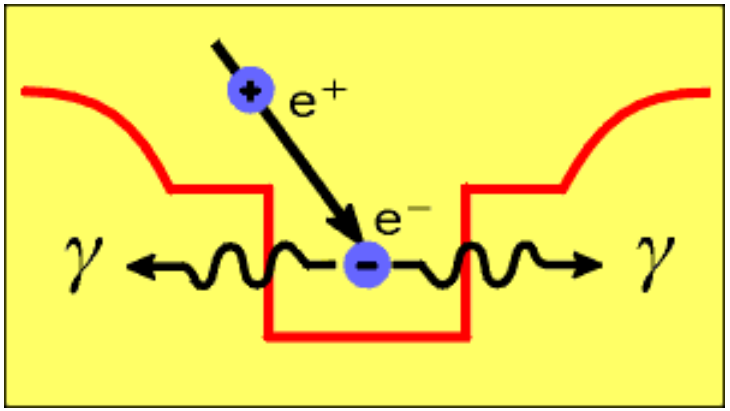
Introduction into Positron Annihilation

- **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



Introduction

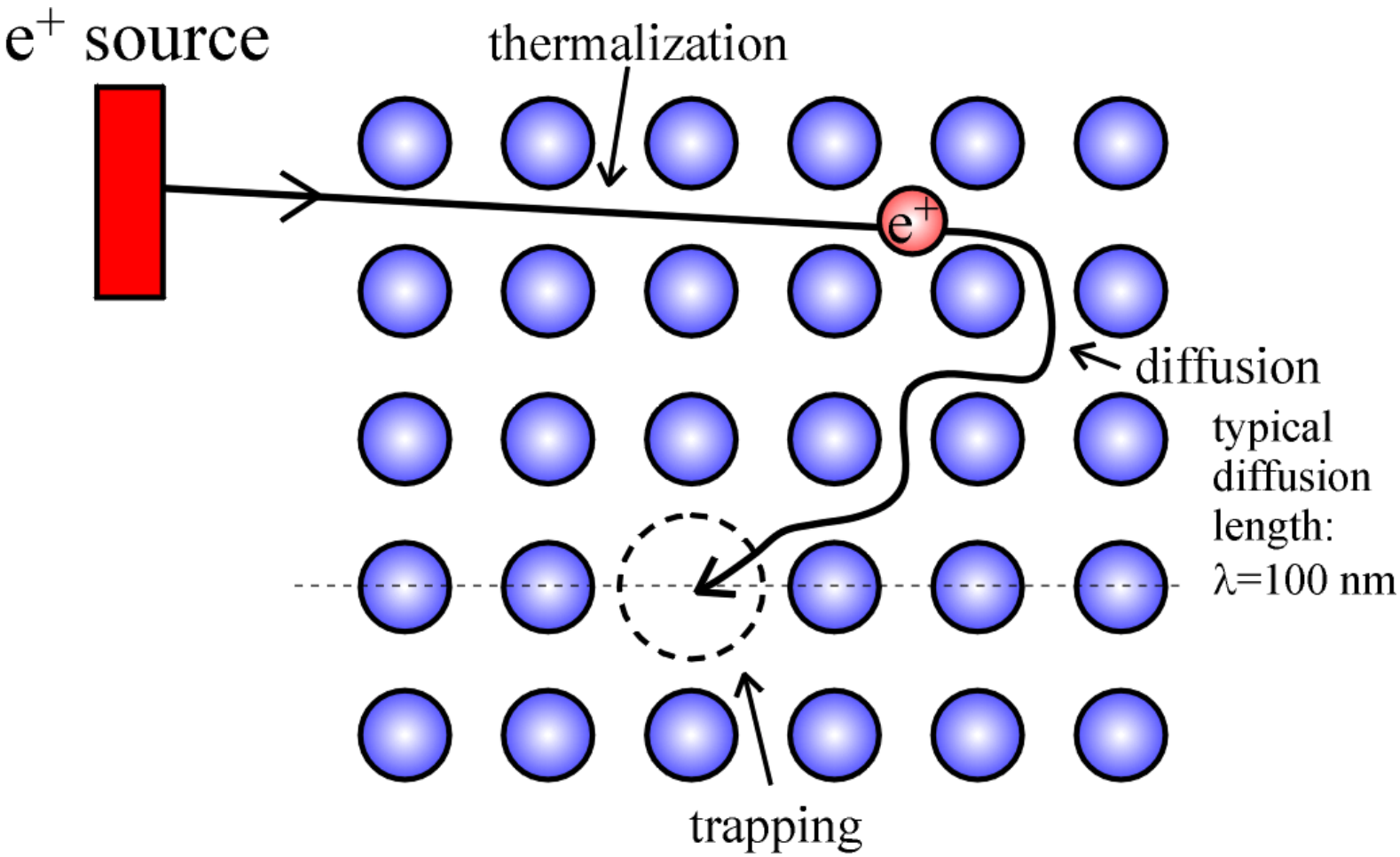
Positrons are obtained either by:

- β^+ decay: $^{22}Na \rightarrow {}^{22}Ne + \beta^+ + \nu_e + \gamma_{(1.27MeV)}$ (half life: 2.6 years, up to 10^6 e^+/s)
- pair production using a beam of MeV-electrons onto a target (Bremsstrahlung creates positrons; $\approx 10^9$ e^+/s; discontinuous positron beam)
- nuclear reaction: $^{113}Cd(n,\gamma)^{114}Cd \rightarrow$ three γ rays and pair production; continuous positron beam; $\approx 10^{10}$ e^+/s (Forschungsreaktor München)

Positrons hit the sample:

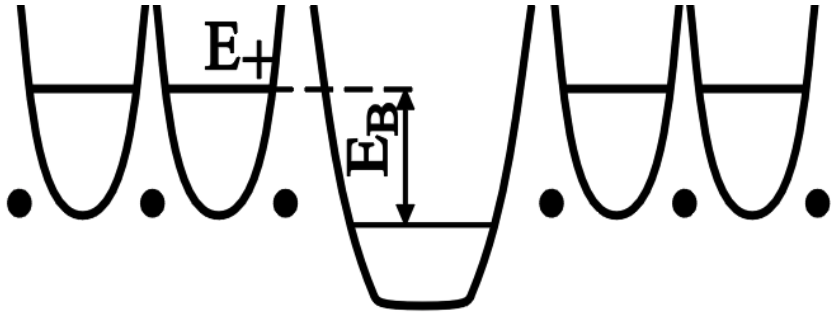
- "Sandwich geometry" (^{22}Na source between two identical samples)
- positron beam (source and sample separated)

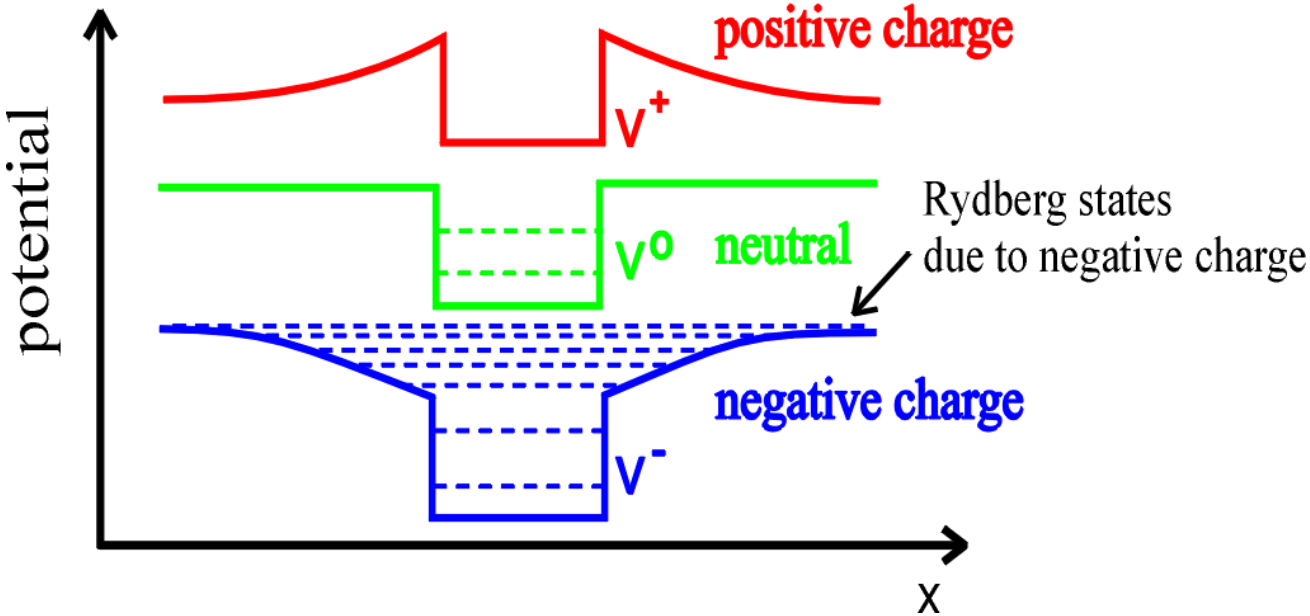
Effect of Positron Trapping in Crystal Lattice Defects



- Positron wavefunction is localized at vacancy site until annihilation
- Positron annihilation parameters change when annihilating in a defect
- Defects can by detected (identification and quantification)

