Positron Beam Application to Materials Science and Intense Accelerator or Reactor based Positron Beam Facilities in Germany

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• Introduction: Positrons detect lattice defects
• Examples:
  - new getter centers in Si after high-energy self-implantation ($R_p/2$ effect)
  - study of defects in GaAs
• Large Positron Facility Projects in Germany
• Conclusions
The positron lifetime spectroscopy

- positron wave-function can be localized in the attractive potential of a defect
- annihilation parameters change in the localized state
- e.g. positron lifetime increases in a vacancy
- lifetime is measured as time difference between 1.27 and 0.51 MeV quanta
- defect identification and quantification possible
Positron lifetime spectroscopy

- Positron lifetime spectra consist of exponential decay components
- Positron trapping in open-volume defects leads to long-lived components
- Longer lifetime due to lower electron density
- Analysis by non-linear fitting: lifetimes $\tau_i$ and intensities $I_i$

Positron lifetime spectrum:

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

- Trapping coefficient

$$\kappa_d = \mu C_d = \frac{I_2}{I_1} \left( \frac{1}{\tau_b} - \frac{1}{\tau_d} \right)$$

- Trapping rate
- Defect concentration

As–grown Cz Si
Plastically deformed Si

$\tau_2 = 320 \text{ ps}$ (divacancies)
$\tau_3 = 520 \text{ ps}$ (vacancy clusters)
$\tau_b = 218 \text{ ps}$ (bulk)
Monoenergetic positron beam by moderation

- positron annihilation was very successful in defect identification in last decades
- semiconductor technology: thin layers (epitaxy, ion implantation)
- broad energy distribution due to $\beta^+$ decay
- some surfaces: negative workfunction $\Rightarrow$ moderation (but rather inefficient)

**Energy distribution after $\beta^+$ decay**

**Effect of moderation**

- W (110) single crystal foil (negative workfunction)
- $\approx 13\%$ annihilation
- $\approx 0.05\%$ monoenergetic positrons $\approx 87\%$ fast positrons up to several 100 keV
Conventional positron beam technique

- positron beam can be formed using mono-energetic positrons
- often: magnetically guided for simplicity

- defect studies by Doppler-broadening spectroscopy
- characterization of defects only by line-shape parameters or positron diffusion length
- for positron lifetime spectroscopy: beam can be bunched
Defects in high-energy self-implanted Si — The $R_{p}/2$ effect

- after high-energy (3.5 MeV) self-implantation of Si ($5 \times 10^{15}$ cm$^{-2}$) and RTA annealing (900°C, 30s): two new gettering zones appear at $R_p$ and $R_{p}/2$ ($R_p =$ projected range of Si$^+$)
- visible by SIMS profiling after intentional Cu contamination

![TEM image by P. Werner, MPI Halle](image1)

- at $R_p$: gettering by interstitial-type dislocation loops (formed by excess interstitials during RTA)
- no defects visible by TEM at $R_{p}/2$
- What type are these defects?

![SIMS graph](graph1)

- Interstitial type [3,4]
- Vacancy type [1,2]

Enhanced depth resolution by using the Munich Scanning Positron Microscope

- Sample is wedge-shaped polished (0.5...2°)
- Layer of polishing defects must be thin compared to \( e^+ \) implantation depth
- Best: chemo-mechanical polishing

![Diagram showing positron beam and scan direction with defect depth and lateral resolution.](image)

- Defect depth: 10 \( \mu \text{m} \)
- Scan direction
- Lateral resolution: 1...2 \( \mu \text{m} \)
- Alpha angle: 0.6°
First defect depth profile using Positron Microscopy

- 45 lifetime spectra: scan along wedge
- separation of 11 µm between two measurements corresponds to depth difference of 155 nm (α = 0.81°)
- beam energy of 8 keV ⇒ mean penetration depth is about 400 nm; represents optimum depth resolution
- no further improvement possible due to positron diffusion: L*(Si @ 300K) ≈ 230 nm
- both regions well visible:
  - vacancy clusters with increasing density down to 2 µm (R_p/2 region)
  - in R_p region: lifetime τ_2 = 330 ps; corresponds to open volume of a divacancy; must be stabilized or being part of interstitial-type dislocation loops

Silicon self-implantation:
- 3.5 MeV, 5×10^{15} cm^{-2}
- annealed 30s 900°C
- Cu contaminated
SIMS profile of Cu
The Nature of the EL2-Defect in GaAs

- one of the most frequently studied crystal lattice defects at all
- responsible for semi-insulating properties of GaAs: large technological importance
- is deep donor, compensates shallow acceptors, e.g. C⁺ impurities
- defect shows metastable state after illumination at low temperatures
- IR-absorption of defect disappears during illumination at T < 100 K
- ground state recovers during annealing at about 110 K
- many structural models proposed
- Dabrowski, Scheffler and Chadi, Chang (1988): simple As⁺Ga⁻-antisite defect responsible
- must show a metastable structural change
The Nature of the EL2-Defect in GaAs

