Positron – theoretical prediction

Schrödinger equation: $$\left[\frac{\hat{\mathbf{p}}^2}{2m}+V(\mathbf{x},t)\right]\psi(\mathbf{x},t)=i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t}$$

- non-relativistic equation of motion for electron

Erwin Schrödinger
1933 Nobel prize

Positron – theoretical prediction

Dirac equation: $$\left(\boldsymbol{\alpha}\hat{\mathbf{p}}\,c+\beta\,mc^{2}\right)\psi\left(\mathbf{x},t\right)=i\hbar\frac{\partial\psi\left(\mathbf{x},t\right)}{\partial t}$$

• relativistic equation of motion for electron

• solutions with positive energy: ’normal electrons’

Paul Adrien Maurice Dirac
1933 Nobel prize

P.A.M. Dirac, Proc. R. Soc. Lond. A 117, 610-624 (1928)

P.A.M. Dirac, Proc. R. Soc. Lond. A 133, 60-72 (1931)

Positron – theoretical prediction

Dirac equation: $$\left(\boldsymbol{\alpha}\hat{\mathbf{p}}c + \beta mc^2\right)\psi(\mathbf{x},t) = i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t}$$

- relativistic equation of motion for electron
- solutions with positive energy: 'normal electrons'
- solutions with negative energy
- energy of a free particle $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ (classical)

Paul Adrien Maurice Dirac
1933 Nobel prize

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Positron – theoretical prediction

Dirac equation: $\left(\boldsymbol{\alpha}\,\hat{\mathbf{p}}\,c + \beta\,mc^2\right)\psi(\mathbf{x},t) = i\hbar\,\frac{\partial\psi(\mathbf{x},t)}{\partial t}$

- relativistic equation of motion for electron
- solutions with positive energy: ’normal electrons’
- solutions with negative energy
- relativistic energy $E^2 = m^2c^4 + p^2c^2$

$$E = \pm\sqrt{m^2c^4 + p^2c^2}$$

Paul Adrien Maurice Dirac
1933 Nobel prize

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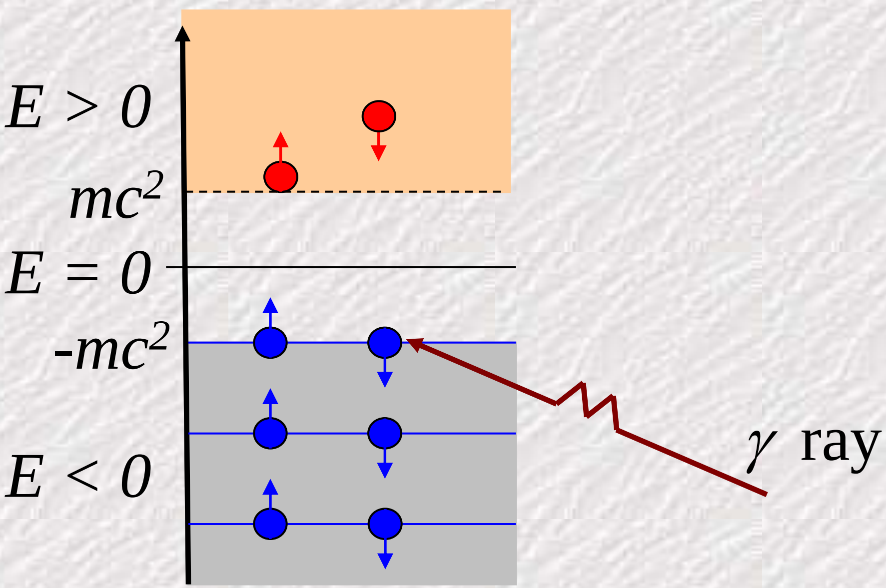
- solutions with positive energy: ’normal electrons’
- vacuum is a see of electrons with negative energy

Paul Adrien Maurice Dirac
1933 Nobel prize



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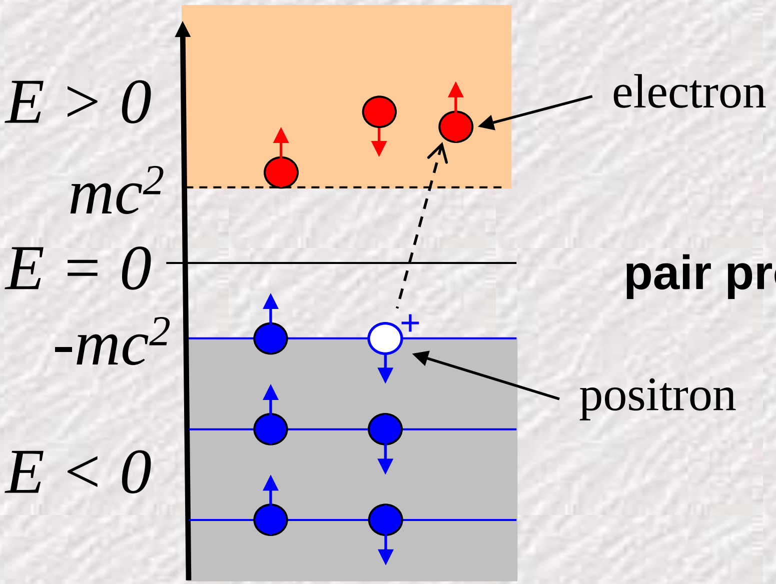
• relativistic equation of motion for electron

• solutions with positive energy: ’normal electrons’

• vacuum is a see of electrons with negative energy

• positron is a “*hole*“ in vacuum



pair production

Paul Adrien Maurice Dirac
1933 Nobel prize

P.A.M. Dirac, Proc. R. Soc. Lond. A 117, 610-624 (1928)

P.A.M. Dirac, Proc. R. Soc. Lond. A 133, 60-72 (1931)

Positron – theoretical prediction

Dirac equation: $\left(\boldsymbol{\alpha}\hat{\mathbf{p}}\,c + \beta\, mc^2\right)\psi(\mathbf{x},t) = i\hbar\,\frac{\partial\psi(\mathbf{x},t)}{\partial t}$

- relativistic equation of motion for electron
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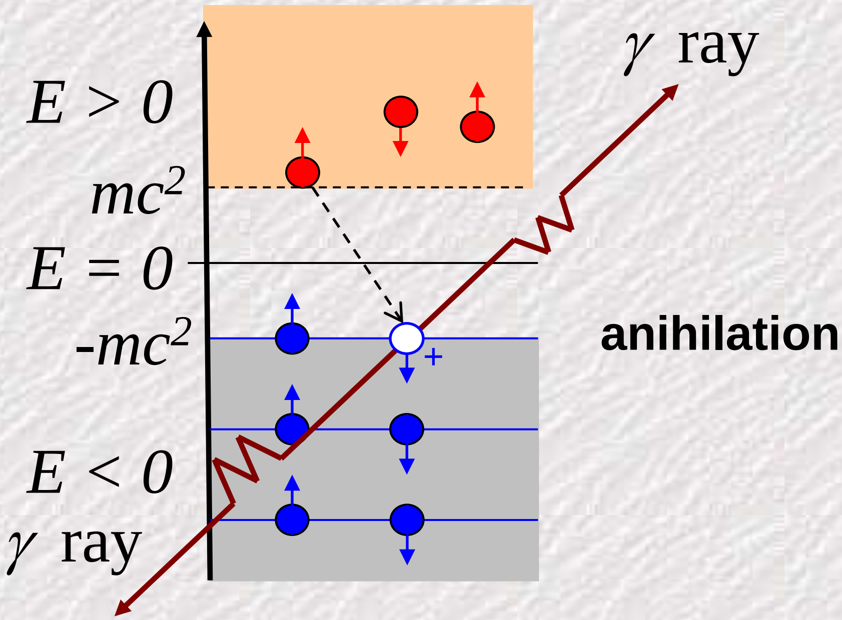
- vacuum is a see of electrons with negative energy
- positron is a “*hole*“ in vacuum



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1933 Nobel prize

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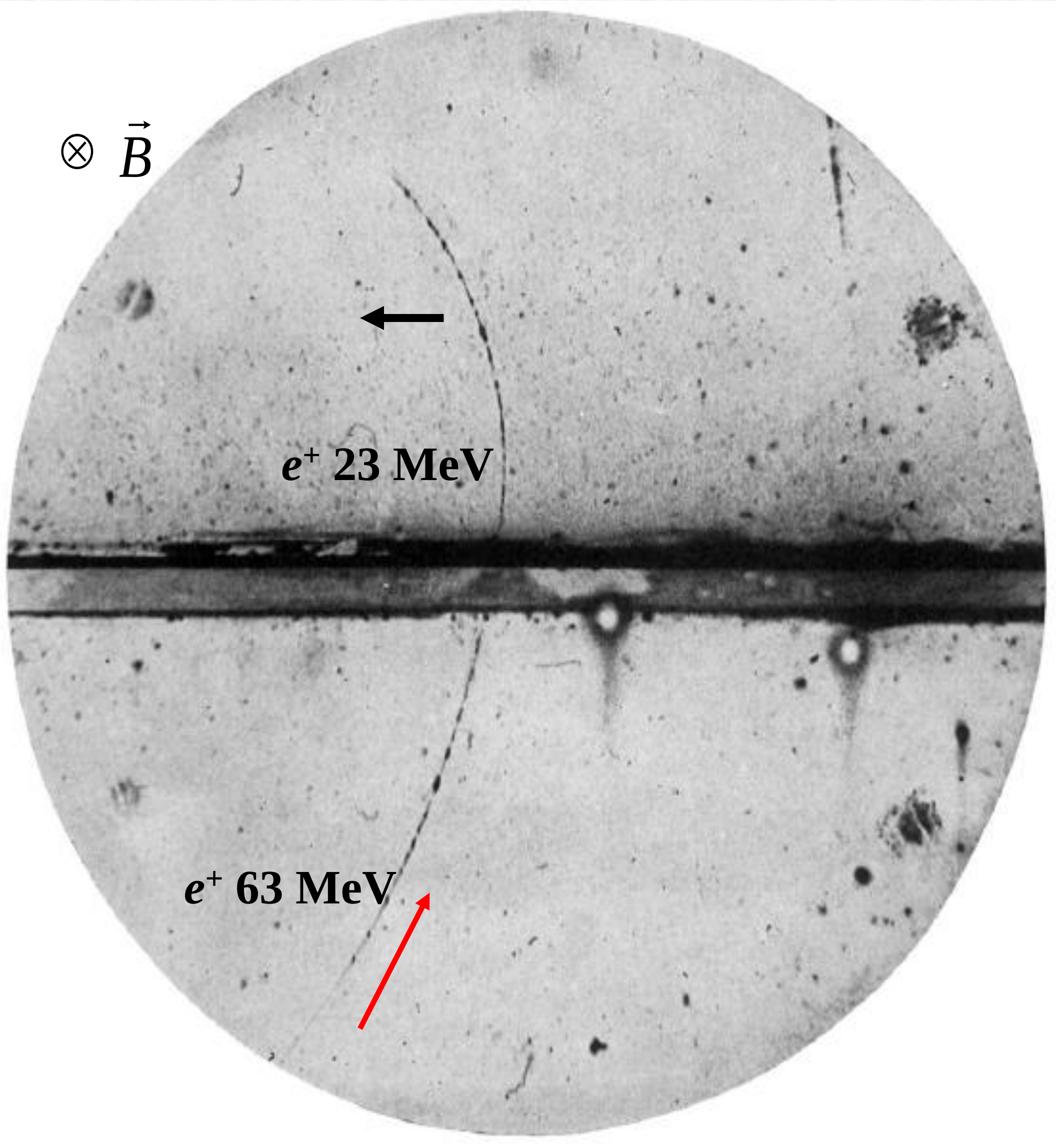
P.A.M. Dirac, Proc. R. Soc. Lond. A 133, 60-72 (1931)

Discovery of positron

Lorentz force

discovery of positron 1932

$$\vec{F} = e\vec{v} \times \vec{B}$$



6 mm Pb foil

Carl David Anderson

1936 Nobel prize

The Positive Electron

CARL D. ANDERSON, *California Institute of Technology, Pasadena, California*
(Received February 28, 1933)

Out of a group of 1300 photographs of cosmic-ray tracks in a vertical Wilson chamber 15 tracks were of positive particles which could not have a mass as great as that of the proton. From an examination of the energy-loss and ionization produced it is concluded that the charge is less than twice, and is probably exactly equal to, that of the proton. If these particles carry unit positive charge the curvatures and ionizations produced require the mass to be less than twenty times the electron mass. These particles will be called positrons. Because they occur in groups associated with other tracks it is concluded that they must be secondary particles ejected from atomic nuclei.