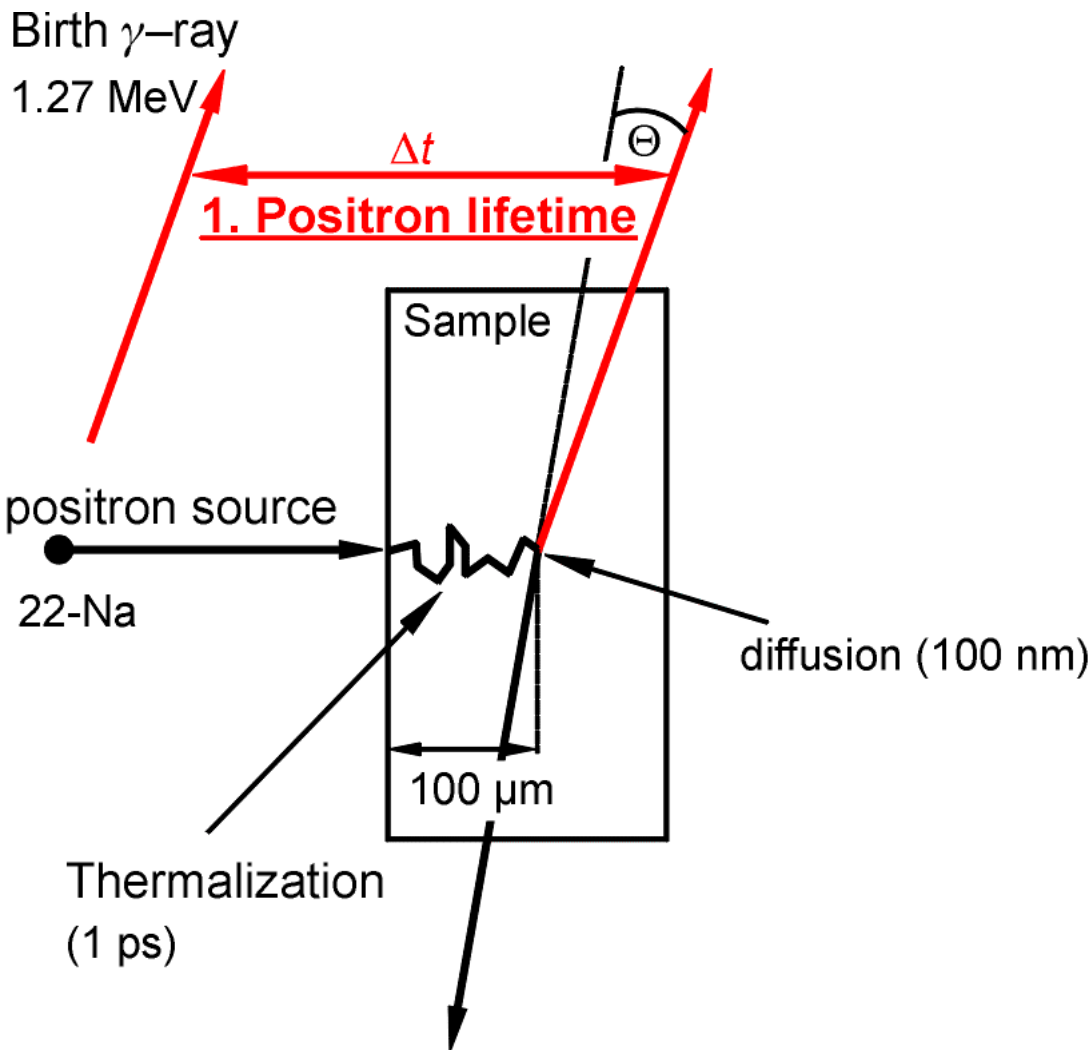
Positron Trapping Potential



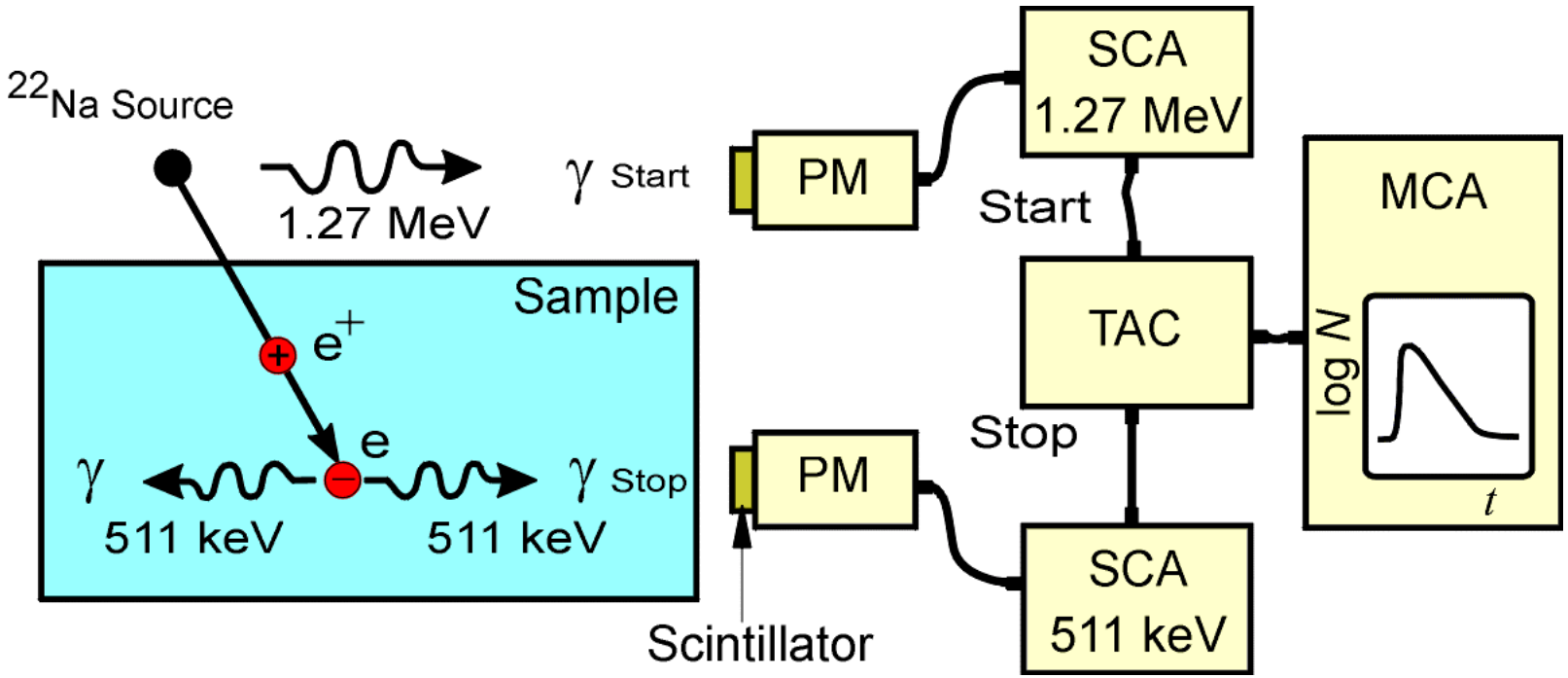


- Attractive potential mainly due to missing ion (repelling core is absent)
- in semiconductors: additional Coulomb tails ($\propto 1/r \rightarrow$ rather extended)
- no positron trapping by positive vacancies

The Methods of Positron Annihilation

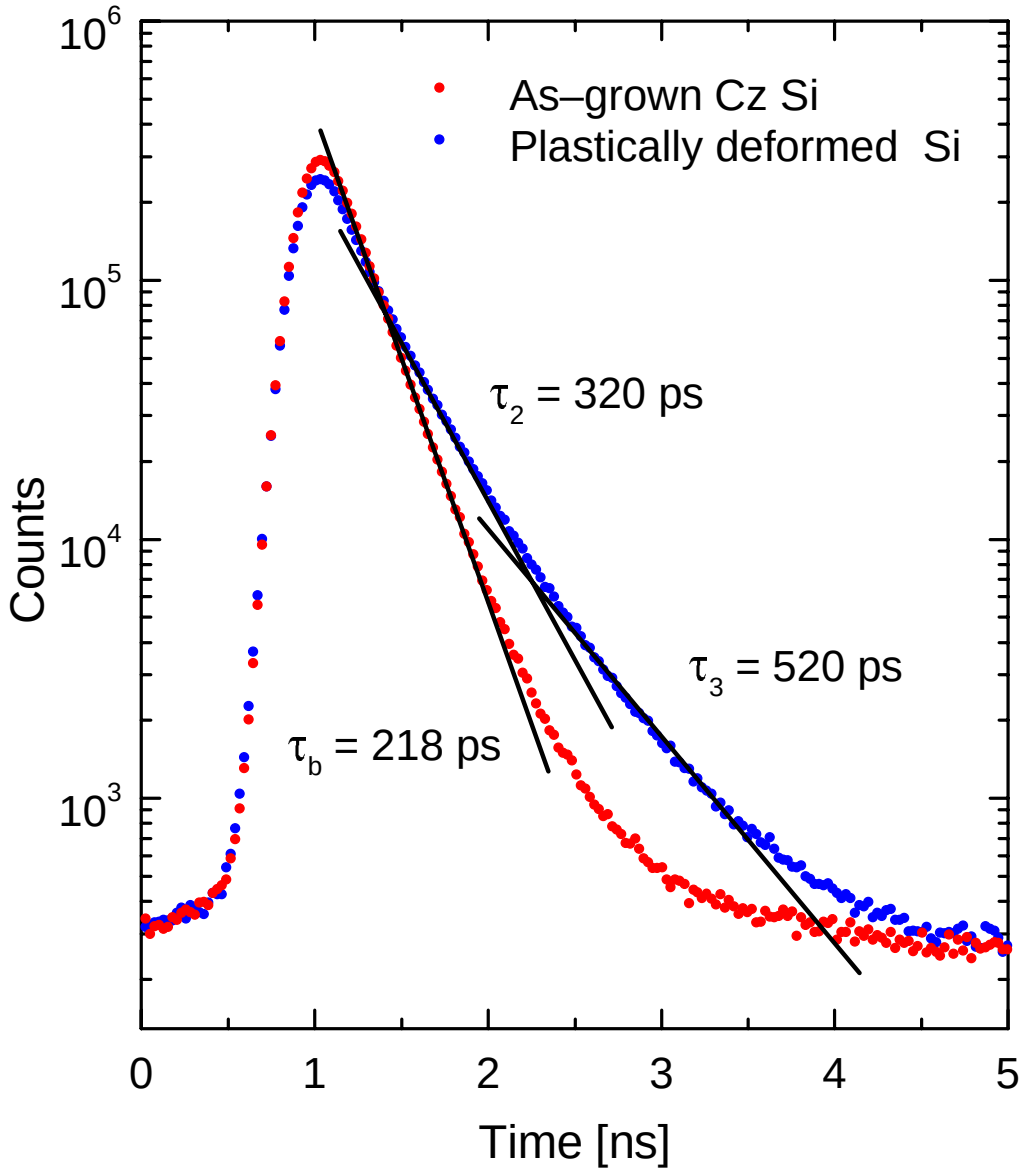


The Positron Lifetime Measurement



- Positron lifetime is measured as time difference between 1.27 MeV quantum (β^+ 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

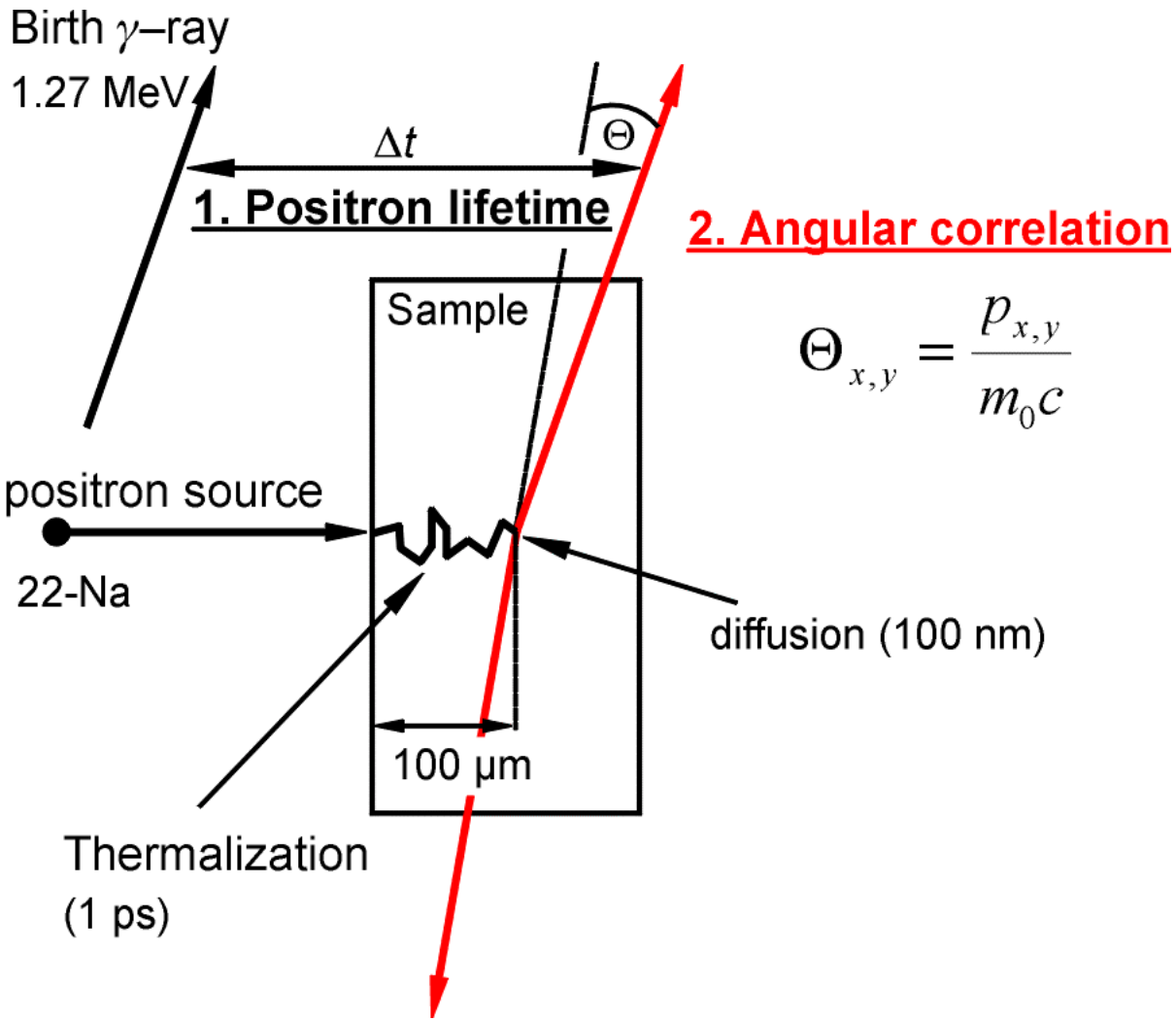
Positron Lifetime Spectra



- 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 τ_i and intensities I_i

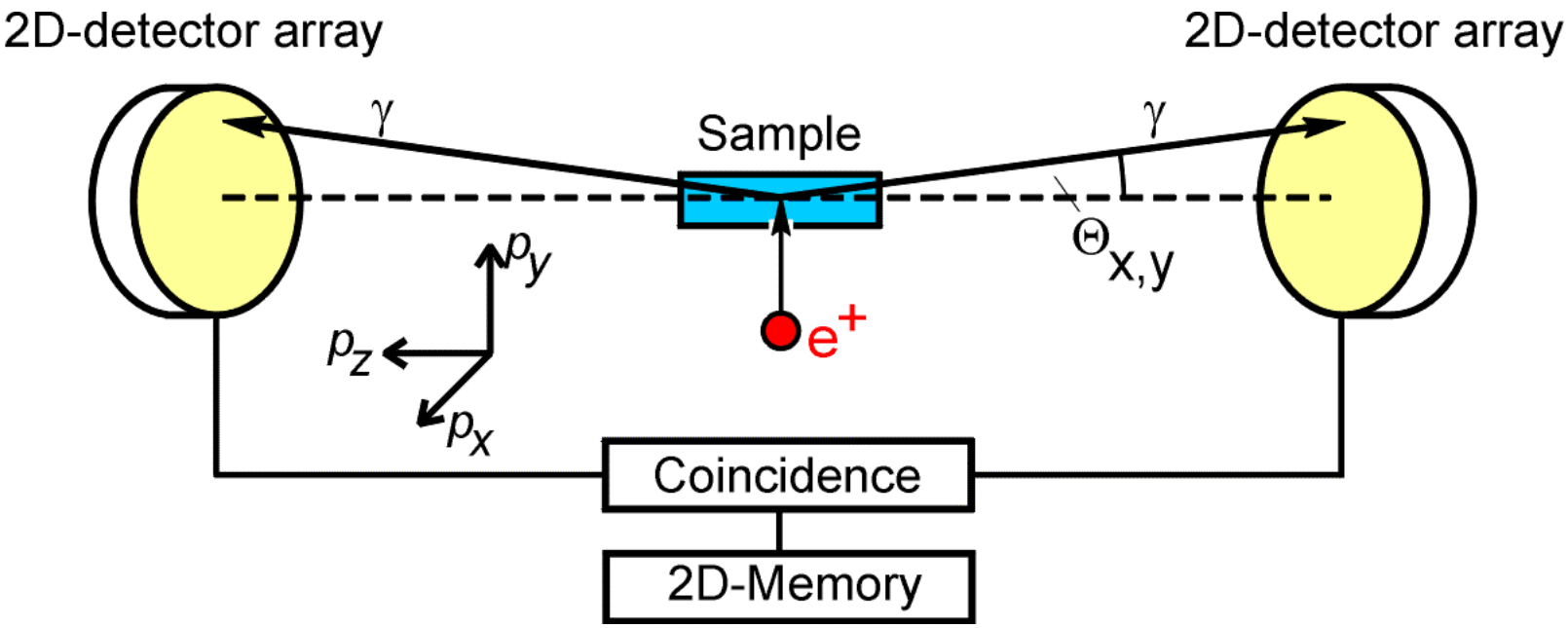
$$N(t) = \sum_{i=1}^{k+1} \frac{I_i}{\tau_i} \exp\left(-\frac{t}{\tau_i}\right)$$