- in metastable state at low temperature: Ga vacancy
- should disappear during annealing at about 110 K
- confirmed by positron lifetime measurements
- kinetics of recovery of ground state is identical for IR- und positron experiment: \( E_A = (0.37 \pm 0.02) \) eV
- evidence of the vacancy in metastable state confirms the proposed structural model

![Graph showing recovery time and positron annihilation](image)

Identification von \( \text{V}_{\text{Ga}} - \text{Si}_{\text{Ga}} \)-Complexes in GaAs:Si

- Scanning tunneling microscopy at GaAs (110)-cleavages planes (by Ph. Ebert, Jülich)
- Defect complex identified as \( \text{V}_{\text{Ga}} - \text{Si}_{\text{Ga}} \)

Mono-vacancies in GaAs:Si are \( \text{V}_{\text{Ga}} - \text{Si}_{\text{Ga}} \)-complexes

electron-irradiated GaAs

- electron irradiation generates vacancies in both sublattices
- very complex annealing behavior
- main annealing stage at 300 K
- similar annealing stage found for doped GaAs

Defects in epitaxially grown LT-GaAs-Layer

- MBE-Growth of GaAs can be performed at 200°C
- thickness of layer ≈ 1 µm
- has unique properties, e.g. very short recombination time
- layer extremely rich of defects
- up to 1% As-excess is compensated by As$_{Ga}$ und V$_{Ga}$
- Ga vacancies are seen by positrons
- during annealing: As-precipitation starts at 400°C
- positrons detect then small vacancy clusters
- clusters are probably bound to precipitates

Large Positron Facility Projects in Germany

- **FRM-II** (Positron source at Research Reactor-II in Garching near Munich)
  - continuous positron beam for different experiments, mainly for:

- **Scanning Positron Microscope** at “Universität der Bundeswehr“, Munich
  - system already working using 22-Na source
  - positron lifetime measurement; lateral resolution about 2 µm

- **EPOS** – European Positron Source for applied Research (project at Research Center Rossendorf, near Dresden)
  - positron source for materials research at superconducting 40 MeV-FEL in Rossendorf
  - primary time structure suitable for positron lifetime spectroscopy
- positron generation by a nuclear reaction: $^{113}\text{Cd}(n,\gamma)^{114}\text{Cd}$
- three $\gamma$ rays $\rightarrow$ pair production
- continuous positron beam
- $\approx 10^{10}$ slow $e^+/s$ expected
Principle of the Positron Source at FRM-II

n\textsubscript{therm} → \gamma → e^+e^-

n - capture

\gamma - emission

\gamma \rightarrow e^+e^-

e^+ - moderation

e^+ - emission

C. Hugenschmidt, 2002
Scanning Positron Microscope in Munich

• Semiconductor devices nm-sized ⇒ Positron microprobes required
• Images show directly distribution of positron traps, i.e. nanoscopic lattice defects
• However: positron diffusion length is fundamental limit for lateral resolution
• No sense to improve resolution much below 500 nm
• First instrument was realized at Univ. Bonn (20 µm; Doppler spectroscopy)
• First realization of scanning positron microscope for lifetime spectroscopy: in Munich
Scheme of the Munich Microscope

- moderated positrons are electrostatically focused, choppered and bunched
- second moderator stage allows focus down to about 2 µm
- positron penetration energy adjustable for depth information
- instrument shall be adopted to the FRM-II positron source when available
Scanning Positron Microscope in Munich
Scanning Positron Microscope in Munich

- defects near a crack in fatigued Cu
- Semiconductor test structure

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EPOS - Positron source at the Free-Electron Laser at ELBE

- electron beam at ELBE FEL is bunched (length: $\approx 1$ ps, repetition time: $\approx 100$ ns, cw-mode, up to $10^8$ e$^-$/bunch)
- beam energy: 40 MeV  power: 40 kW
- FEL-system in Rossendorf under construction (ELBE)
- primary electron beam already available
- direct positron lifetime measurement using time structure of e$^-$ beam possible
- about $2...5 \times 10^8$ slow e$^+$/s; multidetector system for high counting rate
- combination with Doppler-coincidence spectroscopy (DOCOS) and Age-momentum correlation (AMOC)
Conclusions

- vacancy-type defects can be detected in solids by means of positron annihilation
- method very sensitive for early stage of vacancy agglomeration
- tools for thin layers (mono-energetic positron beams)
- scanning positron microbeams available
- intense positron sources under construction in Germany too

This presentation can be found as pdf-files on our Website:
http://www.ep3.uni-halle.de/positrons

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