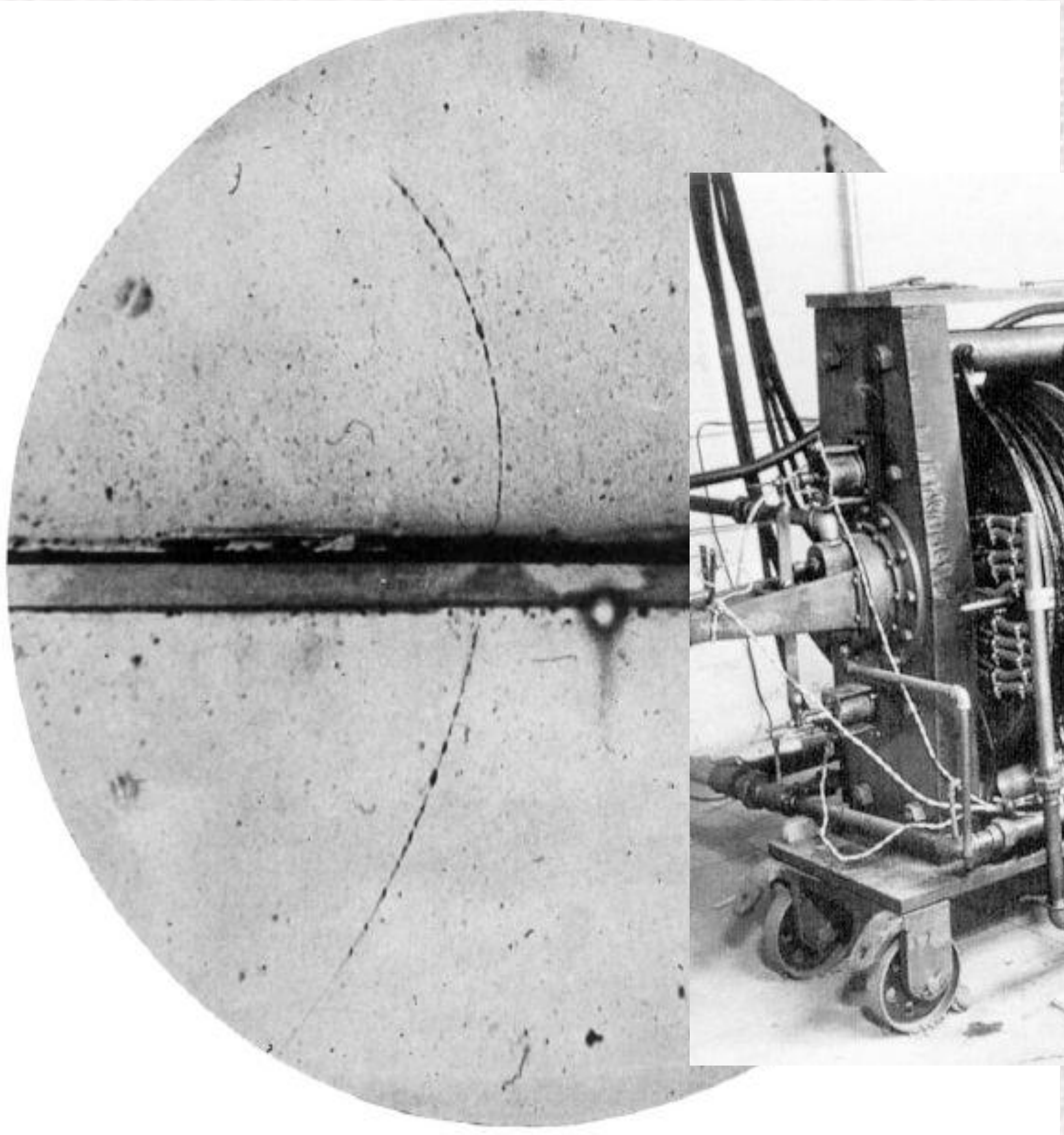
Editor

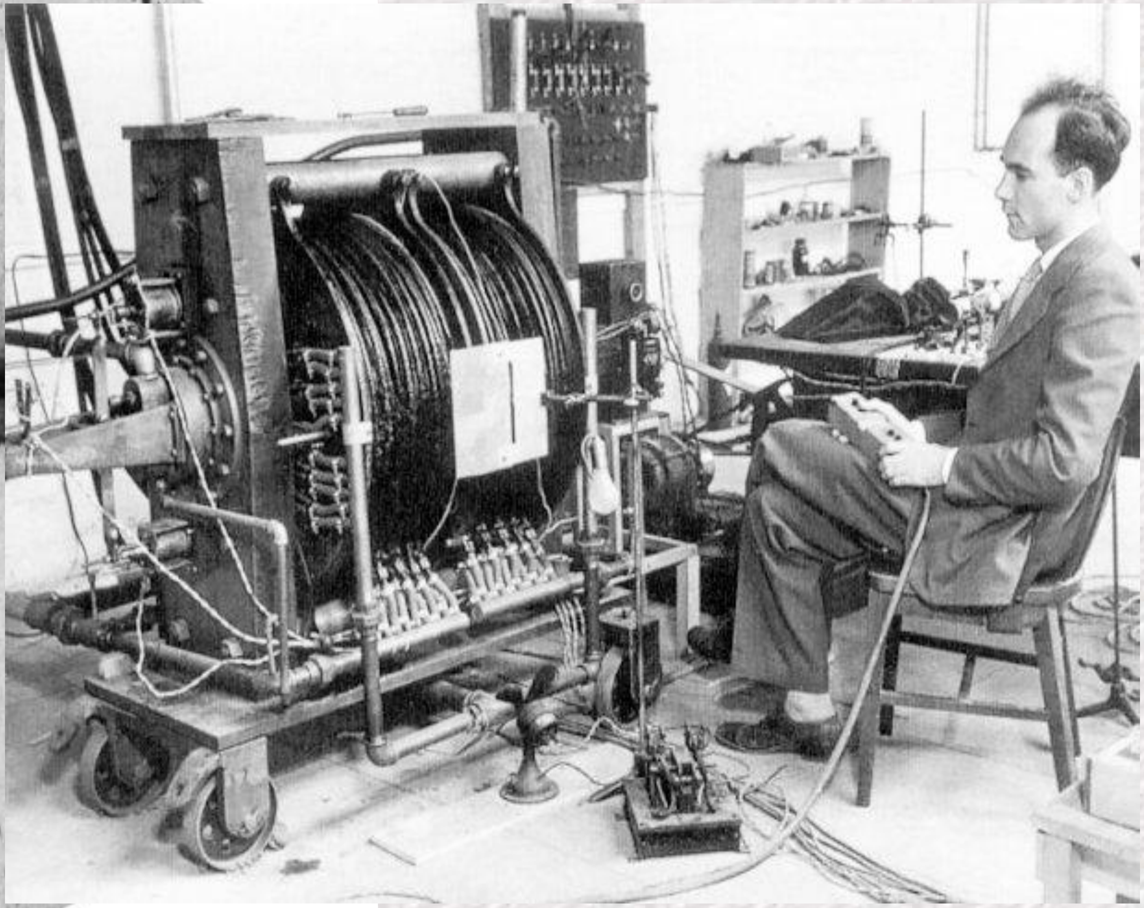
ON August 2, 1932, during the course of photographing cosmic-ray tracks produced in a vertical Wilson chamber (magnetic field of 15,000 gauss) designed in the summer of 1930 by Professor R. A. Millikan and the writer, the tracks shown in Fig. 1 were obtained, which seemed to be interpretable only on the basis of the existence in this case of a particle carrying a positive charge but having a mass of the same order of magnitude as that normally possessed by a free negative electron. Later study of the electrons happened to produce two tracks so placed as to give the impression of a single particle shooting through the lead plate. This assumption was dismissed on a probability basis, since a sharp track of this order of curvature under the experimental conditions prevailing occurred in the chamber only once in some 500 exposures, and since there was practically no chance at all that two such tracks should line up in this way. We also discarded as completely untenable the assumption of an electron of 20