The Methods of Positron Annihilation



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

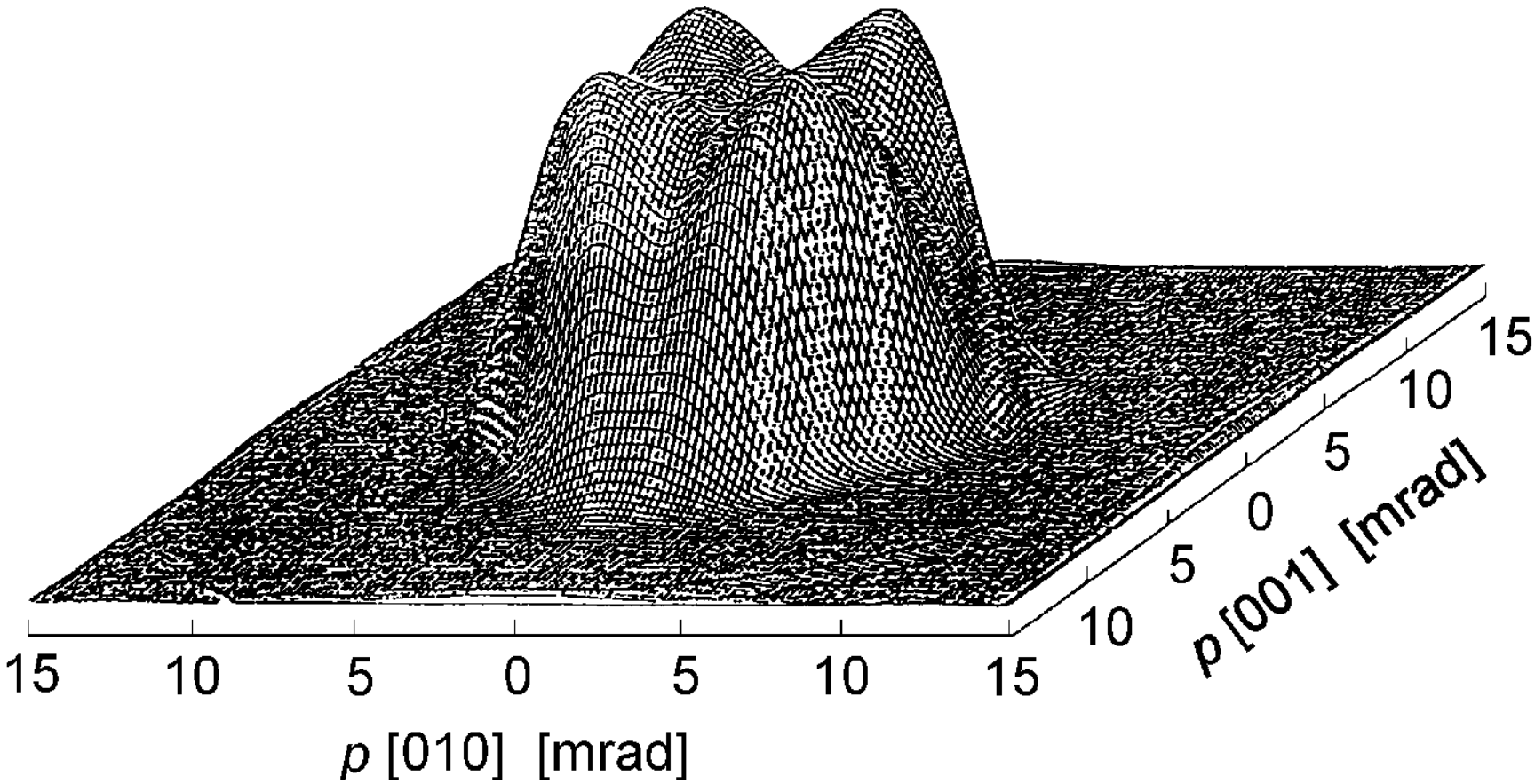
Angular Correlation of Annihilation Radiation - ACAR



Coincidence counting rate N_c:

$$N_c(\Theta_x, \Theta_y) = A_c \int_{-\infty}^{\infty} \sigma(\Theta_x m_0 c, \Theta_y m_0 c, p_z) \mathrm{d}p_z$$

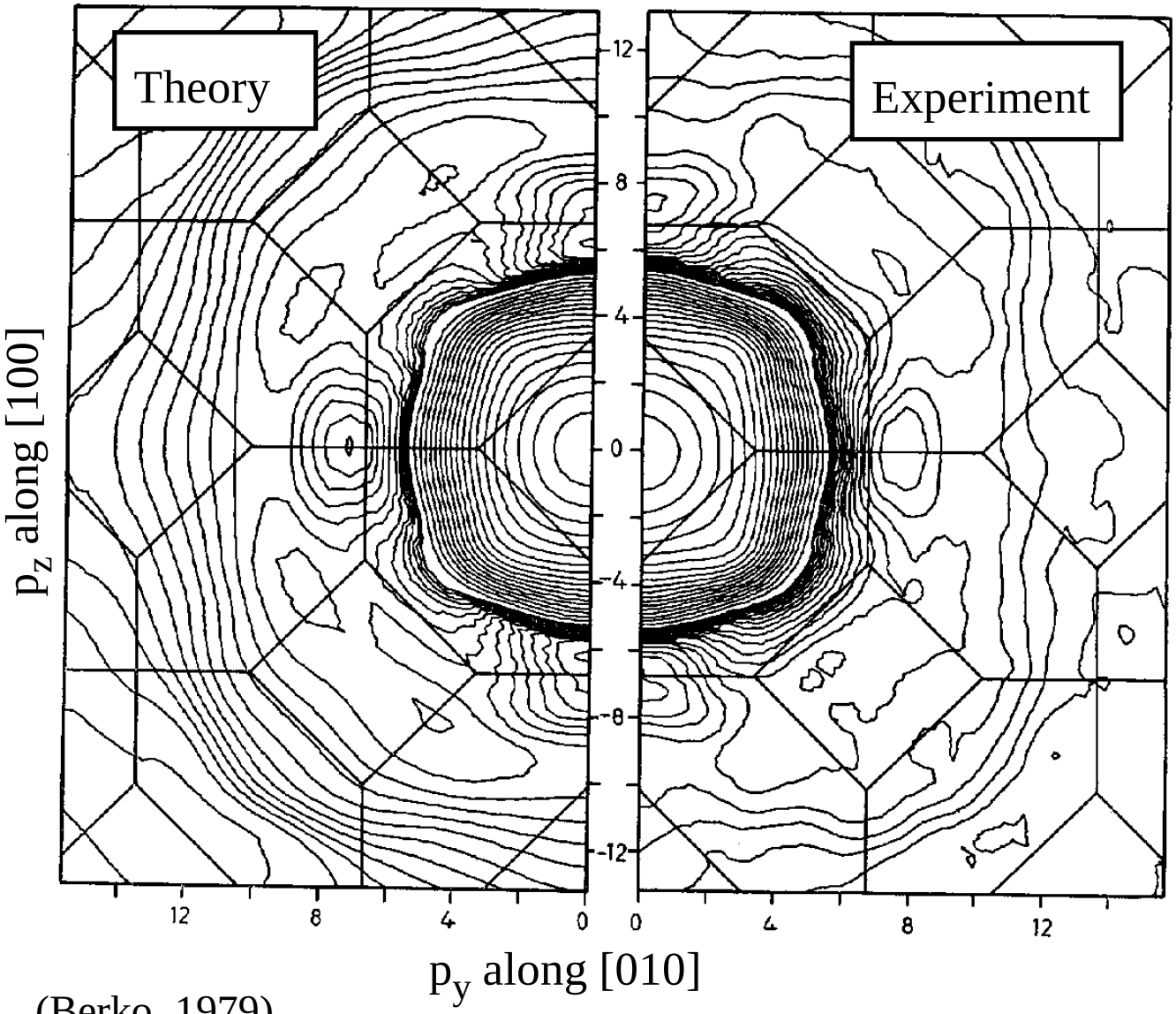
2D-ACAR of defect-free GaAs



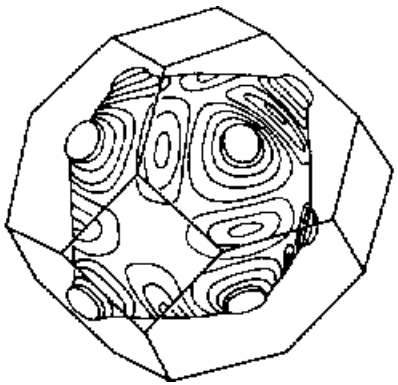
(Tanigawa et al., 1995)

3D-Fermi surface can be reconstructed from measurements in several directions of a single crystal

2D-ACAR of Copper

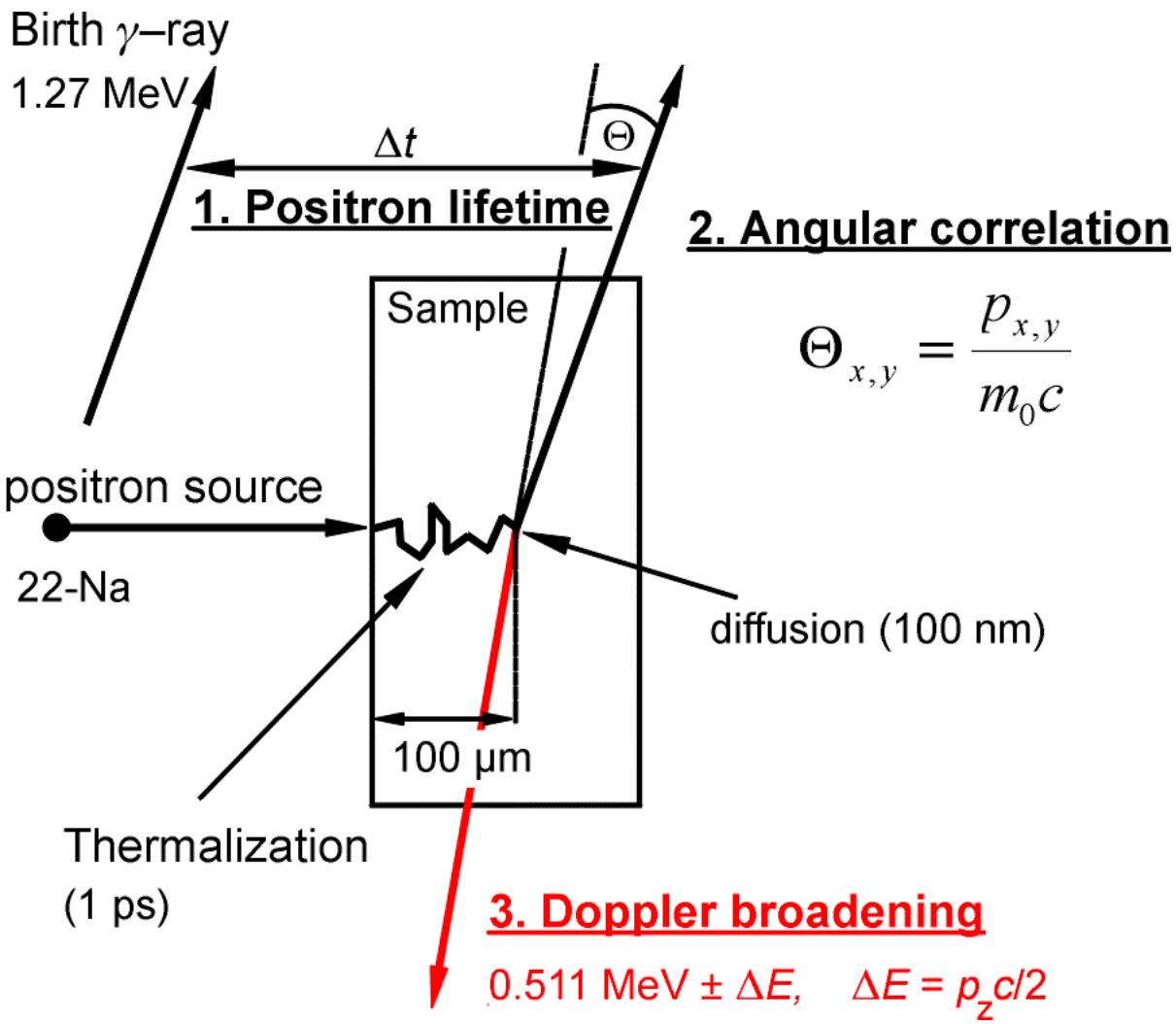


(Berko, 1979)



