppler measurement: 20 min
- time per depth scan: 8 hours

$U_{\text{ExB}}$, $U_{\text{HV}} = 0 \ldots 50 \text{ kV}$, $0 \ldots 5 \mu\text{m}$ penetration depth
The positron beam system at Halle University

- beam valve
- differential pumping
- sample chamber
- Doppler coincidence measurement
- magnetic beam guidance system
- $^{22}$Na Source
- $^{22}$Na Source
- beam valve
- differential pumping
- sample chamber
- Doppler coincidence measurement
- magnetic beam guidance system
The Diffusion of Positrons

Diffusion can be described by the time-dependent diffusion equation:

\[
\frac{\partial}{\partial t} n_+(\mathbf{r}, t) = D_+ \nabla^2 n_+(\mathbf{r}, t) - \nabla \left[ \nu_d n_+ (\mathbf{r}, t) \right] - \lambda_{\text{eff}} n_+ (\mathbf{r}, t). 
\]

\( n_+(\mathbf{r}, t) \) ... positron density \( \nu_d \) ... drift velocity (electric field)

\[
\lambda_{\text{eff}} = \frac{1}{\tau_b} + \kappa(\mathbf{r}) \text{ ... effective annihilation rate}
\]

\[
\kappa = \mu C \quad \mu \text{ ... trapping coefficient} \quad C \text{ ... defect density}
\]

Mean free path \( l \) and positron diffusion length \( L_+ \) in semiconductors is mainly determined by acoustic phonon scattering \( \Rightarrow D \propto T^{-0.5} \)

<table>
<thead>
<tr>
<th></th>
<th>( l ) [nm]</th>
<th>( L ) [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>7</td>
<td>220</td>
</tr>
<tr>
<td>GaAs</td>
<td>5.3</td>
<td>200</td>
</tr>
</tbody>
</table>
Positron Trapping in a Single Defect Type

The $t_i$ and $I_i$ are measured $\Rightarrow k$ is obtained:

$$\kappa_d = \mu C_d = \frac{I_2}{I_1} \left( \frac{1}{\tau_b} - \frac{1}{\tau_d} \right)$$
Positron Trapping in a Dislocation

- $\lambda_i$ ... annihilation rates
- $\kappa_i, \vartheta$ ... trapping rates
- $\delta$ ... detrapping (escape) rate

The dislocation line (shallow trap) acts as a “funnel” for the trapping in deep traps.

b ... bulk
v ... vacancy
t ... deep trap
st ... shallow trap
Determination of absolute Defect Densities

- the trapping coefficient $\mu_k = \mu C$ must be determined by an independent method.

- positron trapping may be strongly temperature-dependent $\Rightarrow \mu = f(T)$

<table>
<thead>
<tr>
<th>Defect in Si$_{300K}$</th>
<th>$\mu$ (10$^{15}$ s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V^-$</td>
<td>1</td>
</tr>
<tr>
<td>$V^{2-}$</td>
<td>2</td>
</tr>
<tr>
<td>$V^0$</td>
<td>0.5</td>
</tr>
<tr>
<td>$V^+$</td>
<td>&lt; 0.1</td>
</tr>
<tr>
<td>Dislocation</td>
<td>1 cm$^2$s$^{-1}$</td>
</tr>
<tr>
<td>Vacancy cluster</td>
<td>$n \cdot \mu_1 V$</td>
</tr>
</tbody>
</table>
Vacancies in thermal Equilibrium

- Vacancy concentration in thermal equilibrium:
  - in metals $H^F \approx 1\ldots4$ eV ⇒
    at $T_m [1v] \approx 10^{-4}\ldots10^{-3}$
  - fits well to the sensitivity range of positron annihilation

\[
C_{1v}(T) = \exp\left(\frac{S_{1v}^F}{k}\right) \exp\left(\frac{H_{1v}^F}{kT}\right)
\]

**Tungsten**

$E^F = (4.0 \pm 0.3)$ eV

(Ziegler, 1979)
Defects in Ge after Electron Irradiation

- electron irradiation generates Frenkel pairs
- vacancy annealing and defect reactions may be studied by positrons

(Polity et al., 1997)
Defects in Si induced by Ion Implantation

- ion implantation is most important doping technique in planar technology
- main problem: generation of defects \( \Rightarrow \) positron beam measurements
Defect density as function of deposited ion energy

Defect generation follows Chadderton’s model of homogenous nucleation:

\[
\text{[defect]} \sim \text{dose}^{0.5}
\]

valid for RBS- and positron data

only exception: Si self-implantation

can be explained: extra Si atoms are interstitials and kill vacancies that are seen by positrons but not by RBS

(Eichler et al., 1997)
Plastic Deformation and Electron Irradiation in Pb

(Petters et al., 1998)
The nature of the EL2 defect in GaAs

- one of mostly investigated defects
- exhibiting metastability at low T under light illumination (Krause et al., 1990)
- stable metastable (Dabrowski 1988, Chadi 1988)
- there were several structural models of EL2
- the above shown model was proven by positron annihilation (Krause et al., 1990)
Other Positron Techniques

- Low-Energy Positron Diffraction (LEPD): more simple theoretical calculation of diffraction pattern (no electron-electron interaction)

- Positron-Annihilation-induced Auger Electron Spectroscopy (PAES): no background due to secondary electrons & very surface-sensitive

- Positron Microprobe/Microscope

- Forschungsreaktor München: very strong continuous positron source and remoderation ⇒ three-dimensional imaging of defect distributions

- Univ. Bonn: combination of Scanning Electron Microscopy and a focussed (1 µm) positron beam of variable energy ⇒ defect imaging
The Positron Microscope at Bonn University

- $e^+$ source
- Prism
- $e^-$ gun
- Moderator
- Condensor
- Objective lens
- Sample
- Ge detector
- Positioning system