Discovery of positron

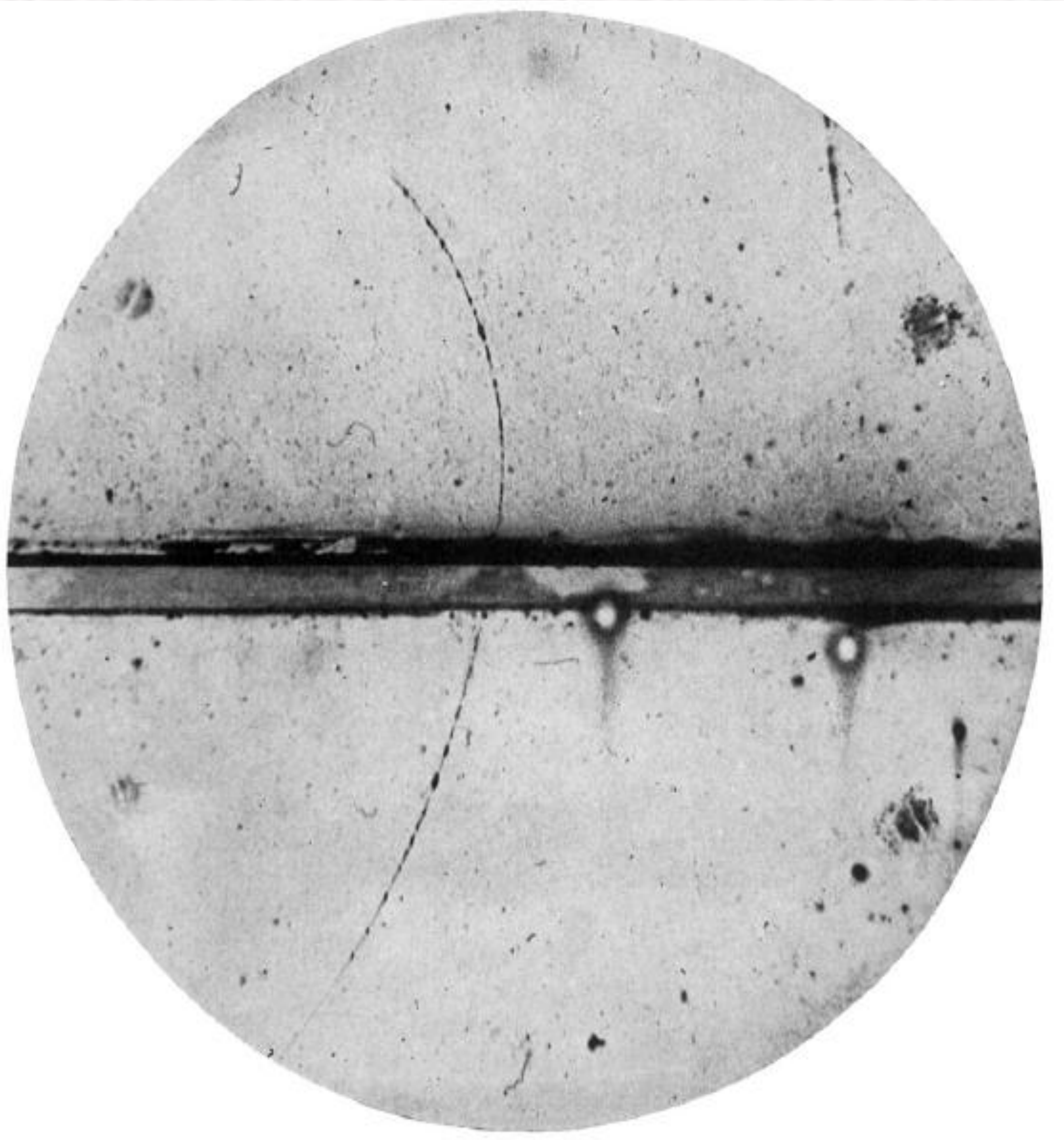
discovery of positron 1932

- $B = 1.7$ T
- $P = 425$ kW
- $m > 3$ t





Positron



positron = antiparticle of electron

- rest mass: m_e
- charge: $+e$
- spin: $1/2$

Positron sources

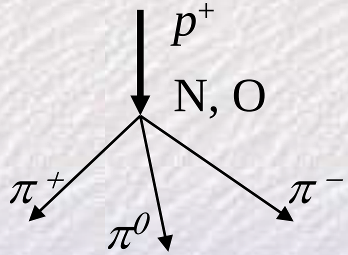
Cosmic rays

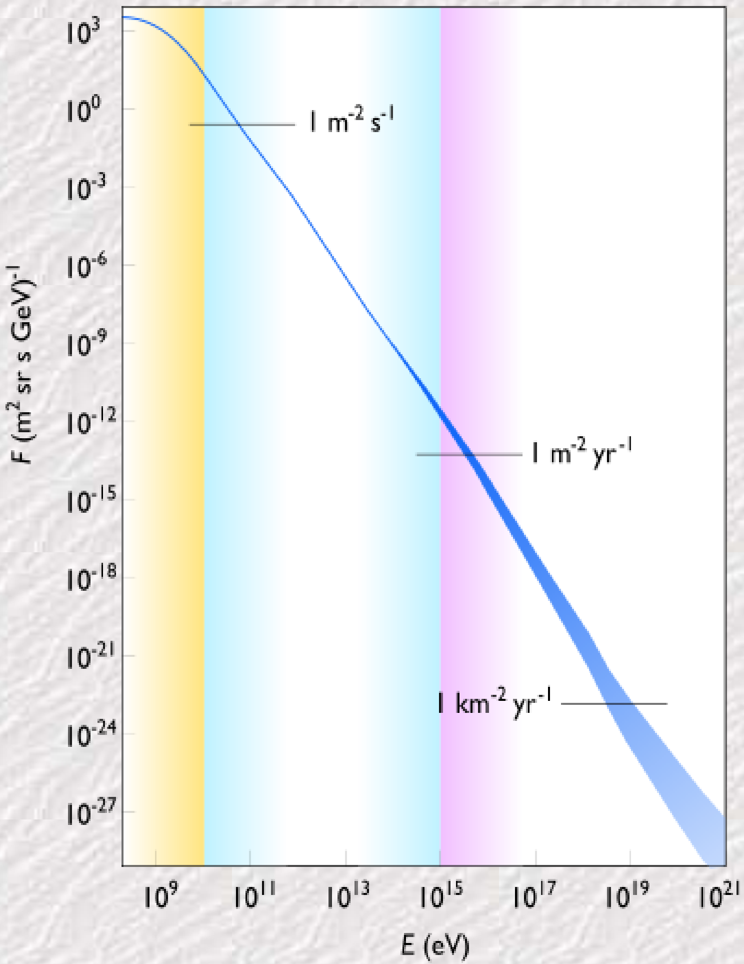
90 % protons

9 % α-particles

1 % heavier nuclei & other particles (e^-, e^+, p^-)

interaction with atmosphere





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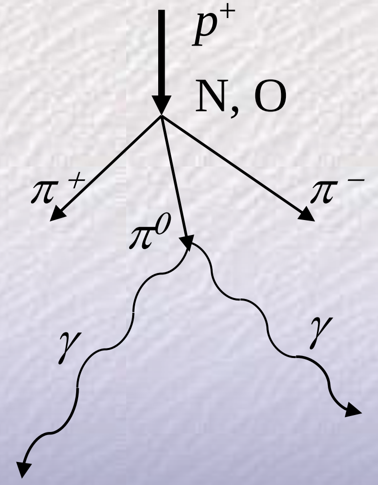

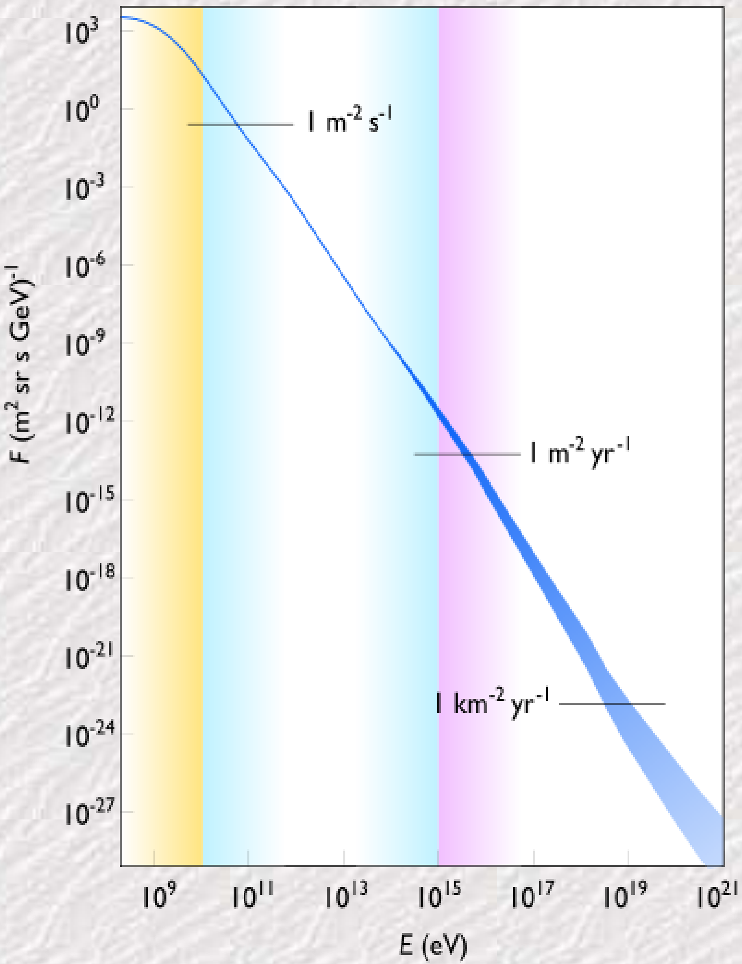

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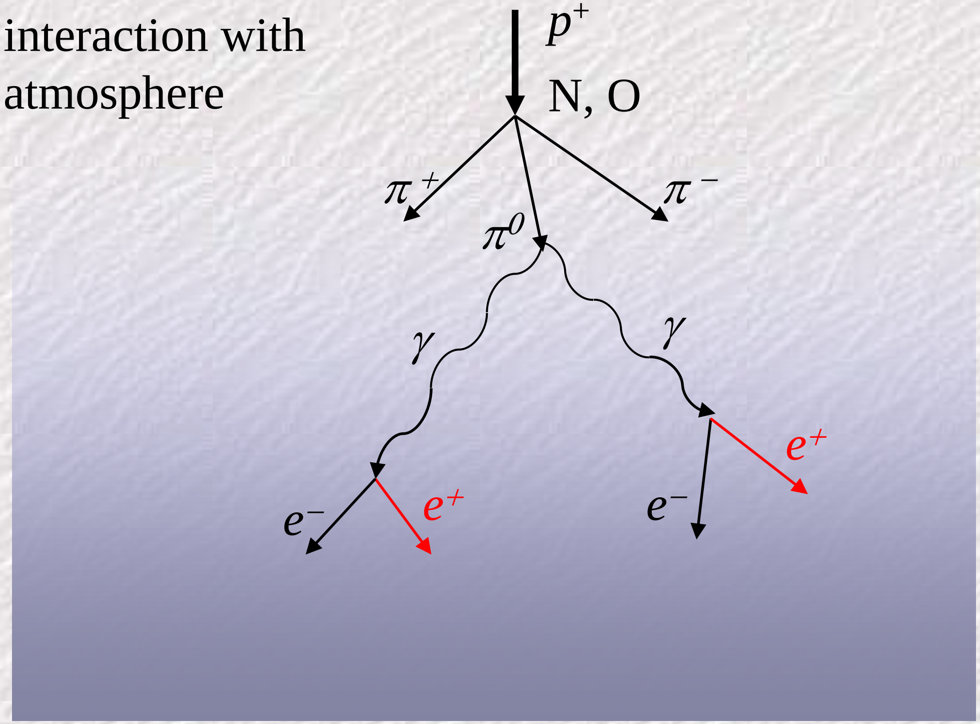

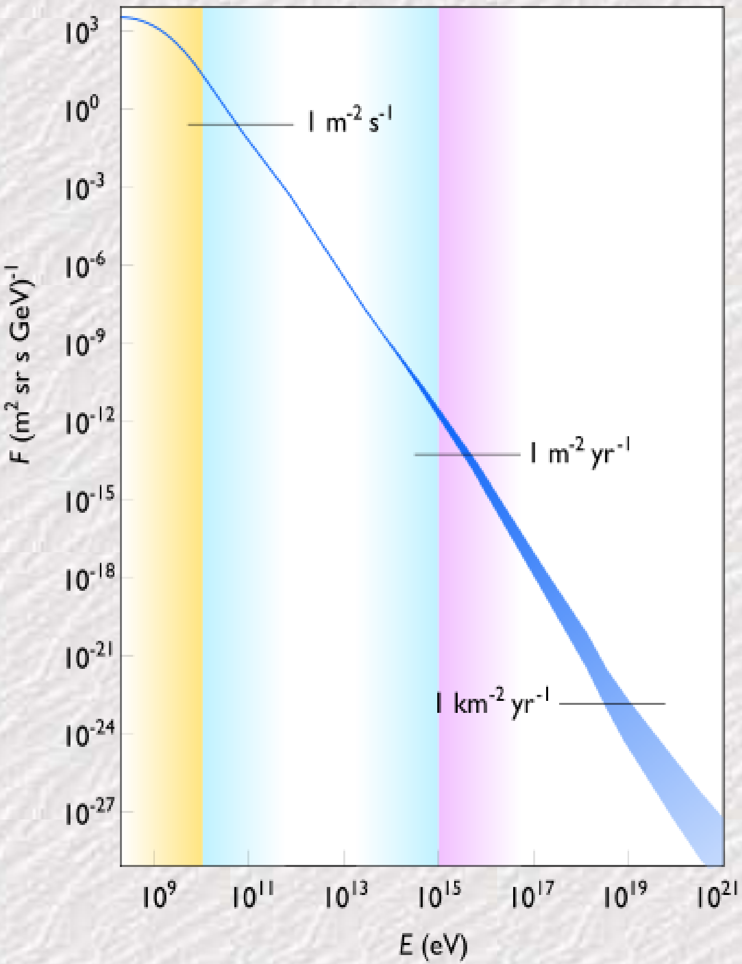

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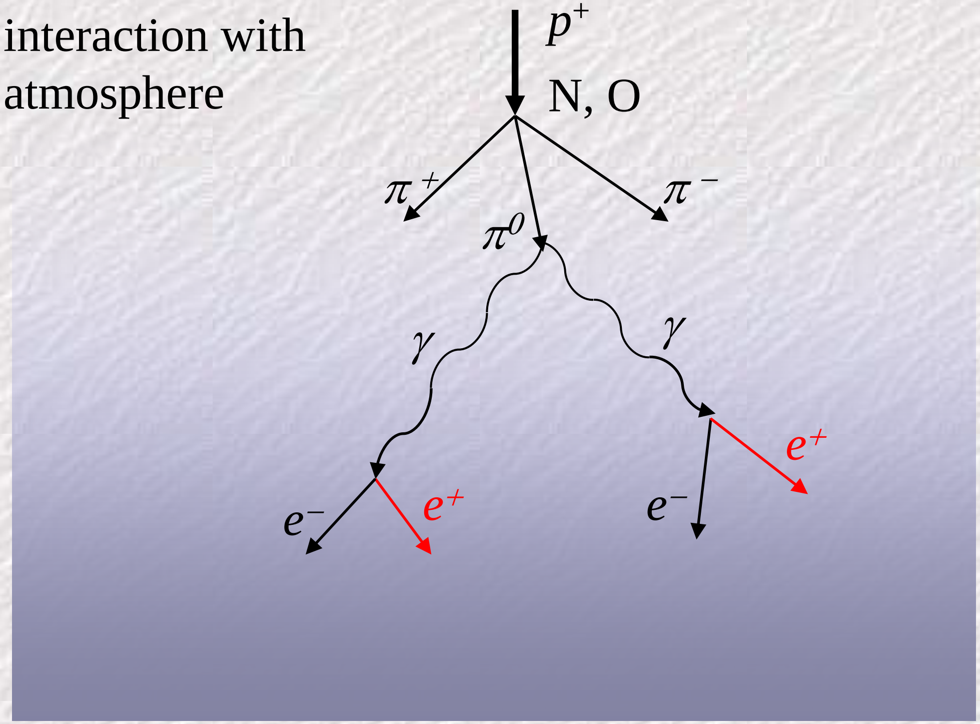