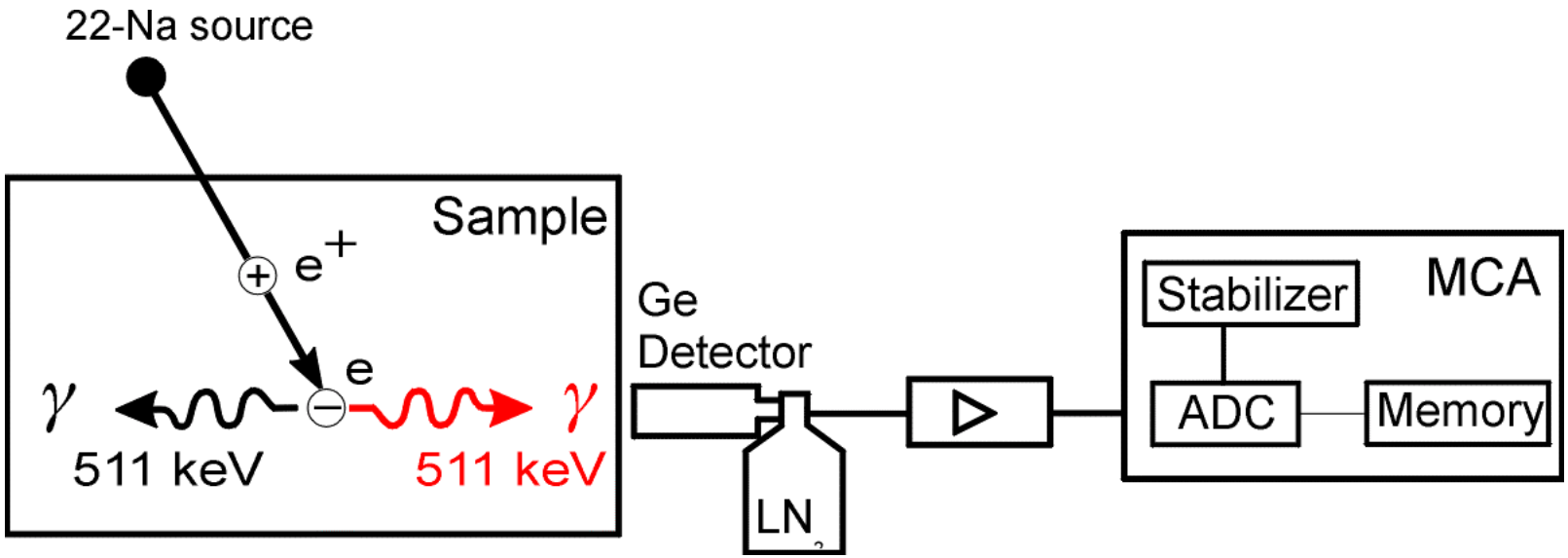
Fermi surface of copper

Three Methods of Positron Annihilation



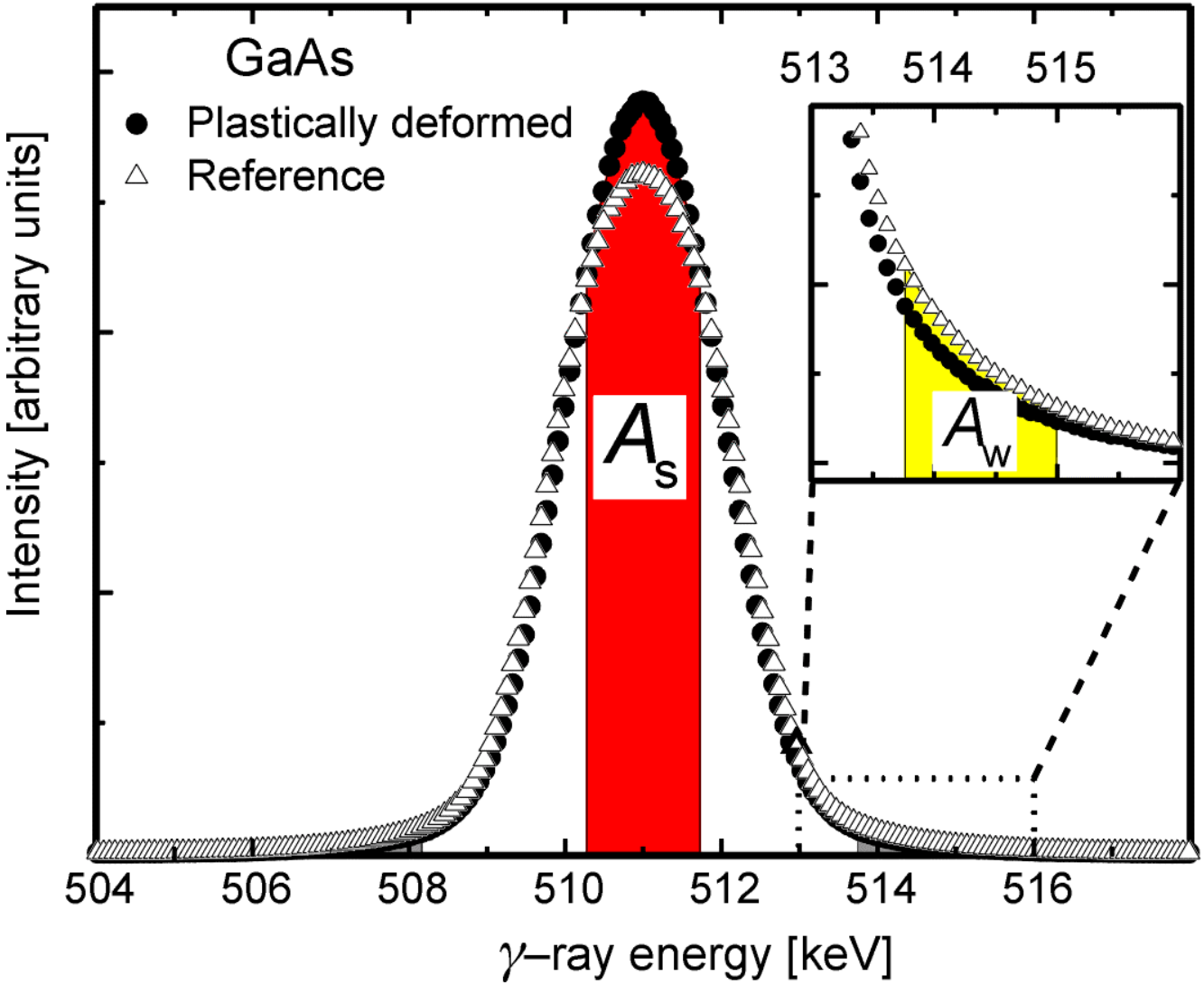
$$\Theta_{x,y} = \frac{p_{x,y}}{m_0 c}$$

Measurement of Doppler Broadening



- electron momentum in propagation direction of 511 keV γ-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:

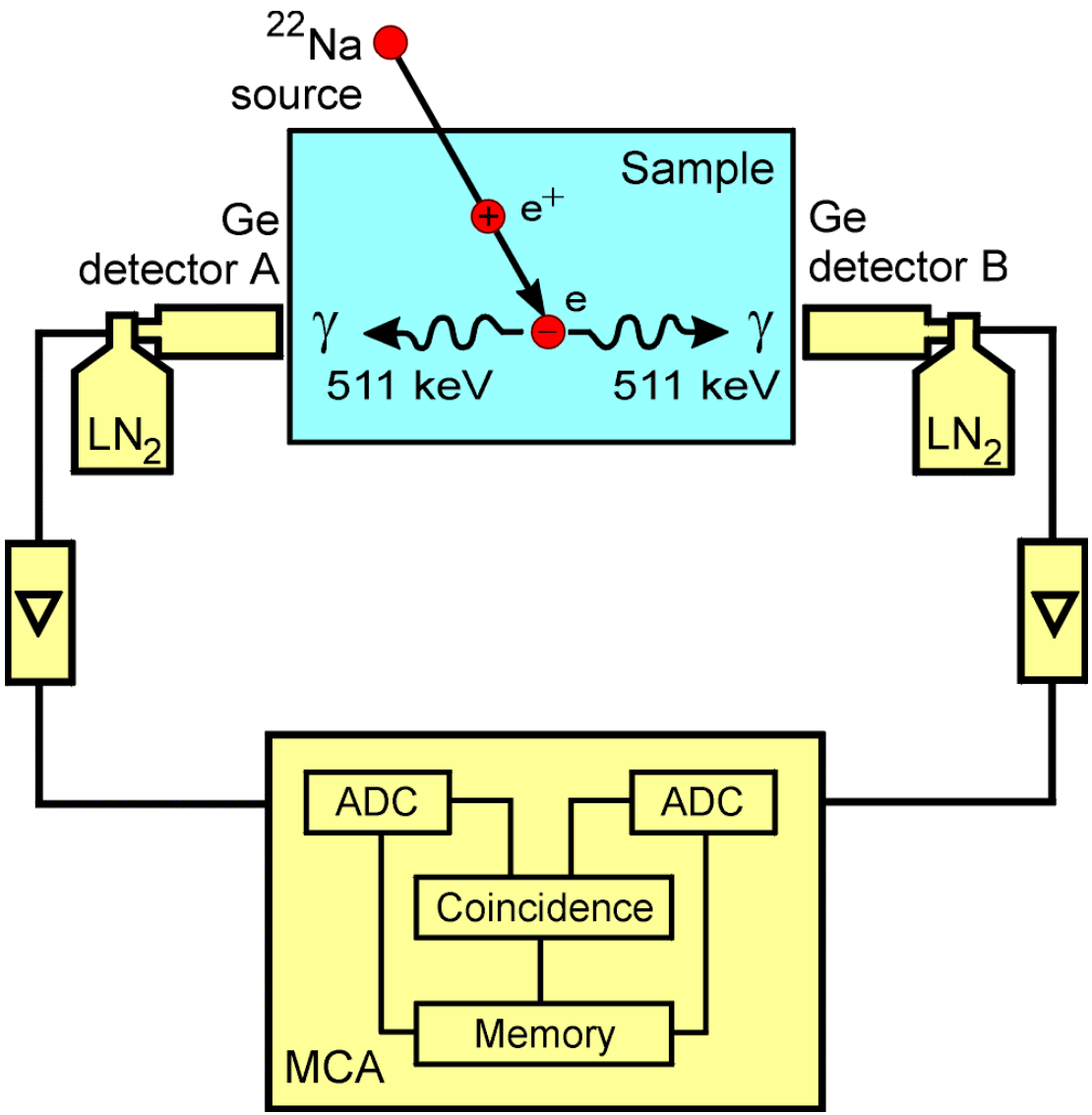
$S = A_S/A_0$

W parameter:

$W = A_W/A_0$

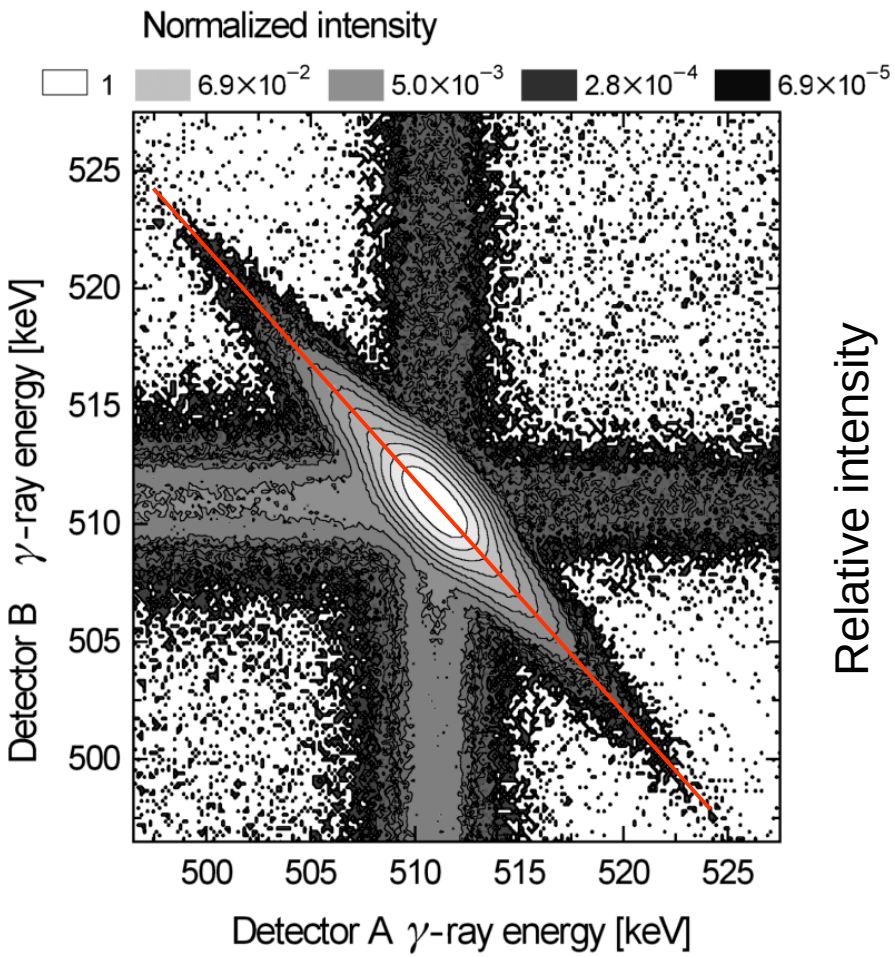
W parameter mainly determined by annihilations of core electrons (chemical information)

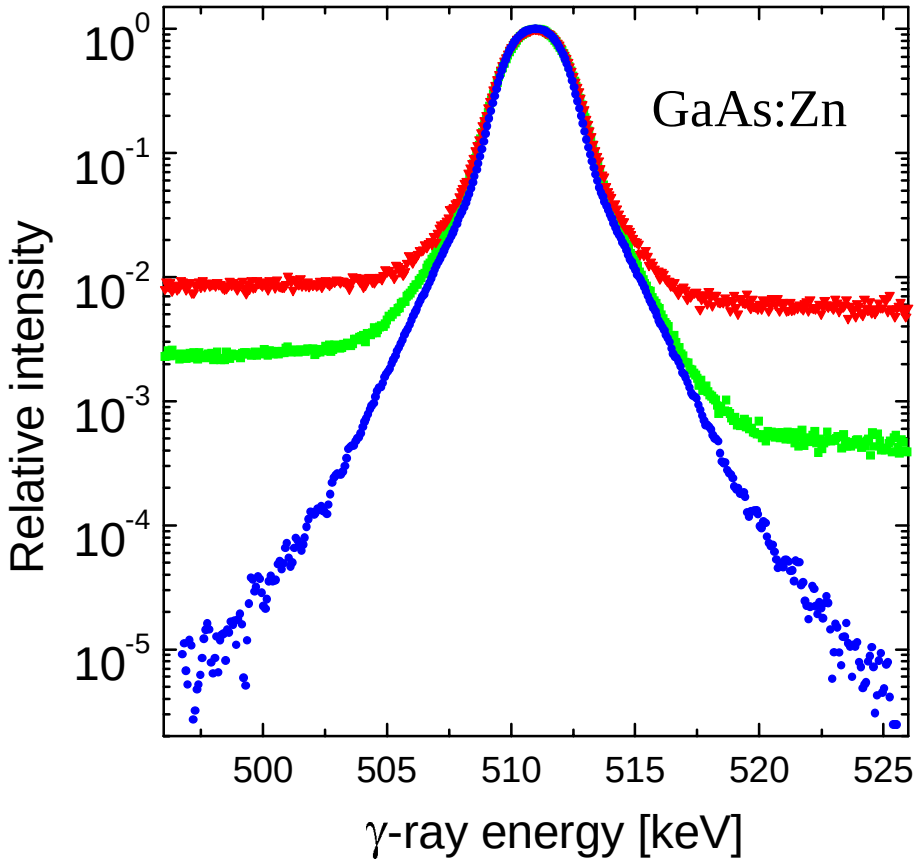
Doppler Coincidence Spectroscopy



- coincident detection of second annihilation γ reduces background
- use of a second Ge detector improves energy resolution of system