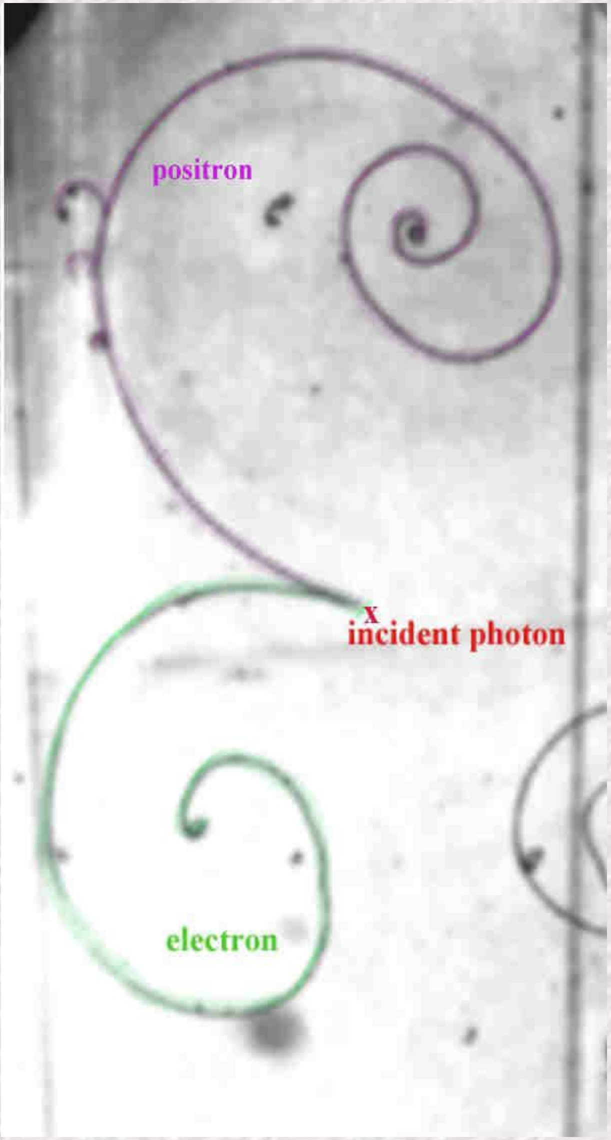

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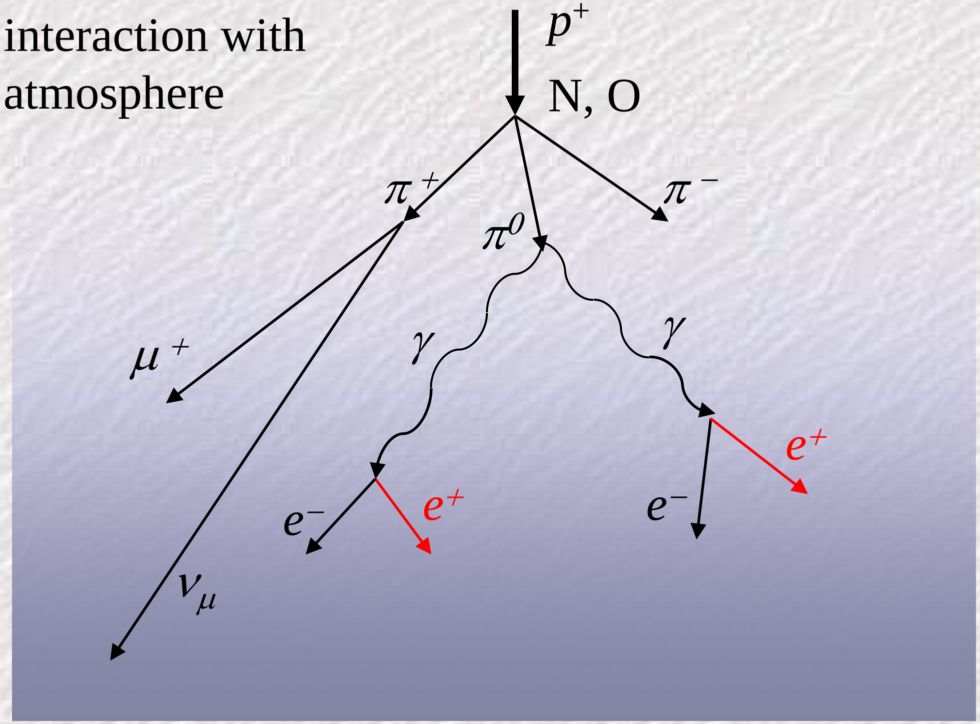

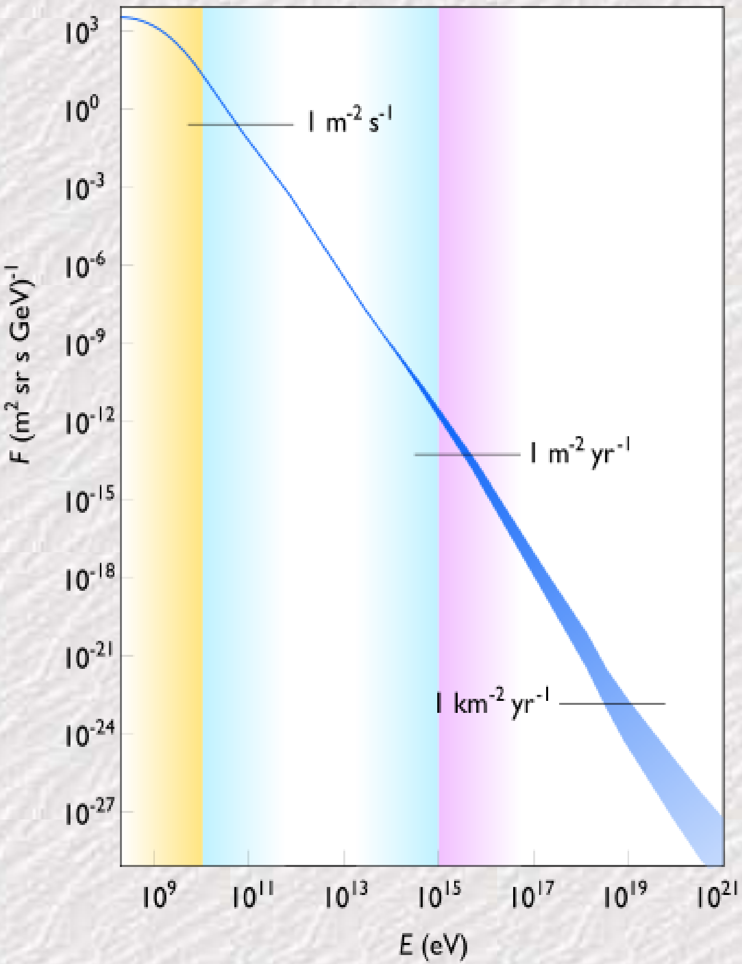

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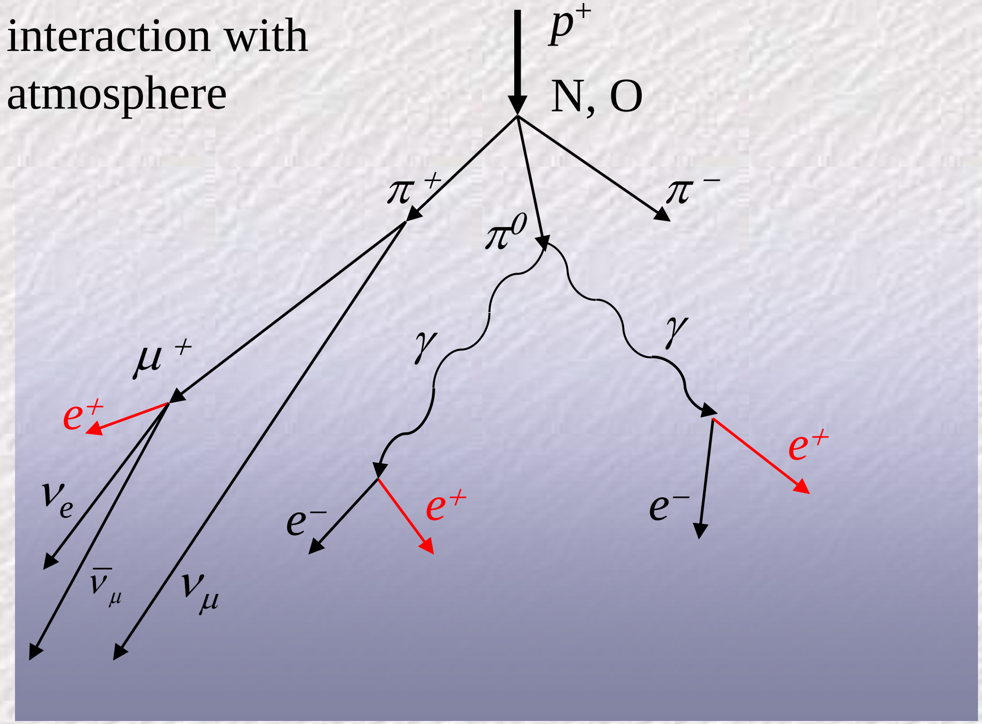
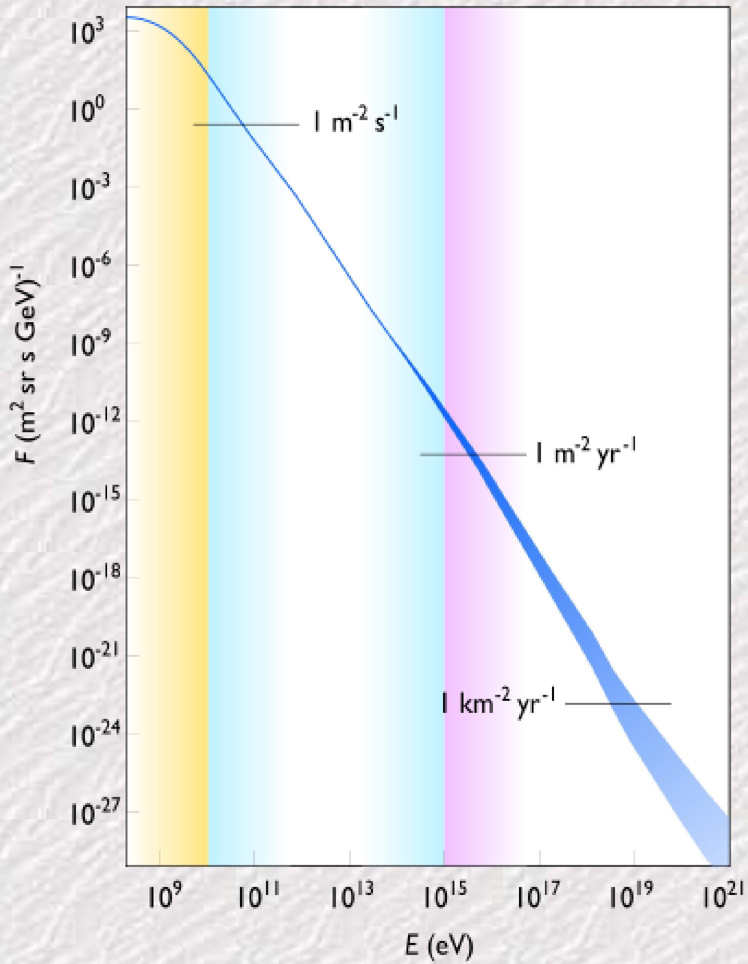




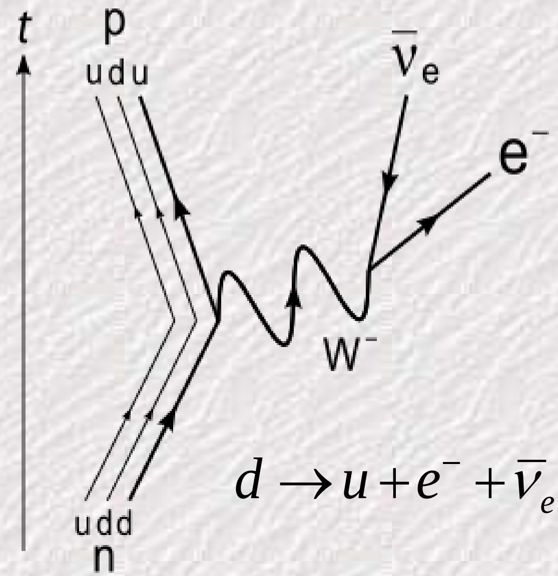
Positron sources

β - decay

β⁻ decay: $${}^{A}_{Z}X \rightarrow {}^{A}_{Z+1}X' + e^{-} + \bar{\nu}_e$$

$$n \rightarrow p^{+} + e^{-} + \bar{\nu}_e$$

$${}^{137}_{55}\mathrm{Cs} \rightarrow {}^{137}_{56}\mathrm{Ba} + e^{-} + \bar{\nu}_e$$



$$d \rightarrow u + e^{-} + \bar{\nu}_e$$

β⁺ decay: $${}^{A}_{Z}X \rightarrow {}^{A}_{Z-1}X' + e^{+} + \nu_e$$

$$p^{+} \rightarrow n + e^{+} + \nu_e$$

$${}^{22}_{11}\mathrm{Na} \rightarrow {}^{22}_{10}\mathrm{Ne} + e^{+} + \nu_e$$

Positron sources

β - decay

β^- decay: $${}^{A}_{Z}X \rightarrow {}^{A}_{Z+1}X' + e^- + \bar{\nu}_e$$

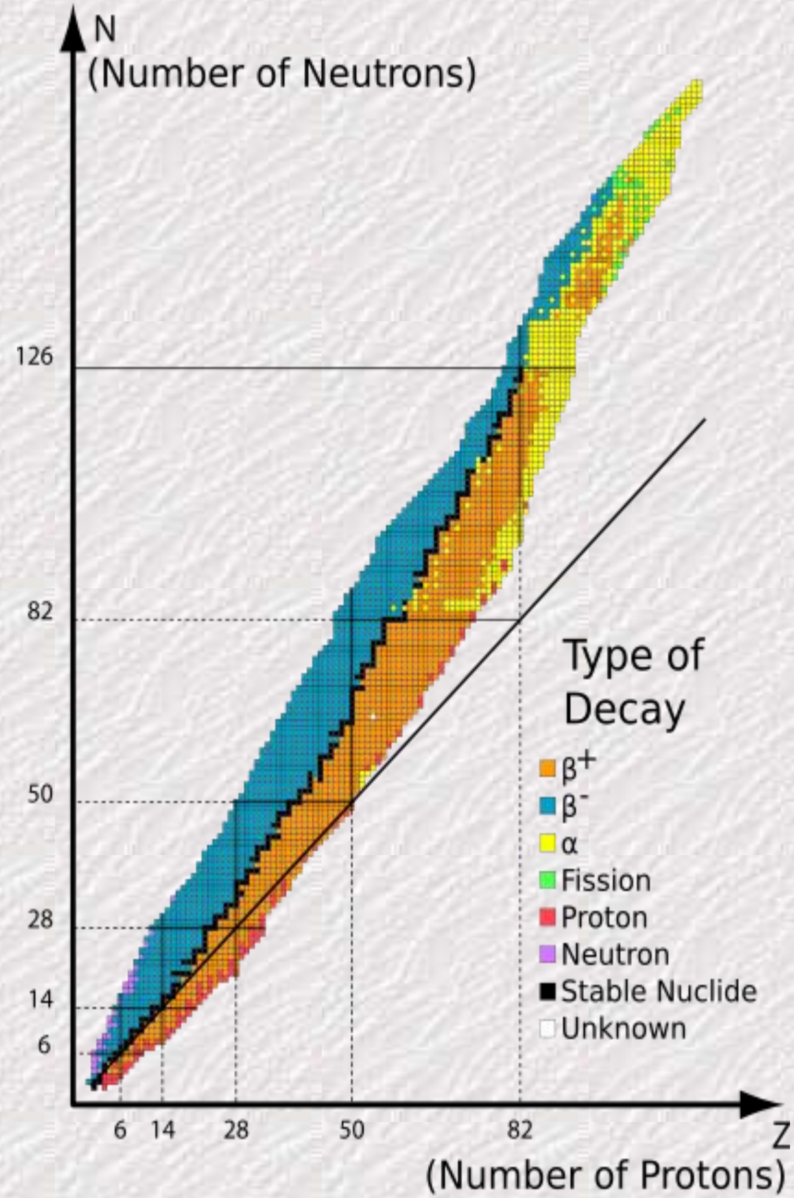
$$n \rightarrow p^+ + e^- + \bar{\nu}_e$$

$${}^{137}_{55}\mathrm{Cs} \rightarrow {}^{137}_{56}\mathrm{Ba} + e^- + \bar{\nu}_e$$

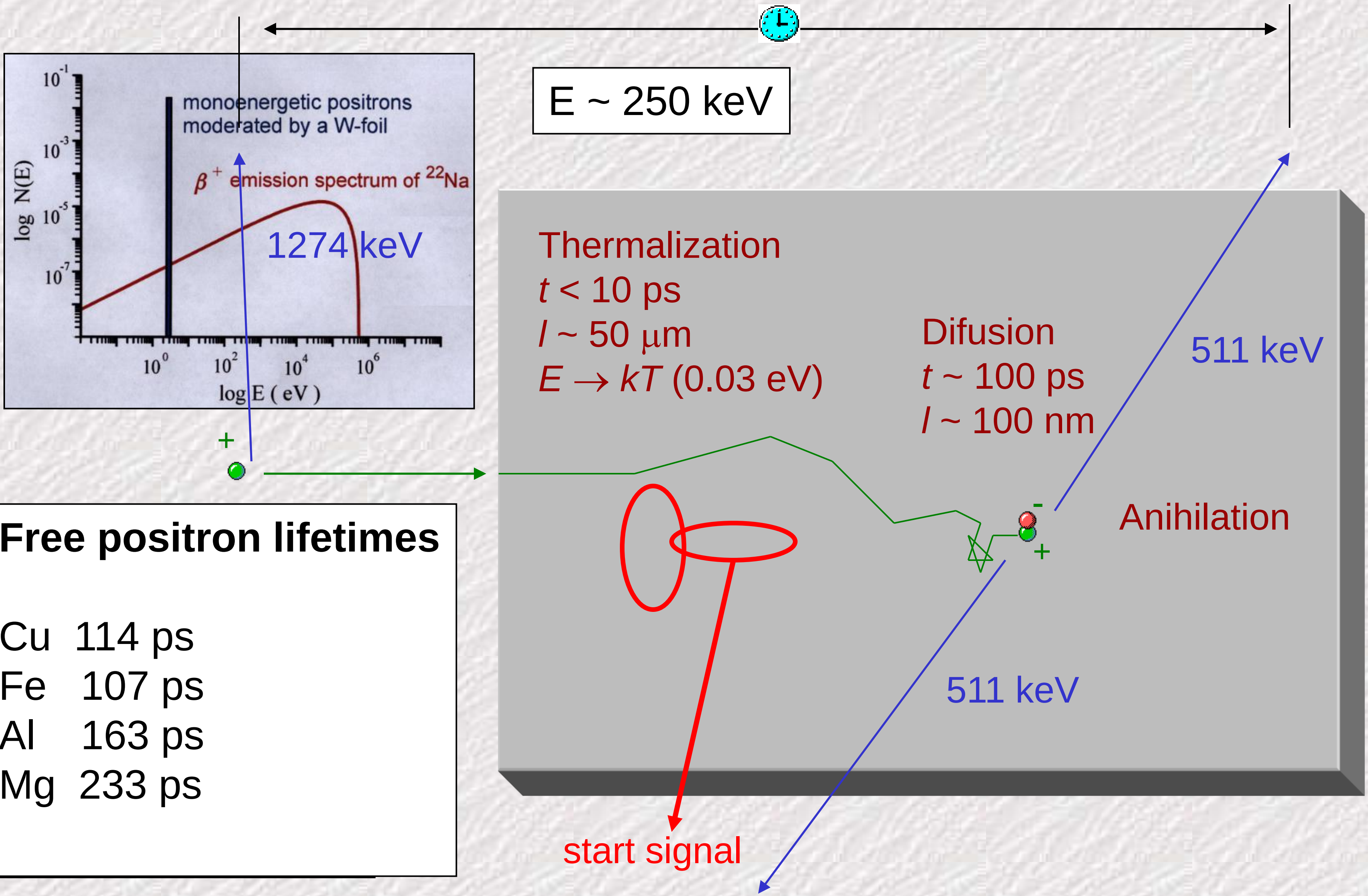
β^+ decay: $${}^{A}_{Z}X \rightarrow {}^{A}_{Z-1}X' + e^+ + \nu_e$$

$$p^+ \rightarrow n + e^+ + \nu_e$$

$${}^{22}_{11}\mathrm{Na} \rightarrow {}^{22}_{10}\mathrm{Ne} + e^+ + \nu_e$$



Interaction of e^+ with solid



Free positron lifetimes

Cu 114 ps
Fe 107 ps
Al 163 ps
Mg 233 ps

Positron lifetime

N*(t)* - probability that e⁺ is alive at time *t* : $\frac{\mathrm{dN}(t)}{\mathrm{d}t} = -\lambda N(t)$ $\quad N(0) = 1$

positron annihilation rate: $\lambda = \pi r_0 c \int n_+(\mathbf{r}) n_-(\mathbf{r}) \gamma \mathrm{d}\mathbf{r}$

$$N(t) = e^{-\lambda t}$$

positron lifetime spectrum: $-\frac{\mathrm{d}N(t)}{\mathrm{d}t} = \lambda e^{-\lambda t}$

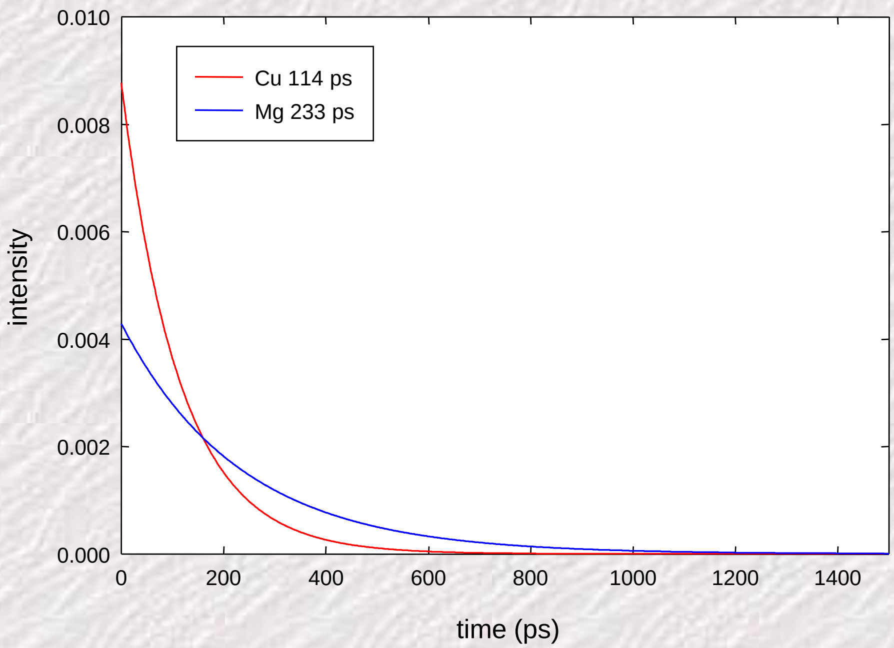
mean time of positron life:

$$\int_0^\infty t \frac{\mathrm{d}N(t)}{\mathrm{d}t} \mathrm{d}t = \int_0^\infty \lambda t e^{-\lambda t} \mathrm{d}t = \left[-t e^{-\lambda t}\right]_0^\infty + \int_0^\infty e^{-\lambda t} \mathrm{d}t = \left[-\frac{1}{\lambda} e^{-\lambda t}\right]_0^\infty = \frac{1}{\lambda}$$