Doppler Coincidence Spectra

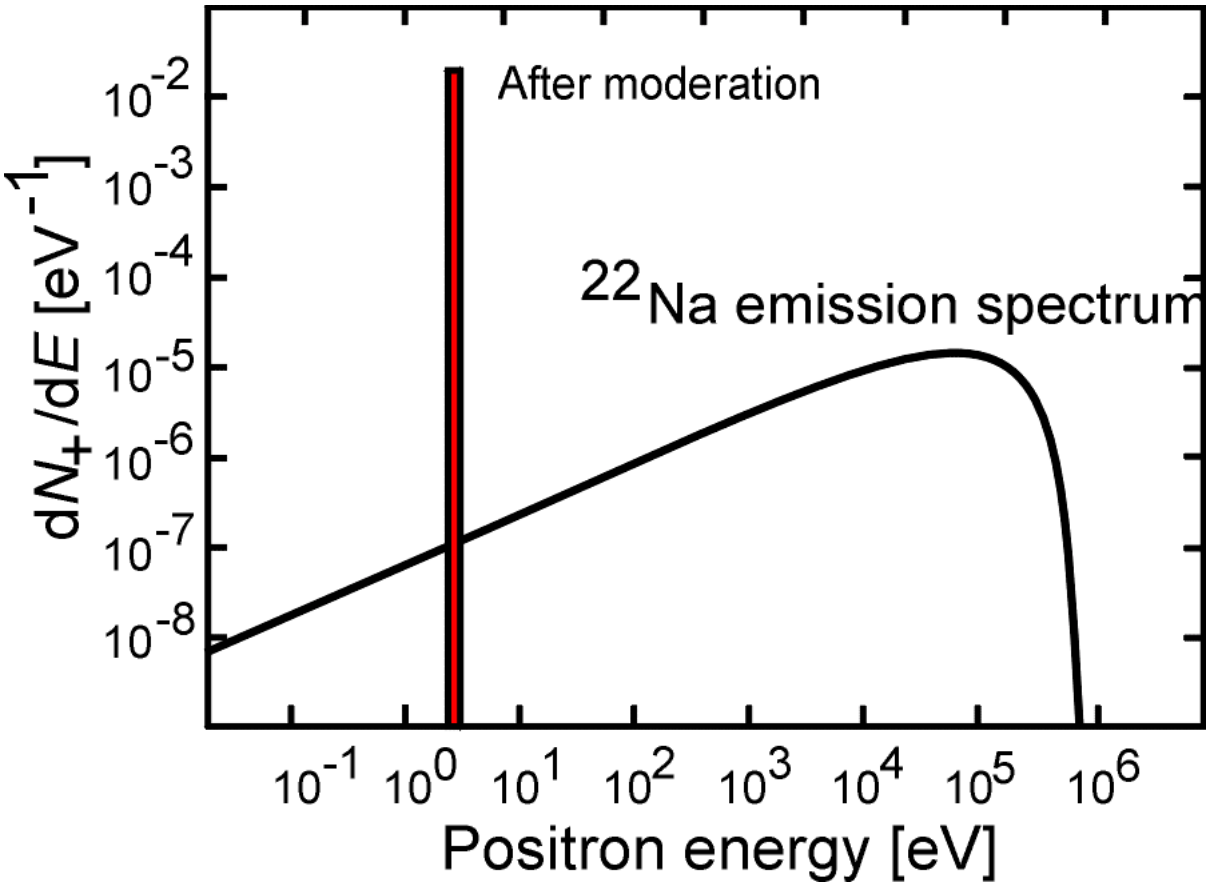




$$E_1 + E_2 = 2\, m_0\, c^2$$

$$= 1022 \text{ keV}$$

Thermalization in Solids

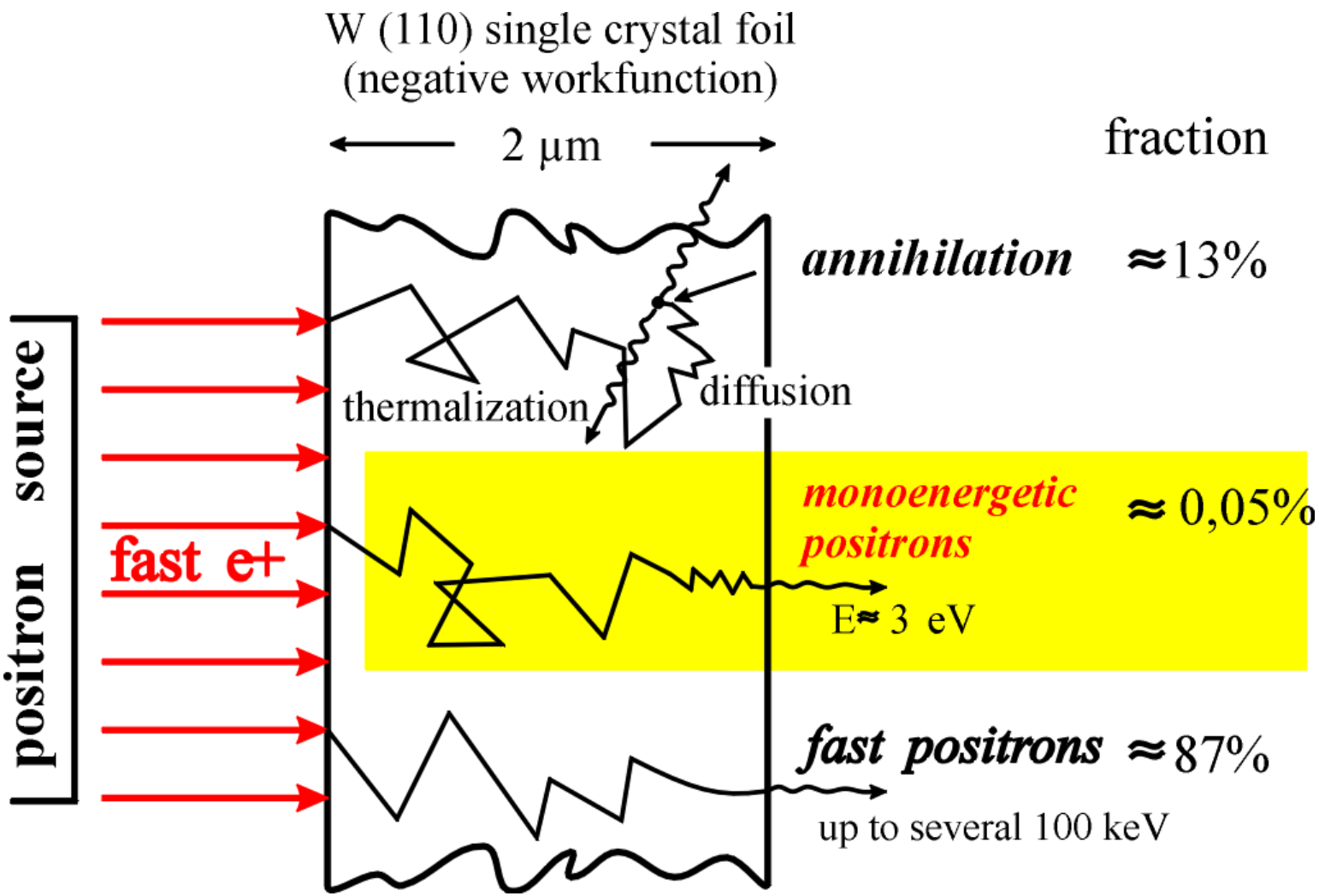


- broad positron emission spectrum
- deep implantation into solids
- no use for study of defects in thin layers
- moderation necessary

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

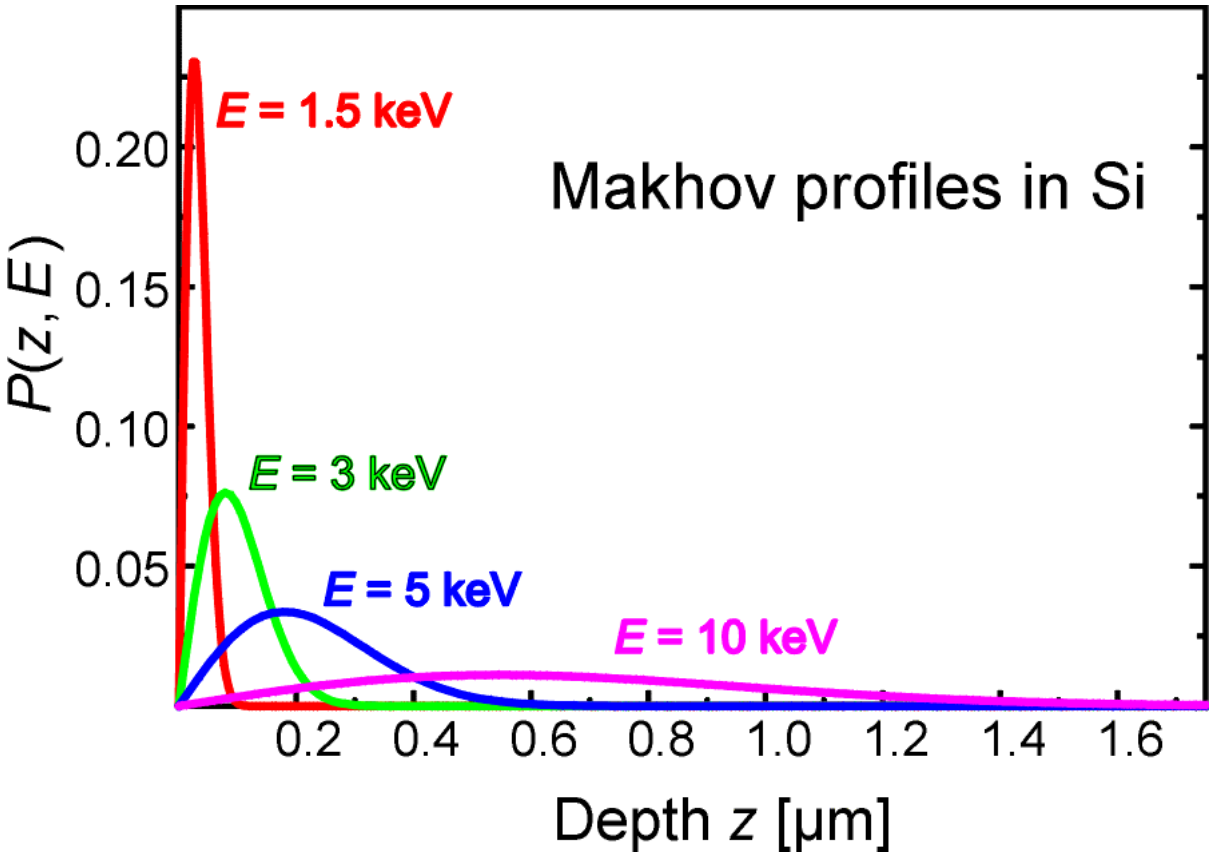
Si: 50µm (770µm) GaAs: 22µm (330µm) PbS: 15µm (220µm)

Moderation of Positrons



moderation efficiency: 10^{-4}

Implantation Profiles of monoenergetic Positrons



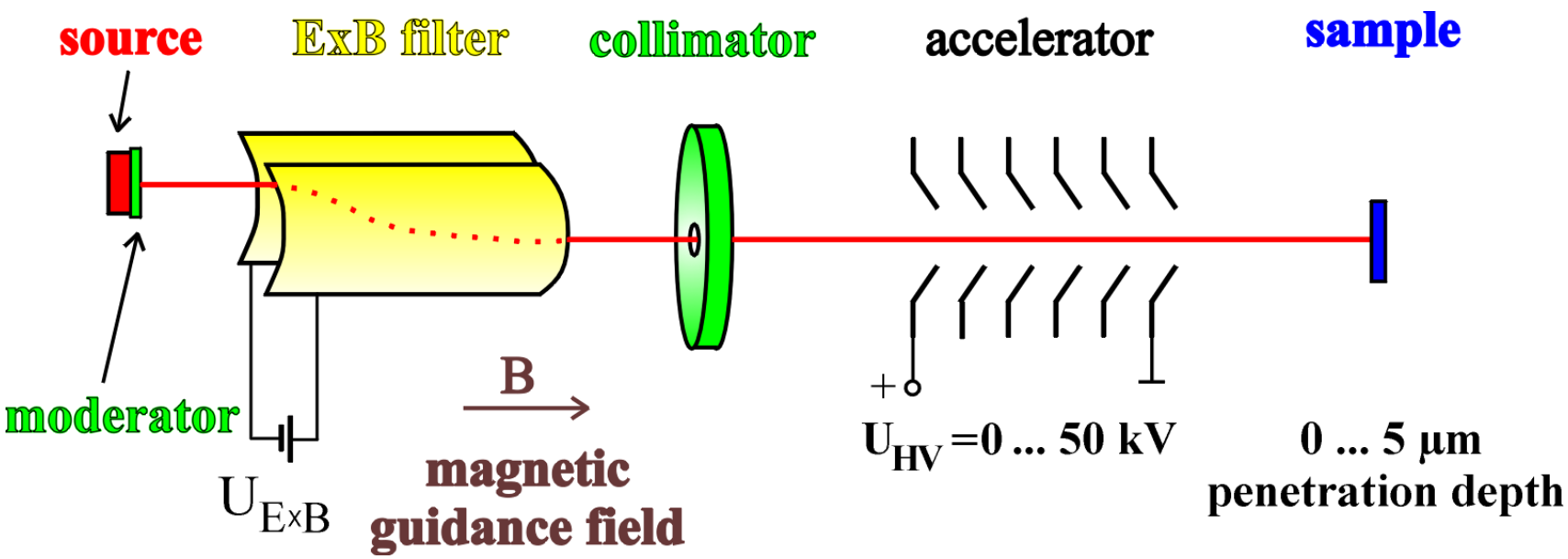
- depth resolution is function of implantation depth
- exact implantation profiles are obtained by Monte-Carlo simulations