free positron lifetime: $\tau = \frac{1}{\lambda}$

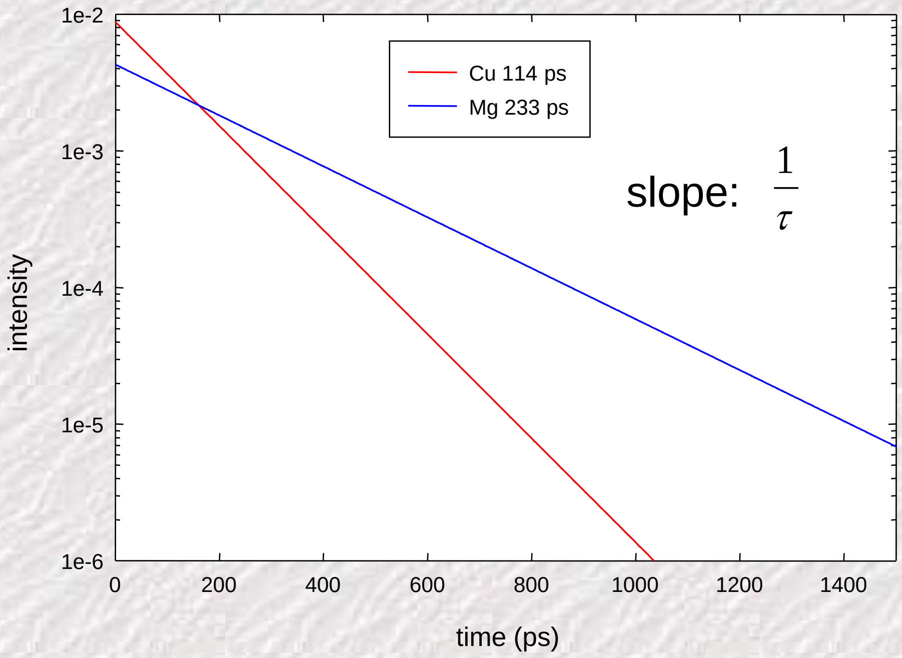
Positron lifetime spectrum

positron lifetime spectrum: $$S_{\mathrm{id}} = -\frac{\mathrm{d}N(t)}{t} = \lambda e^{-\lambda t}$$



Positron lifetime spectrum

positron lifetime spectrum: $$S_{id} = -\frac{dN(t)}{t} = \lambda e^{-\lambda t}$$



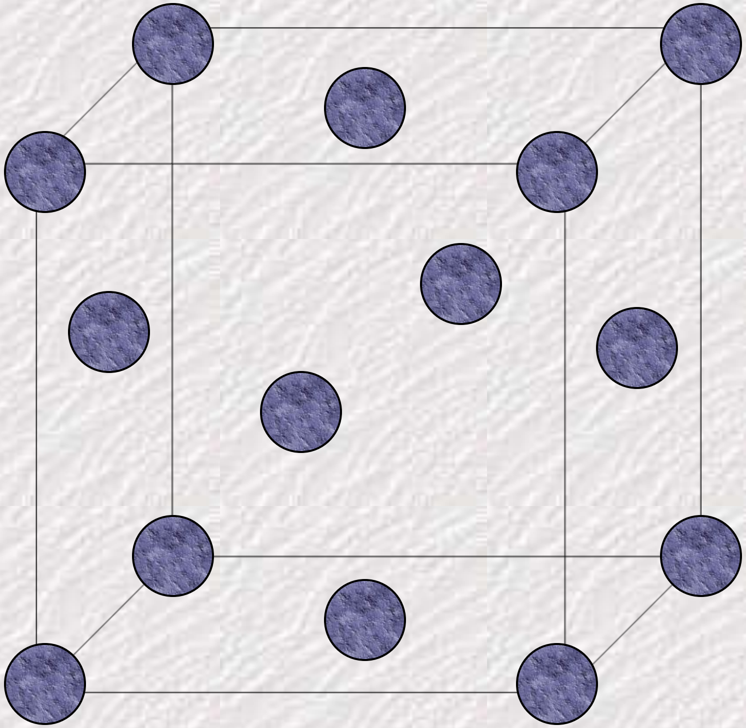
real positron lifetime spectrum: $$S_{real}(t) = \int_{-\infty}^{+\infty} S_{id}(t-\xi)\, R(\xi)\, d\xi + B$$

background

resolution function of spectrometer

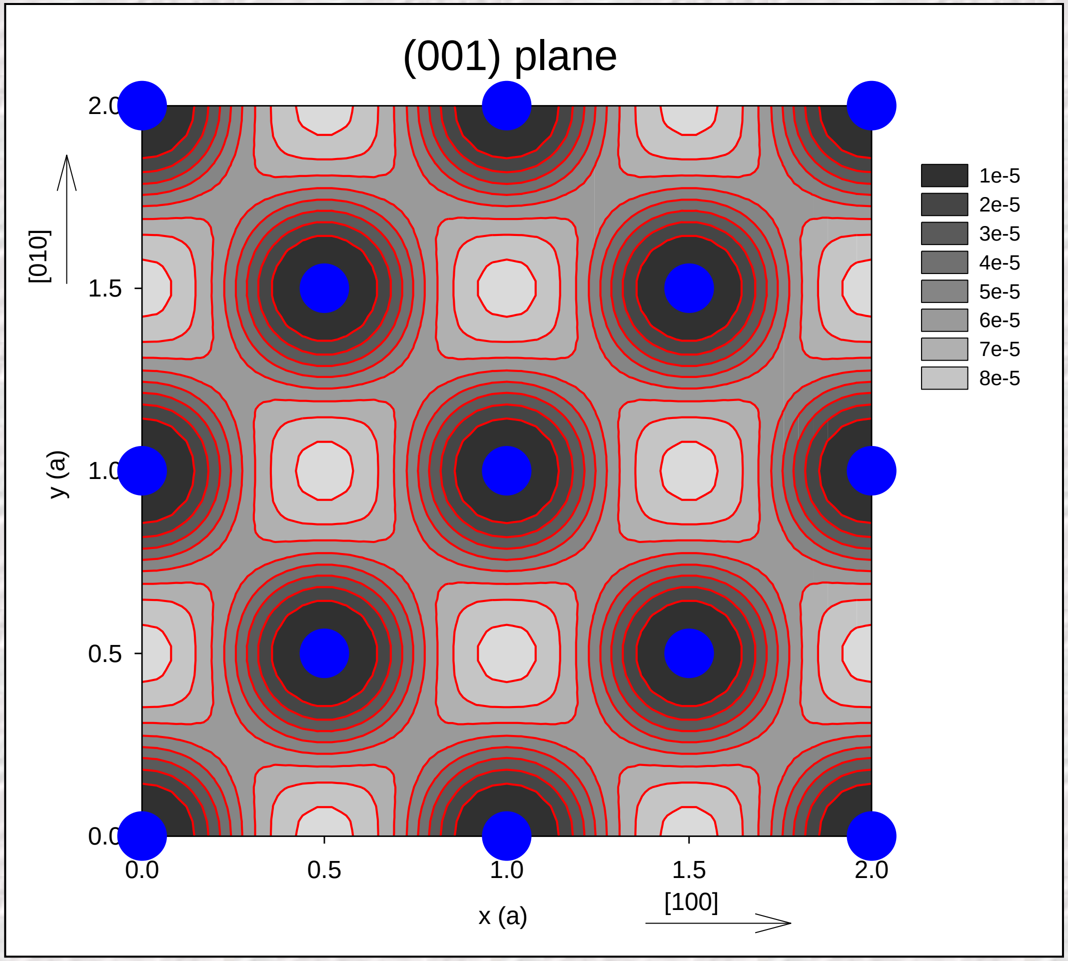
Positron trapping

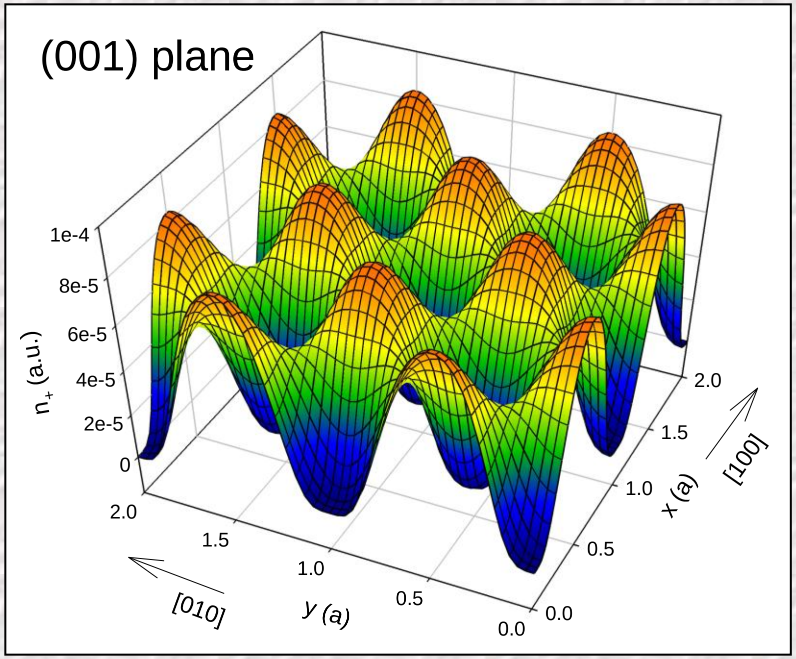
Cu: fcc



$$\tau = \left(\pi r_0 c \int n_-(\mathbf{r}) n_+(\mathbf{r}) \gamma(n_-)\, d\mathbf{r} \right)^{-1}$$

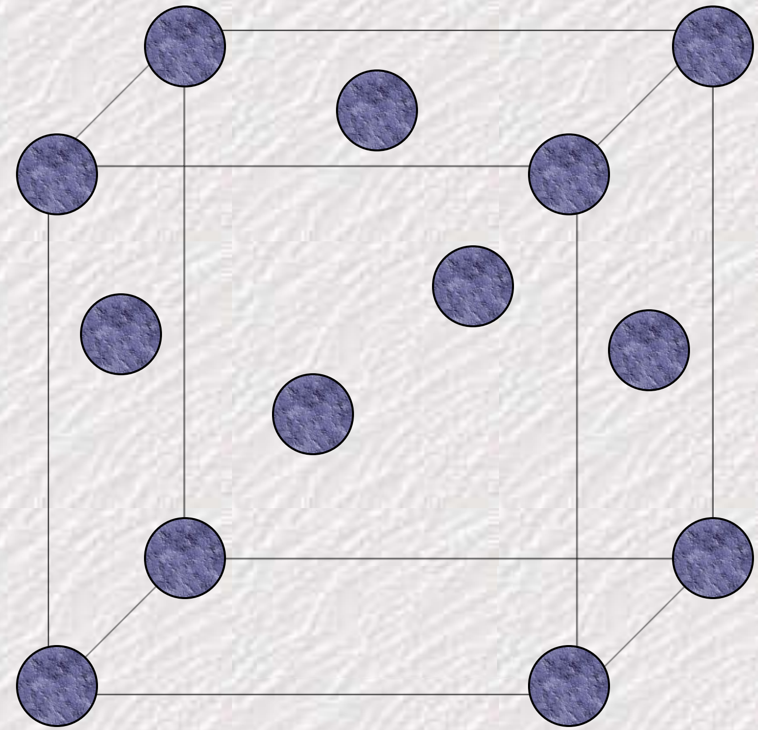
lifetime τ_B = 114 ps





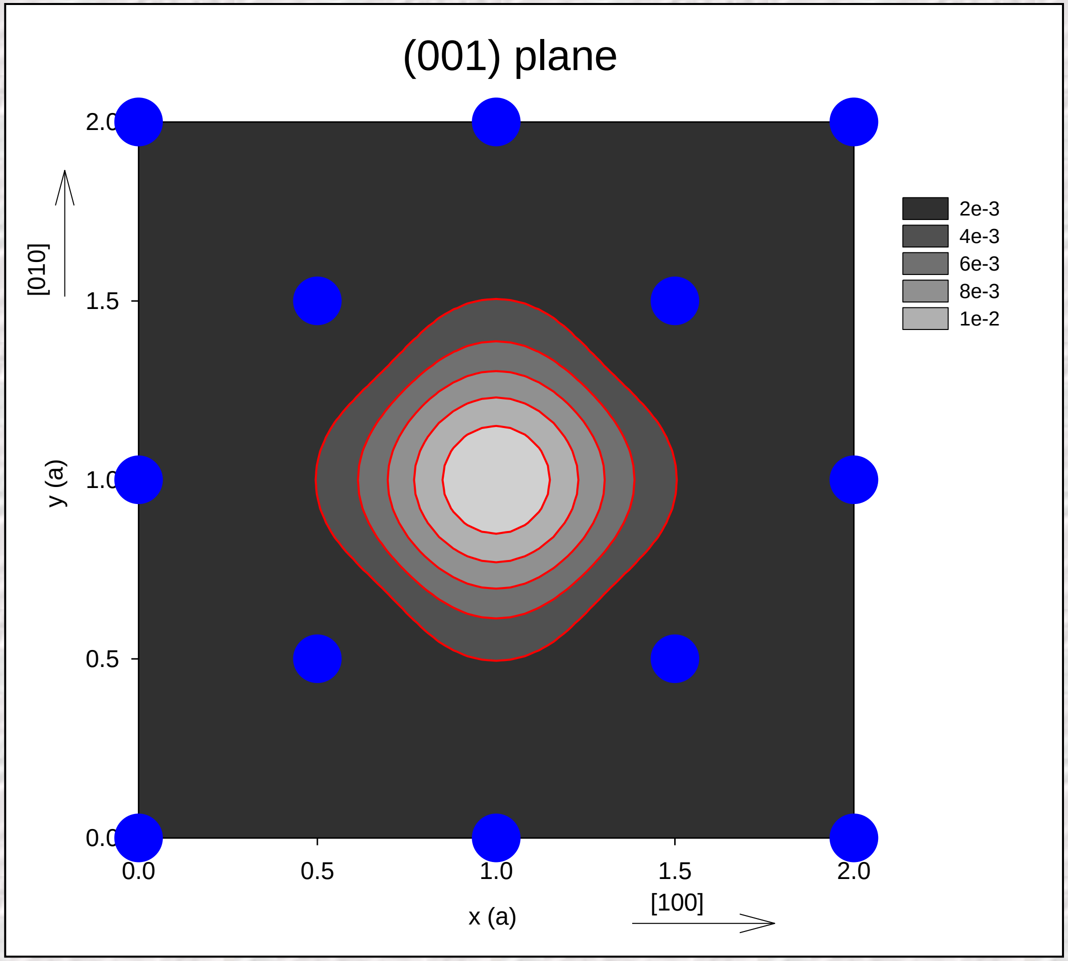
Positron trapping

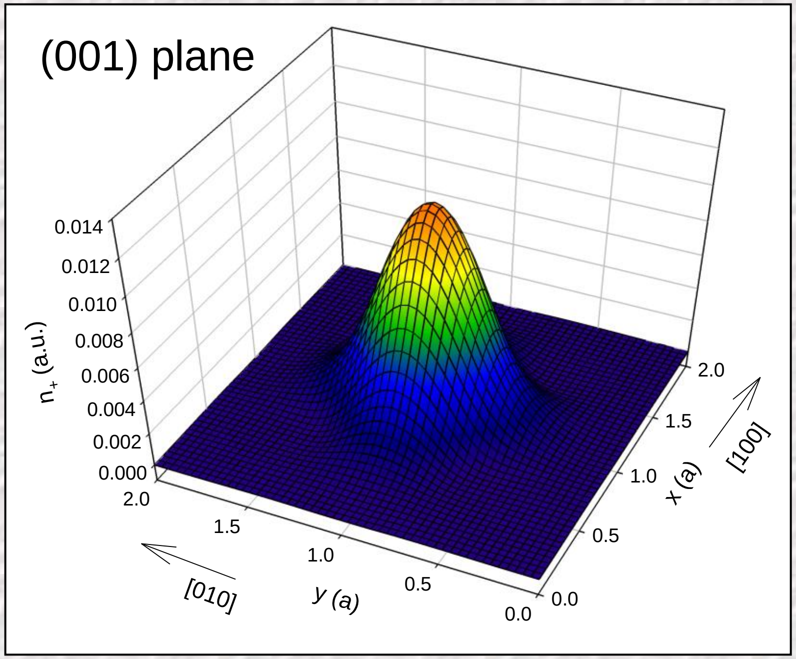
Cu: fcc



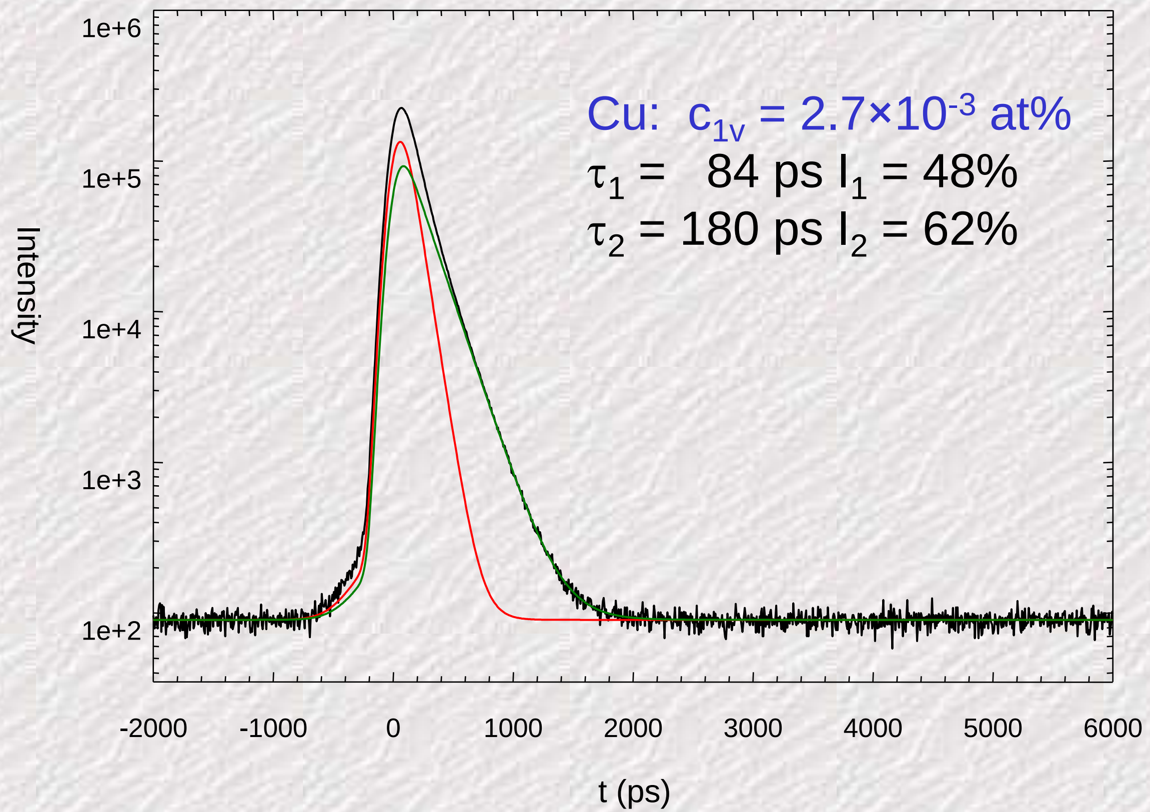
vacancy in [1/2,1/2,0] position

lifetime τ_{1v} = 180 ps





Positron lifetime spectrum

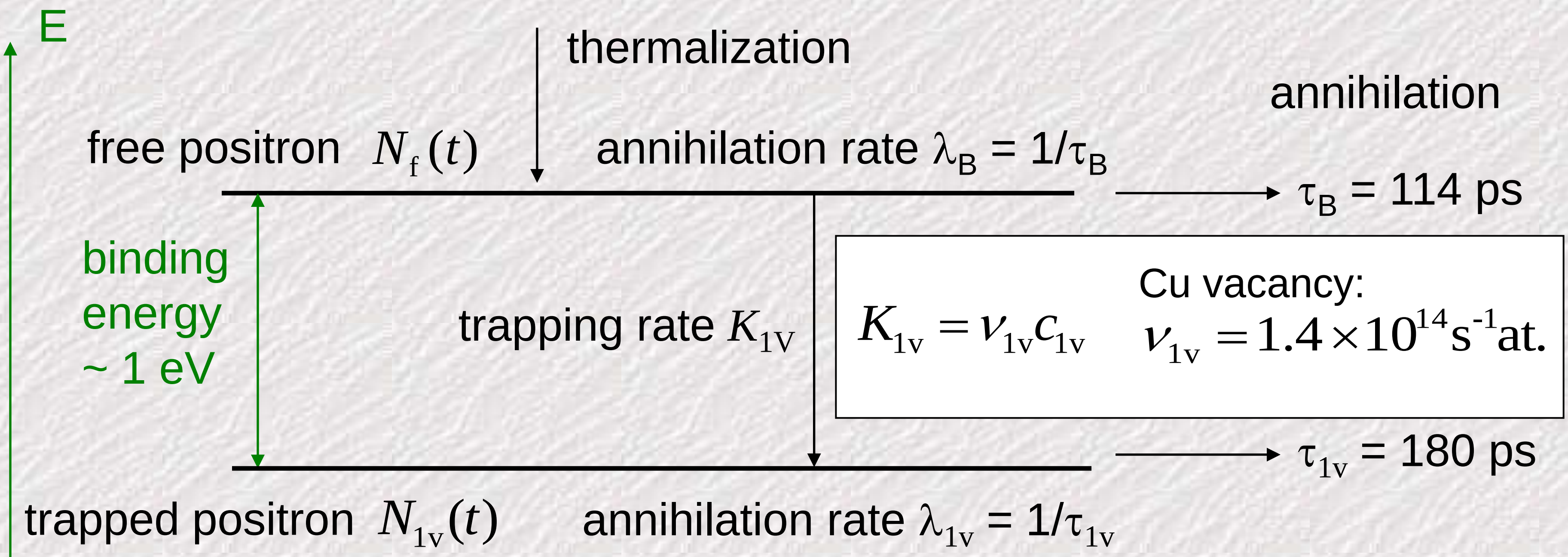


decomposition of PL spectrum:

lifetimes τ_i $\rightarrow$ type of defects present

intensities $I_i \rightarrow$ defect densities

Simple positron trapping model: Cu with vacancies



two-component spectrum: $S_{id} = \frac{1}{\tau_1} I_1 e^{-\frac{t}{\tau_1}} + \frac{1}{\tau_2} I_2 e^{-\frac{t}{\tau_2}}$

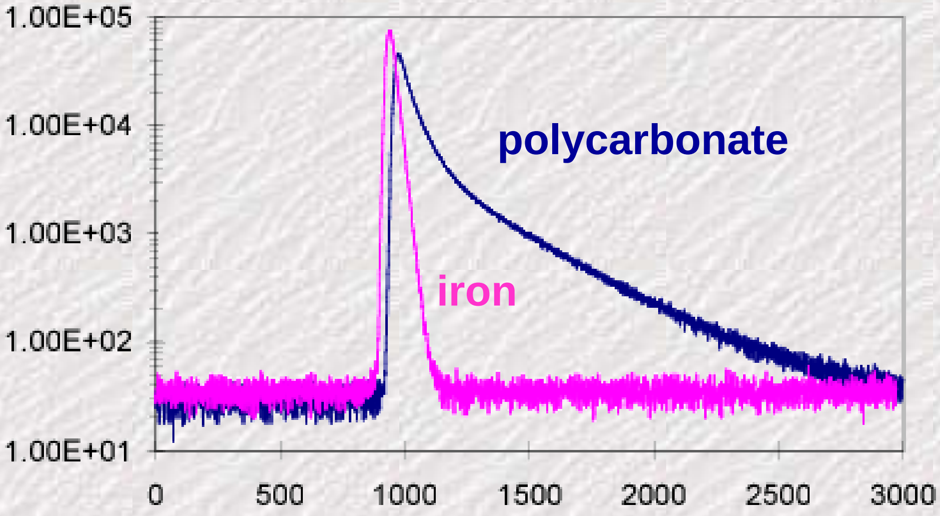
$\tau_1 = \frac{1}{\lambda_B + K_{1v}}$ $I_1 = 1 - I_2$ free positrons