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

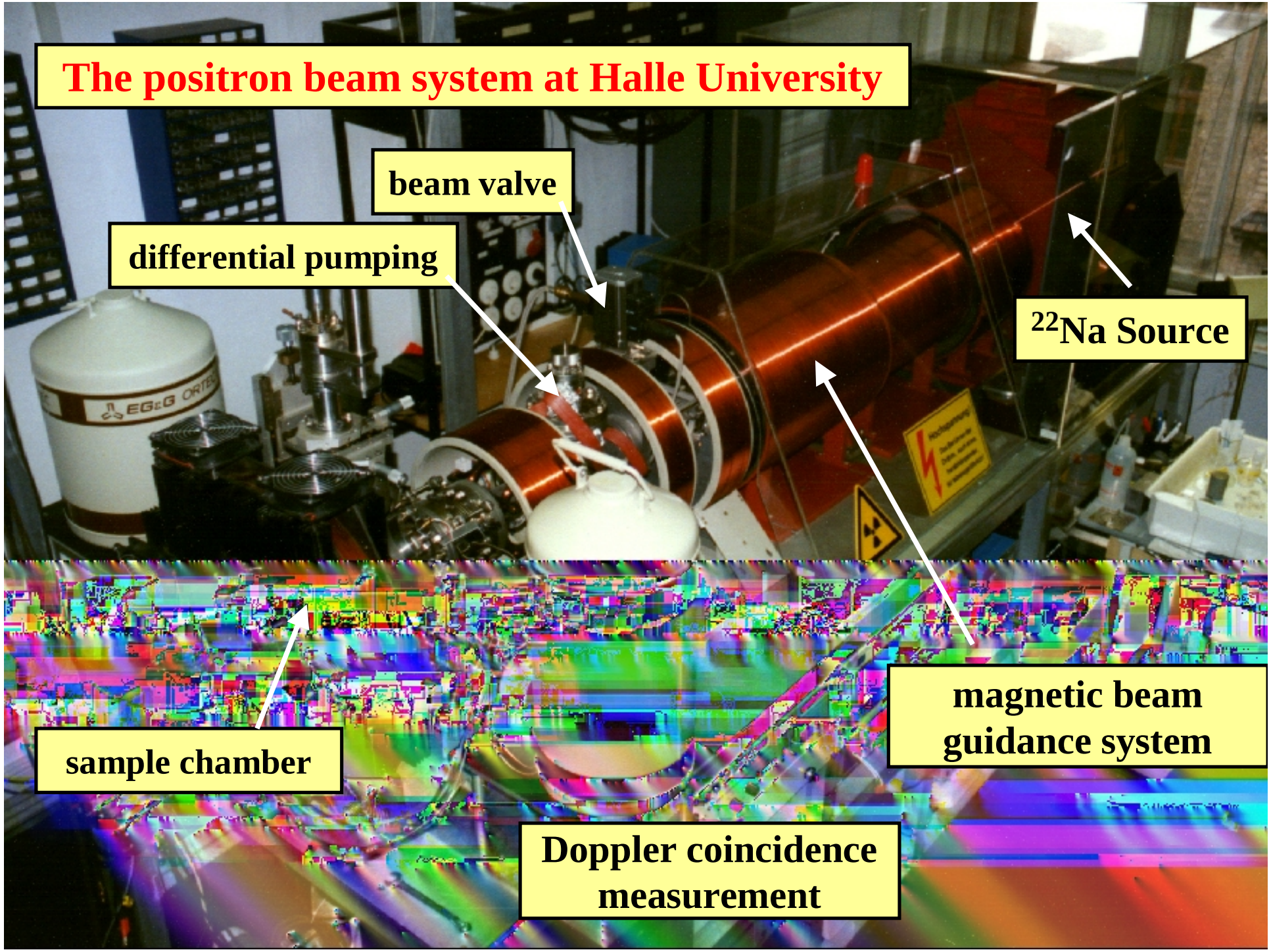
$z = f(E,\rho)$ $z_0 = \text{const.}$ $m = 2$

(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


The positron beam system at Halle University
beam valve
differential pumping
^{22}Na Source
sample chamber
magnetic beam guidance system
Doppler coincidence measurement

The Diffusion of Positrons

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

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

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

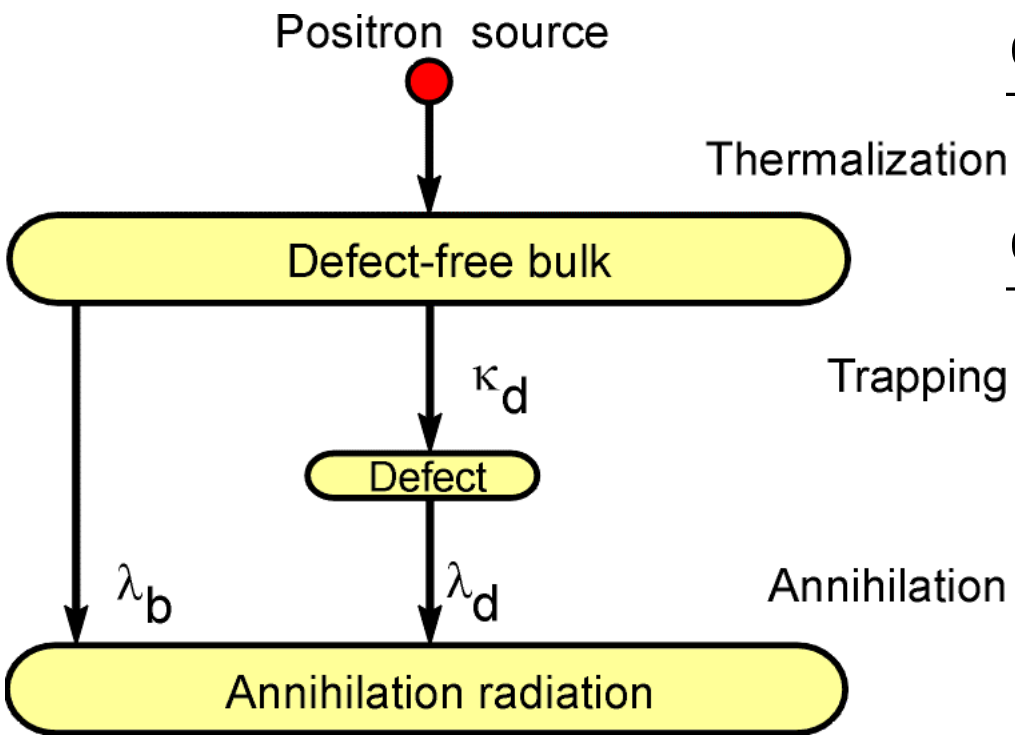
$\lambda_{eff} = 1/\tau_b + \kappa(\mathbf{r})$ ... effective annihilation rate

$\boxed{\kappa = \mu C}$ $\quad$ μ ... trapping coefficient $\quad$ C ... defect density

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

at 300 K:	l [nm]	L [nm]
Si	7	220
GaAs	5.3	200

Positron Trapping in a Single Defect Type



$$\frac{\mathrm{d}n_\mathrm{b}(t)}{\mathrm{d}t} = -(\lambda_\mathrm{b} + \kappa_\mathrm{d})n_\mathrm{b}(t)$$

$$\frac{\mathrm{d}n_\mathrm{d}(t)}{\mathrm{d}t} = -\lambda_\mathrm{d} n_\mathrm{d}(t) + \kappa_\mathrm{d} n_\mathrm{b}(t)$$

solution: decay spectrum

$$D(t) = I_1 \exp\left(-\frac{t}{\tau_1}\right) + I_2 \exp\left(-\frac{t}{\tau_2}\right)$$

abbreviations:

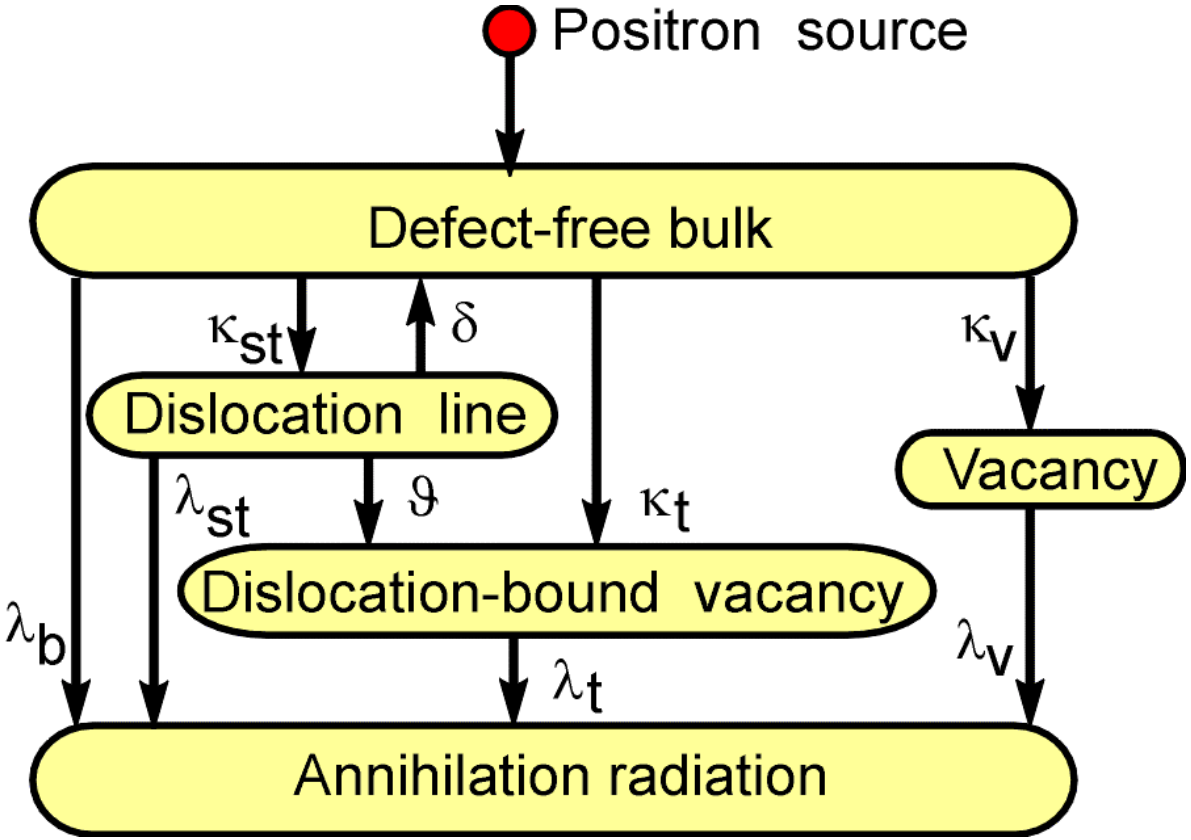
$$\tau_1 = \frac{1}{\lambda_\mathrm{b} + \kappa_\mathrm{d}}, \quad \tau_2 = \frac{1}{\lambda_\mathrm{d}},$$

$$I_1 = 1 - I_2, \qquad I_2 = \frac{\kappa_\mathrm{d}}{\lambda_\mathrm{b} - \lambda_\mathrm{d} + \kappa_\mathrm{d}}$$

The t_i and I_i are measured ⇒ k is obtained:

$$\boxed{\kappa_\mathrm{d} = \mu C_\mathrm{d}} = \frac{I_2}{I_1}\left(\frac{1}{\tau_\mathrm{b}} - \frac{1}{\tau_\mathrm{d}}\right)$$

Positron Trapping in a Dislocation



the dislocation line (shallow trap) acts as a "funnel" for the trapping in deep traps

b ... bulk

v ... vacancy

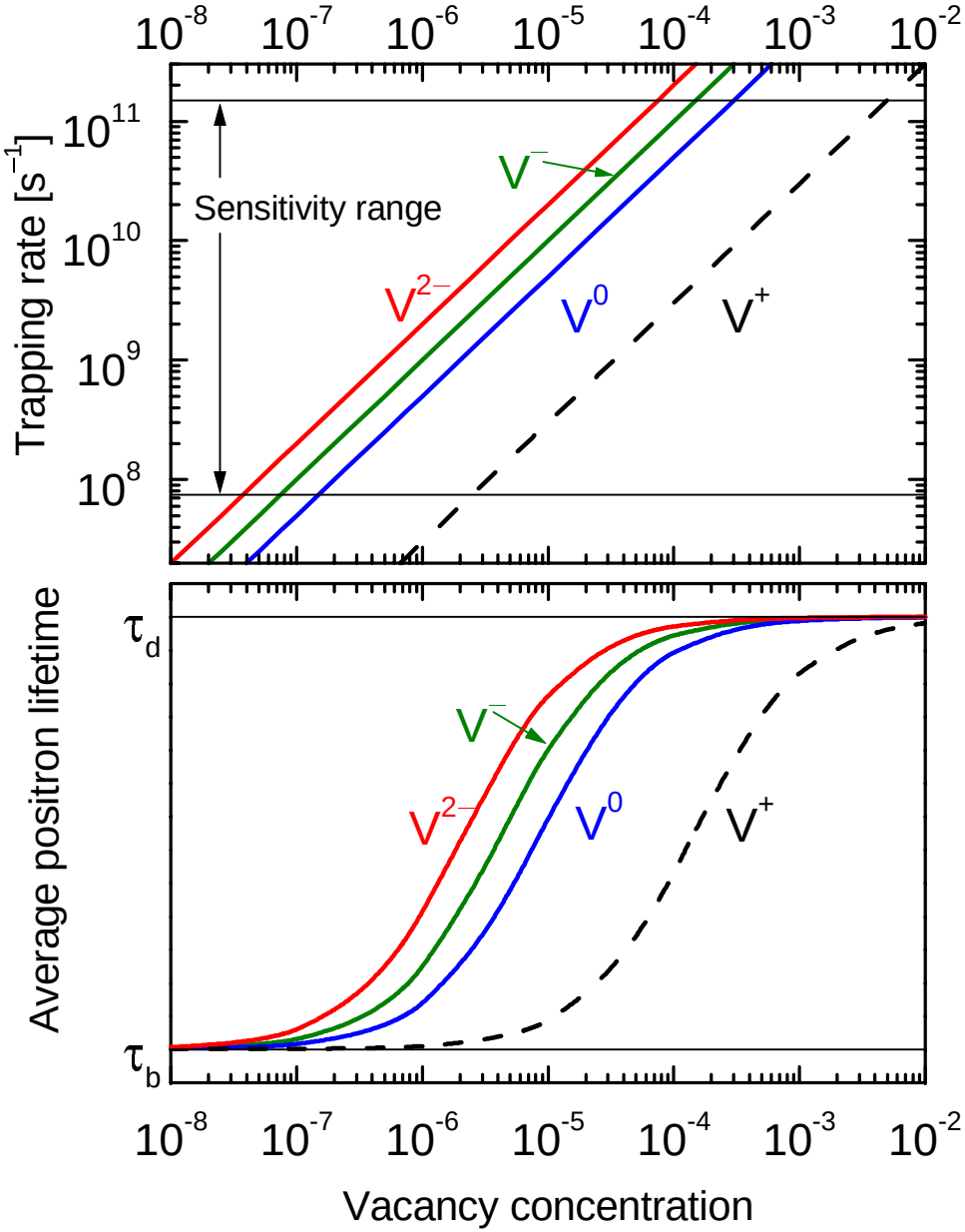
t ... deep trap

st ... shallow trap

λ_i ... annihilation rates κ_i, ϑ ... trapping rates

δ ... detrapping (escape) rate

Determination of absolute Defect Densities



- the trapping coefficient μ

  $$k = \mu C$$

  must be determined by an independent method

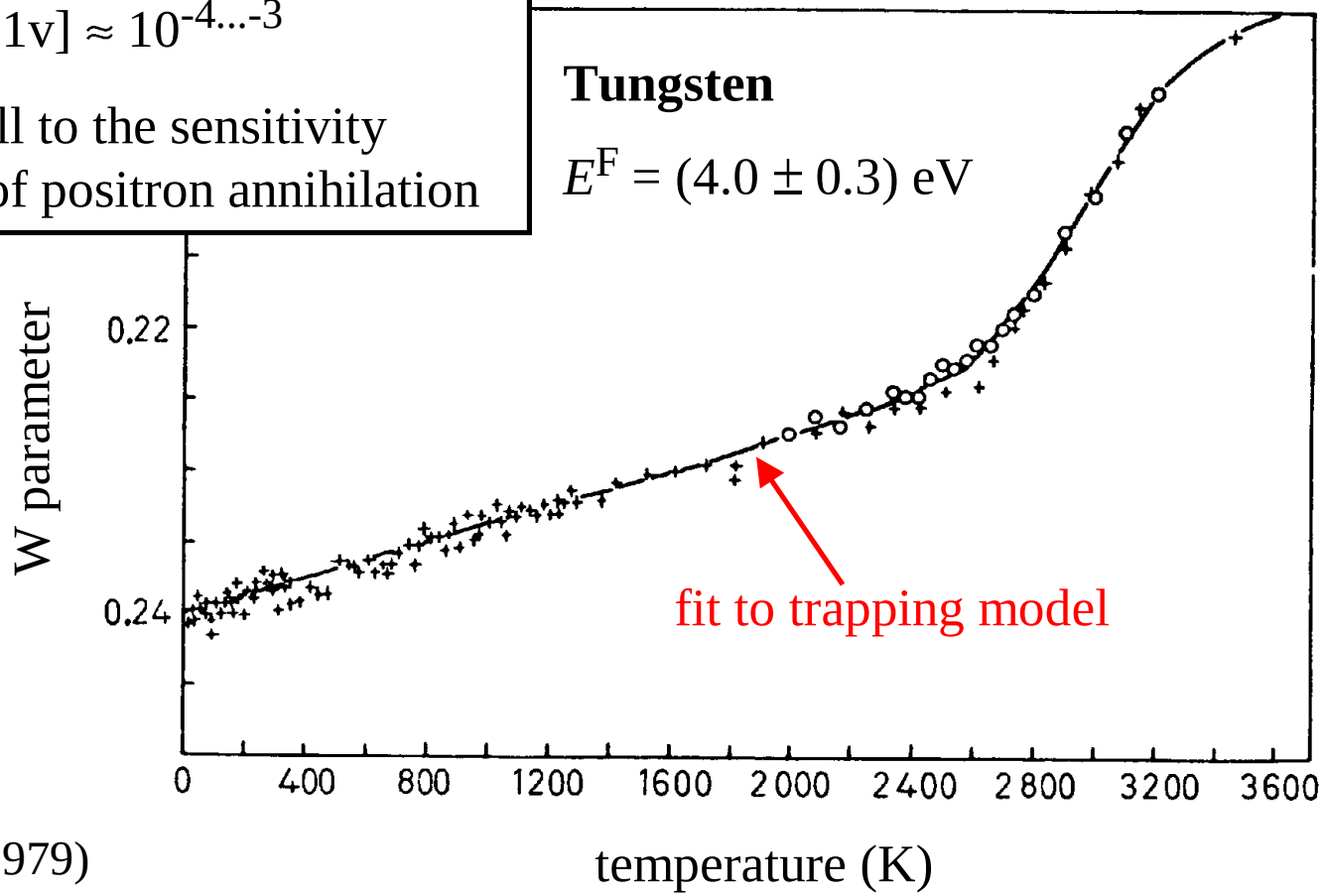
- positron trapping may be strongly temperature-dependent ⇒ $\mu = f(T)$

defect in Si_{300K}	μ (10^{15} s^{-1})
V^-	1
V^{2-}	2
V^0	0.5
V^+	< 0.1
dislocation	1 $cm^2 s^{-1}$
vacancy cluster	$n \cdot \mu_{1V}$

Vacancies in thermal Equilibrium

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

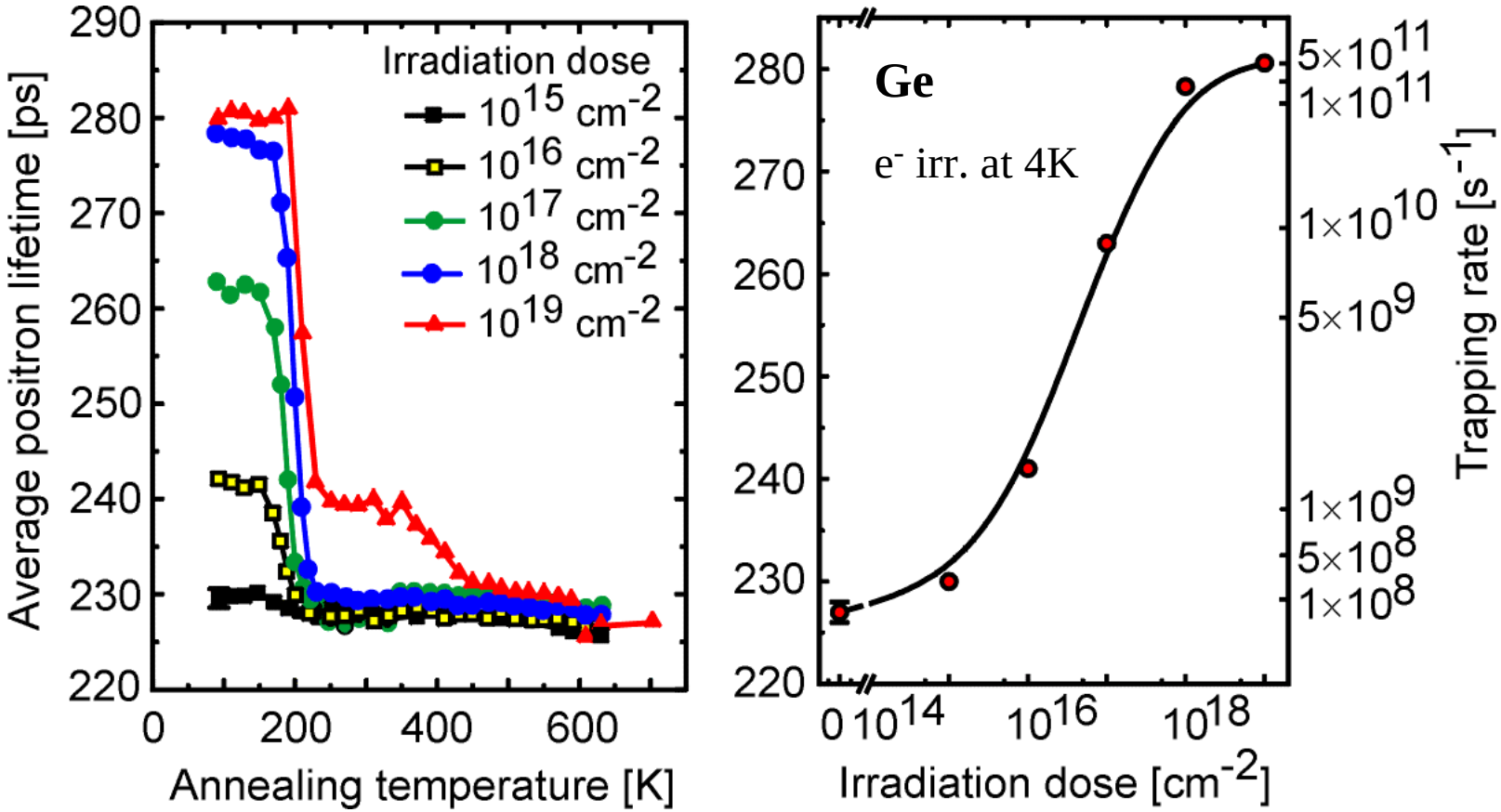
$$C_{1v}(T) = \exp\left(\frac{S_{1v}^F}{k}\right)\exp\left(\frac{H_{1v}^F}{kT}\right)$$



(Ziegler, 1979)

Defects in Ge after Electron Irradiation

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

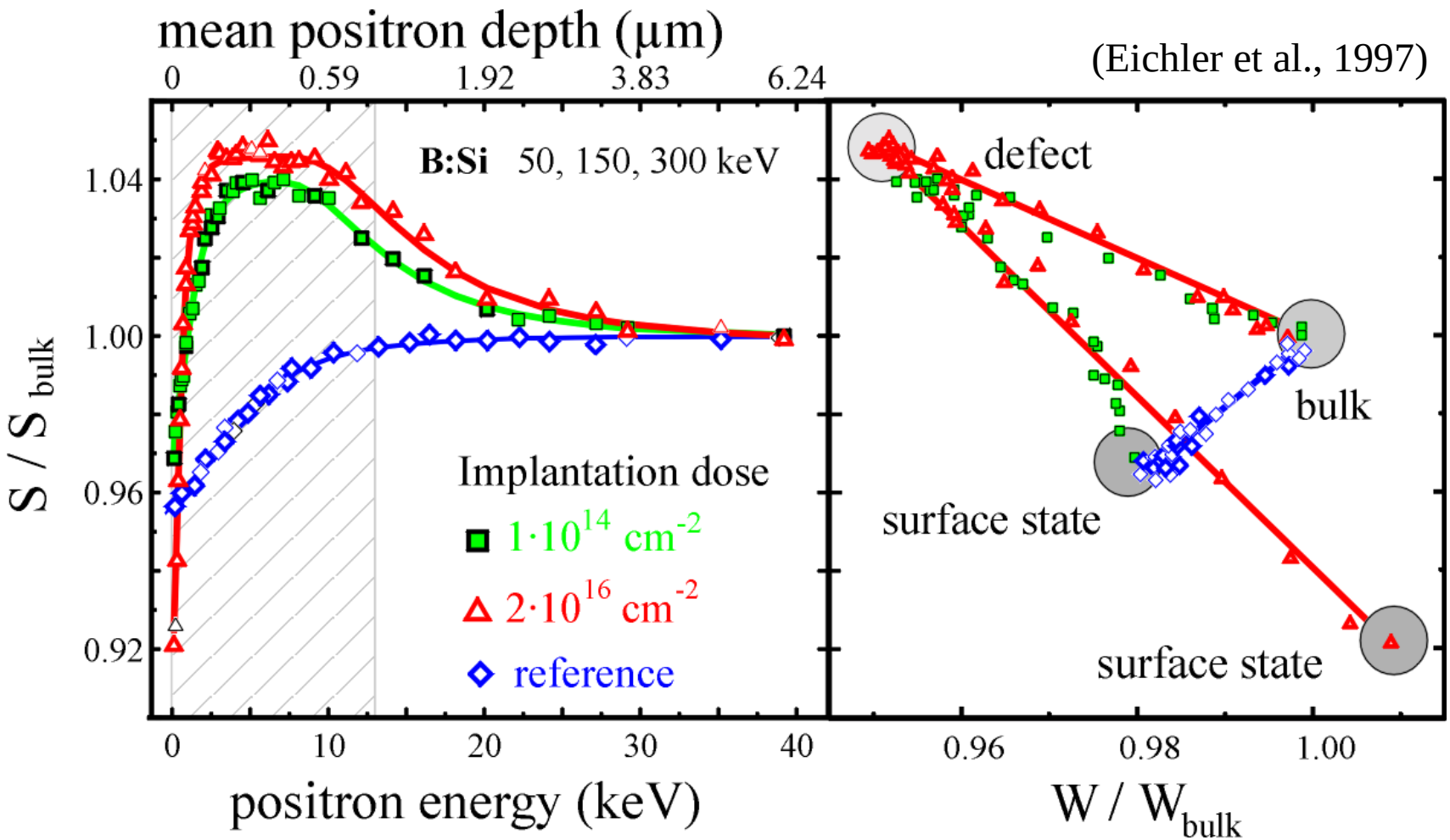


(Polity et al., 1997)

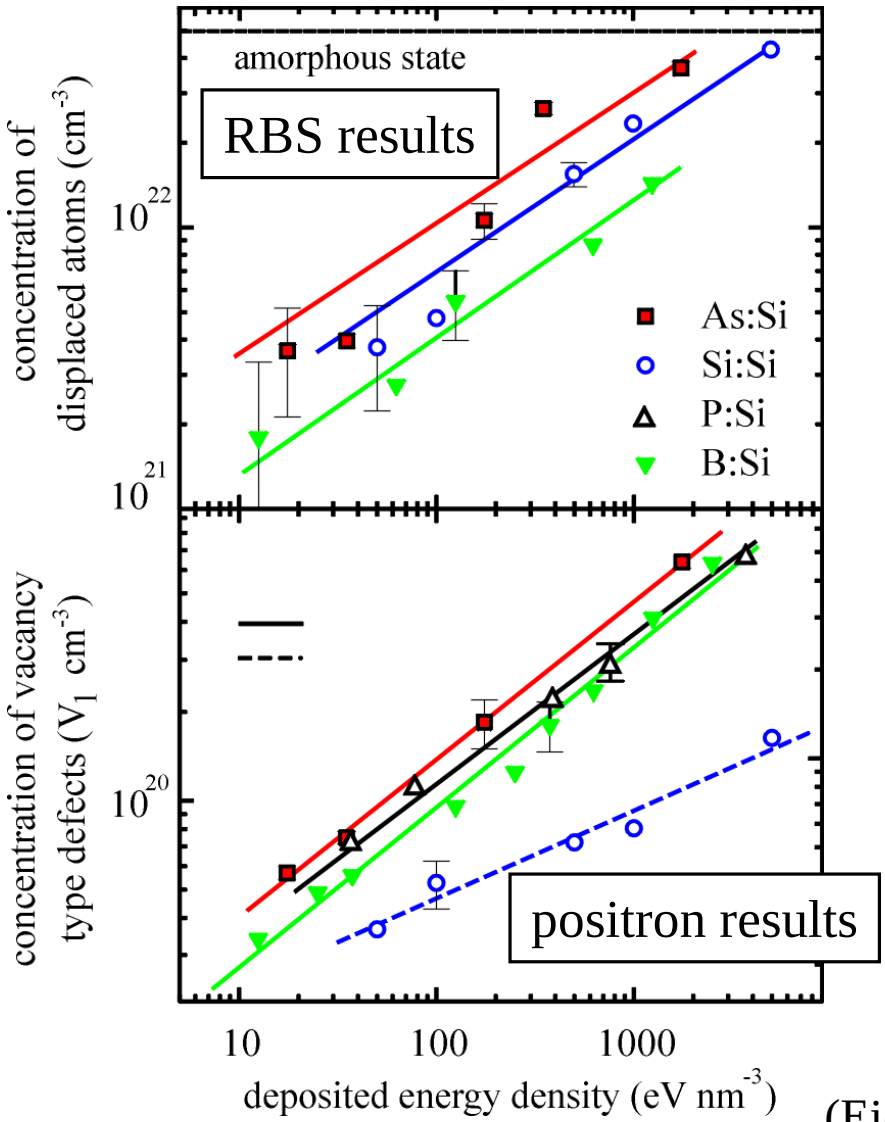
Defects in Si induced by Ion Implantation

- ion implantation is most important doping technique in planar technology
- main problem: generation of defects ⇒ positron beam measurements

(Eichler et al., 1997)



Defect density as function of deposited ion energy

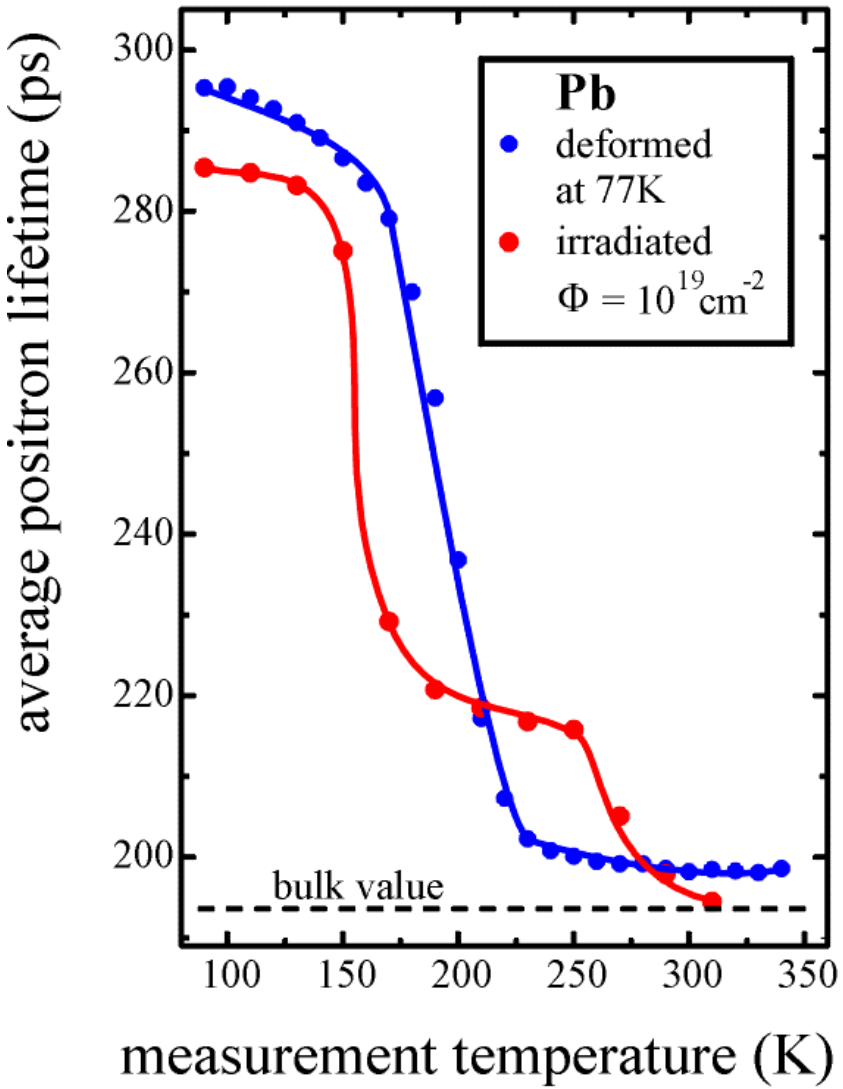


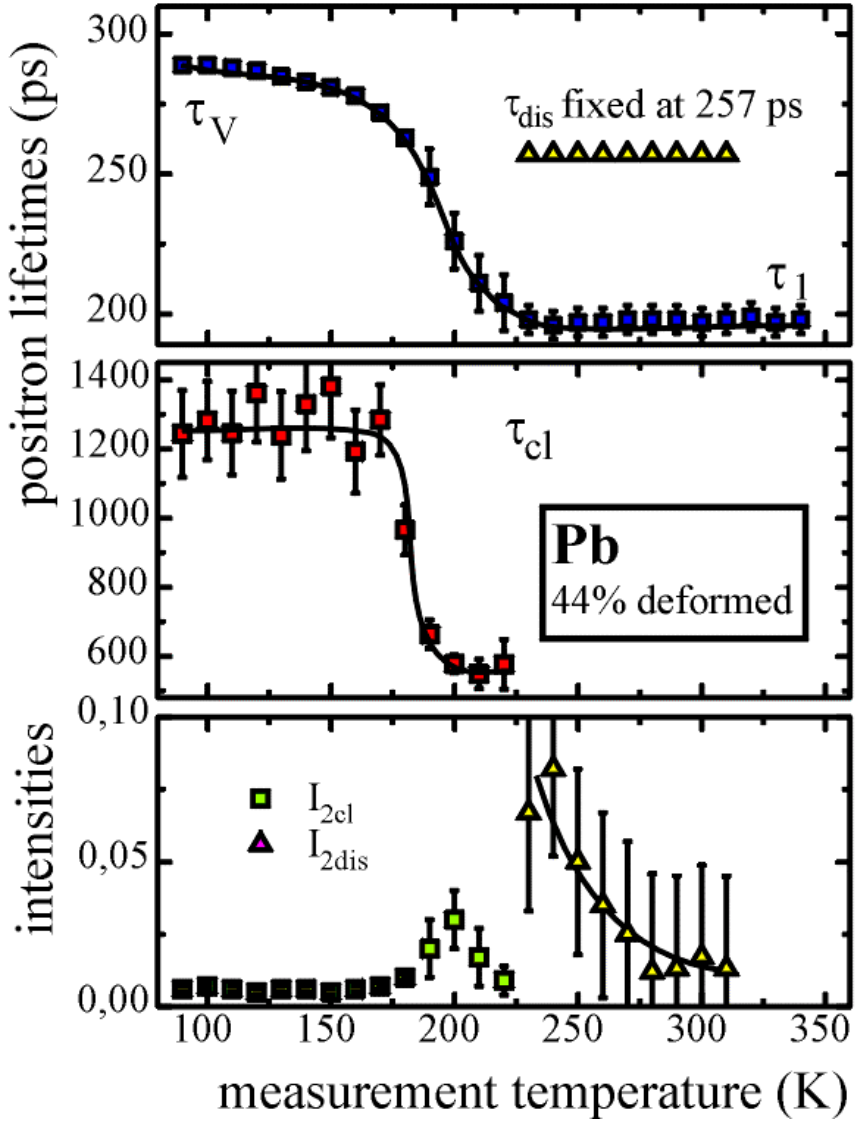
(Eichler et al., 1997)

- Defect generation follows Chadderton's model of homogenous nucleation:

  (L.T. Chadderton, Rad. Eff. 8 (1971) 1)
- [defect] ~ 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

Plastic Deformation and Electron Irradiation in Pb

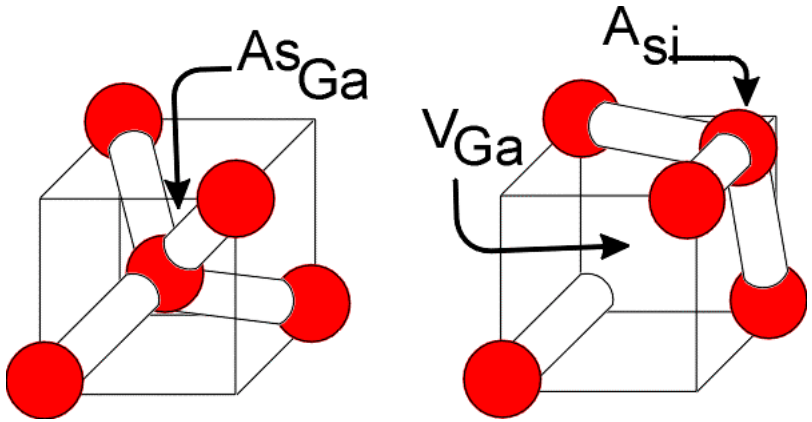




(Petters et al., 1998)

The nature of the EL2 defect in GaAs

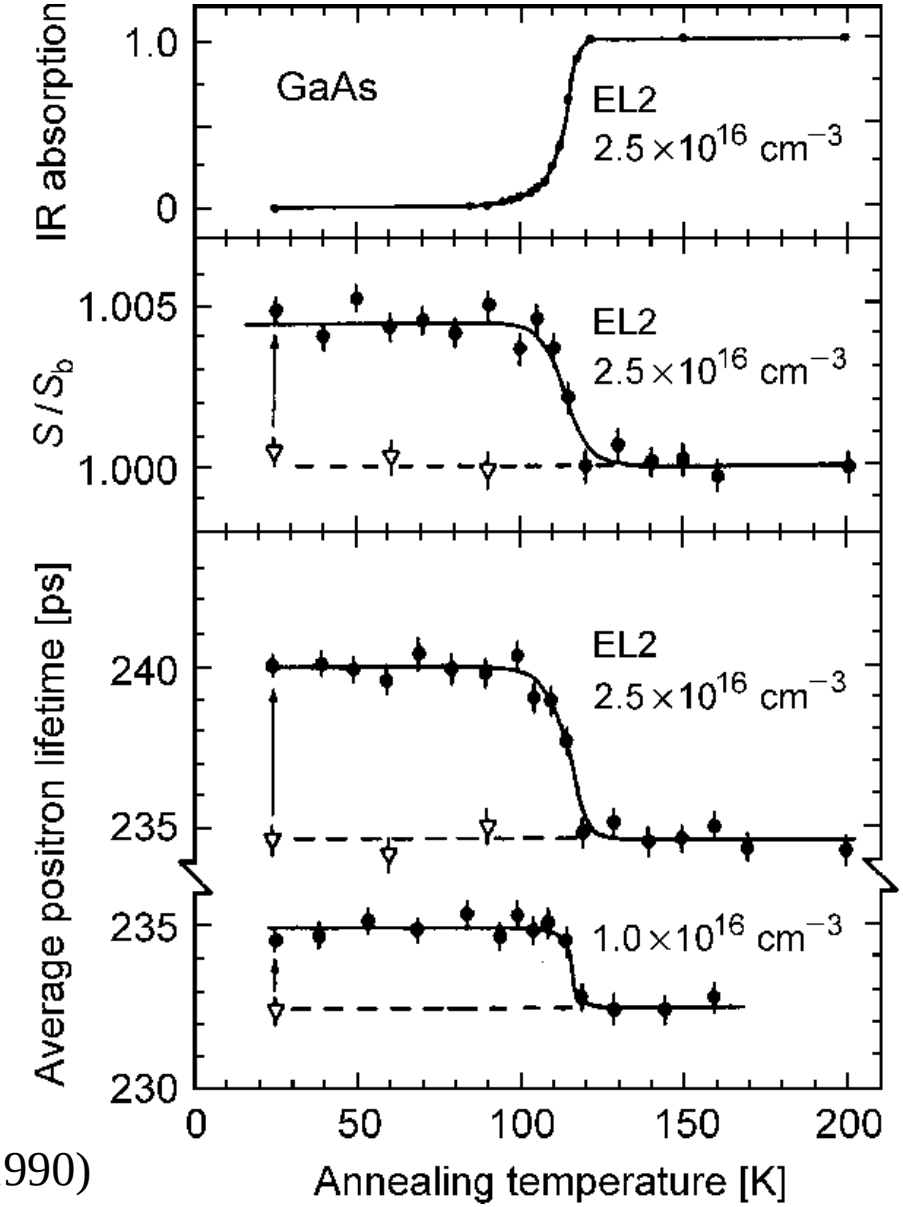
- one of mostly investigated defects
- exhibiting metastability at low T under light illumination



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 $\Rightarrow$ three-dimensional imaging of defect distributions
- Univ. Bonn: combination of Scanning Electron Microscopy and a focussed (1 μm) positron beam of variable energy $\Rightarrow$ defect imaging

The Positron Microscope at Bonn University