$\tau_2 = \frac{1}{\lambda_{1v}}$ $I_2 = \frac{K_{1v}}{\lambda_B + K_{1v} - \lambda_{1v}}$ positrons trapped at vacancies

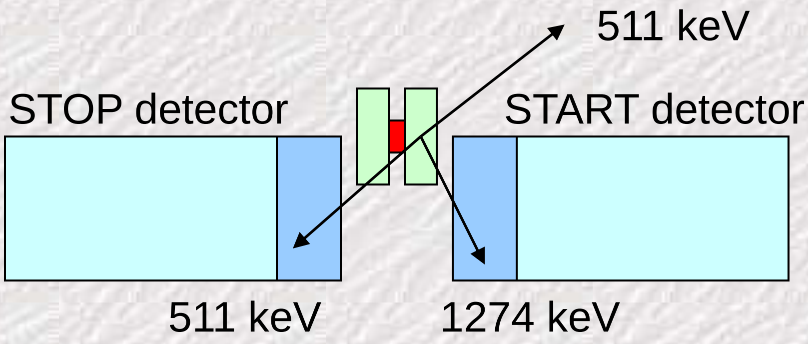
Positronium

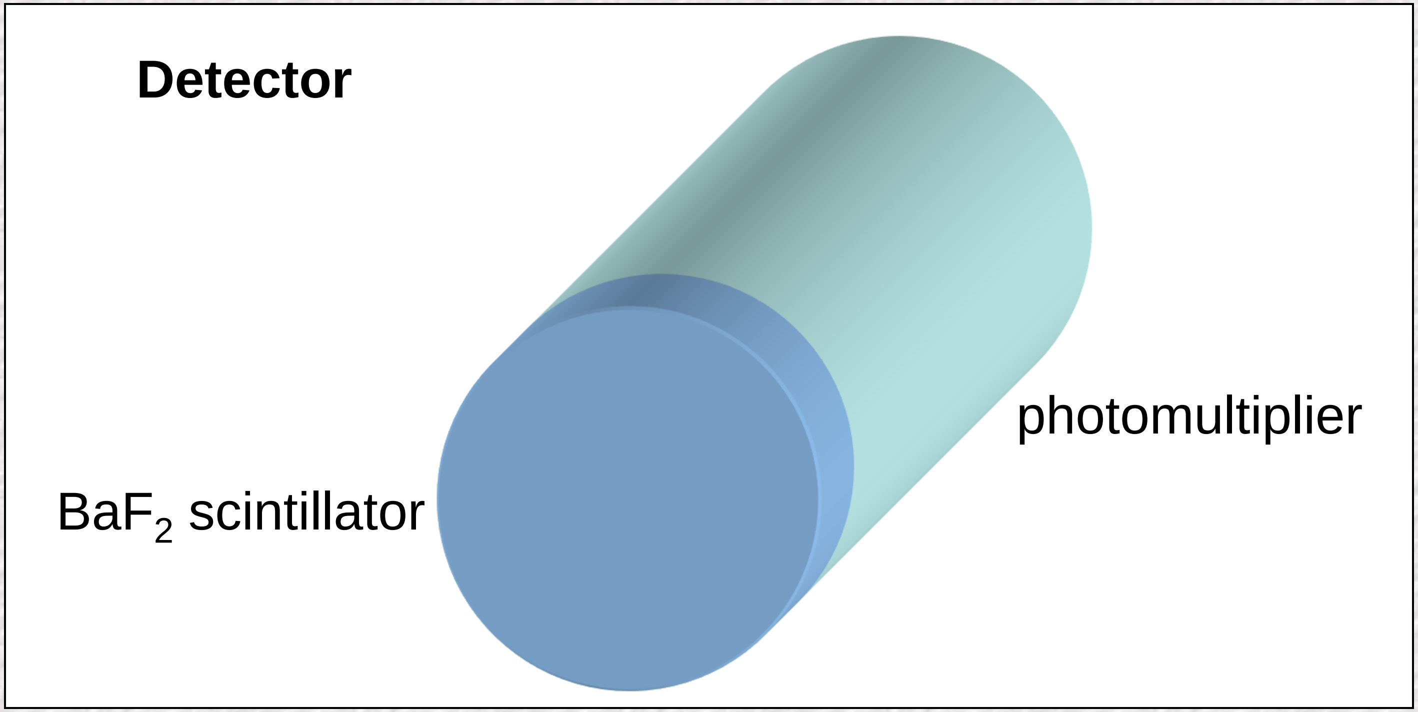
- hydrogen-like bound state of positron and electron
- **parapositronium p-Ps**
  $^1S_0$, singlet state, antiparallel spins, lifetime $\tau_{\text{p-Ps}}$ = 125 ps, 2-γ
- **orthopositronium o-Ps**
  $^3S_1$, triplet state, parallel spins, lifetime $\tau_{\text{o-Ps}}$ = 142 ns, 3-γ
- formed in large open volumes: e.g. in polymers

- in solids
  ⇒ "pick-off" annihilation of o-Ps
  $\tau_{\text{o-Ps}}$ reduced to several ns



Positron – lifetime spectrometer





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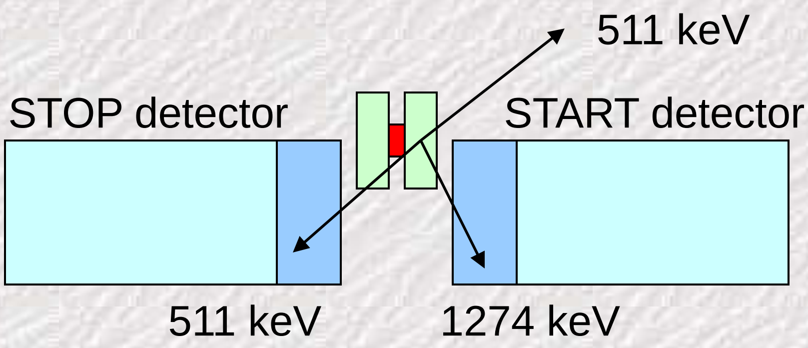


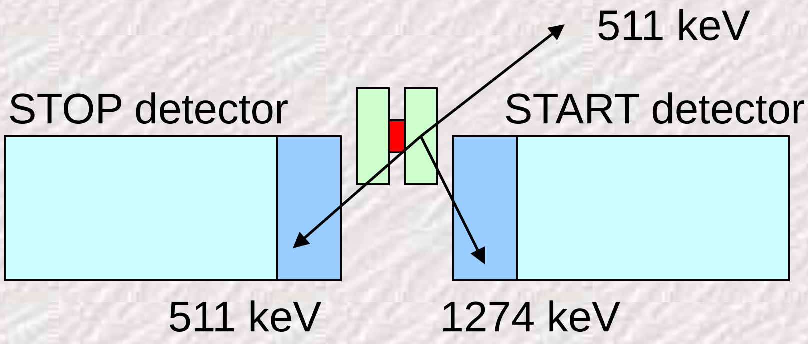
Detector

BaF_2 scintillator

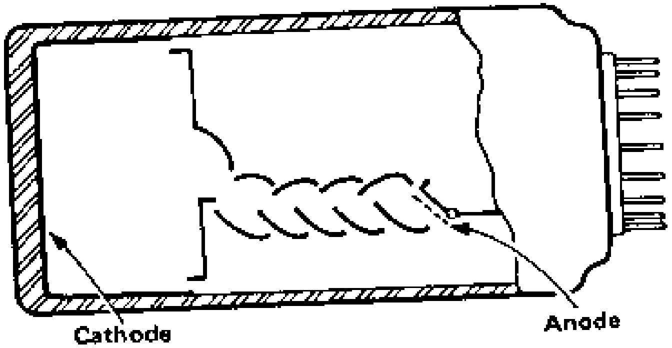
Fast component: λ_1 = 220 nm, τ_1 = 0.6 ns

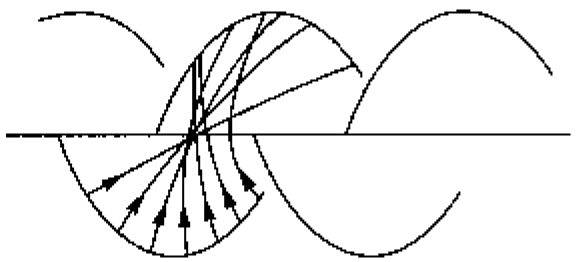
Slow component: λ_2 = 310 nm, τ_2 = 630 ns

Positron – lifetime spectrometer



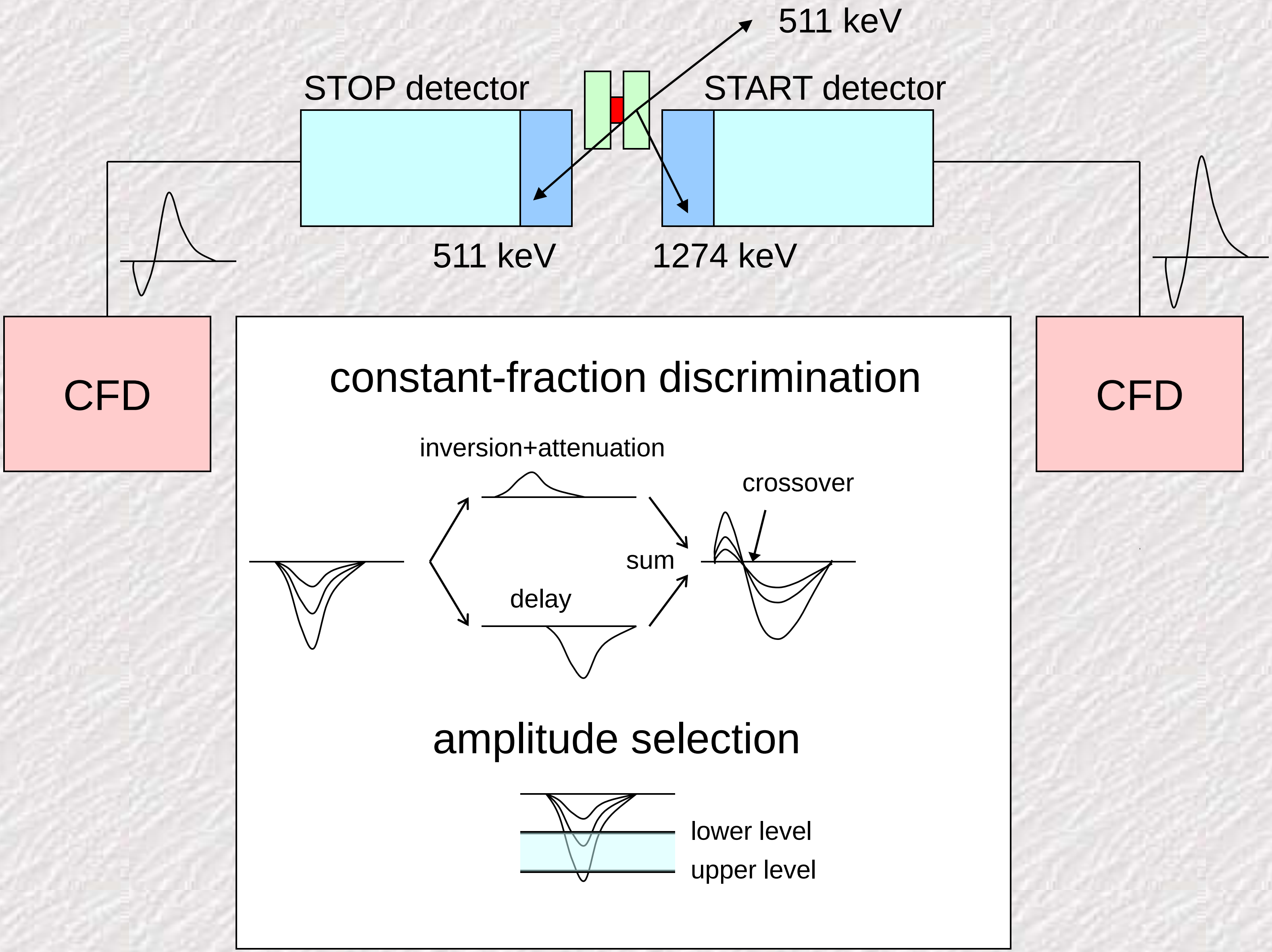
Detector



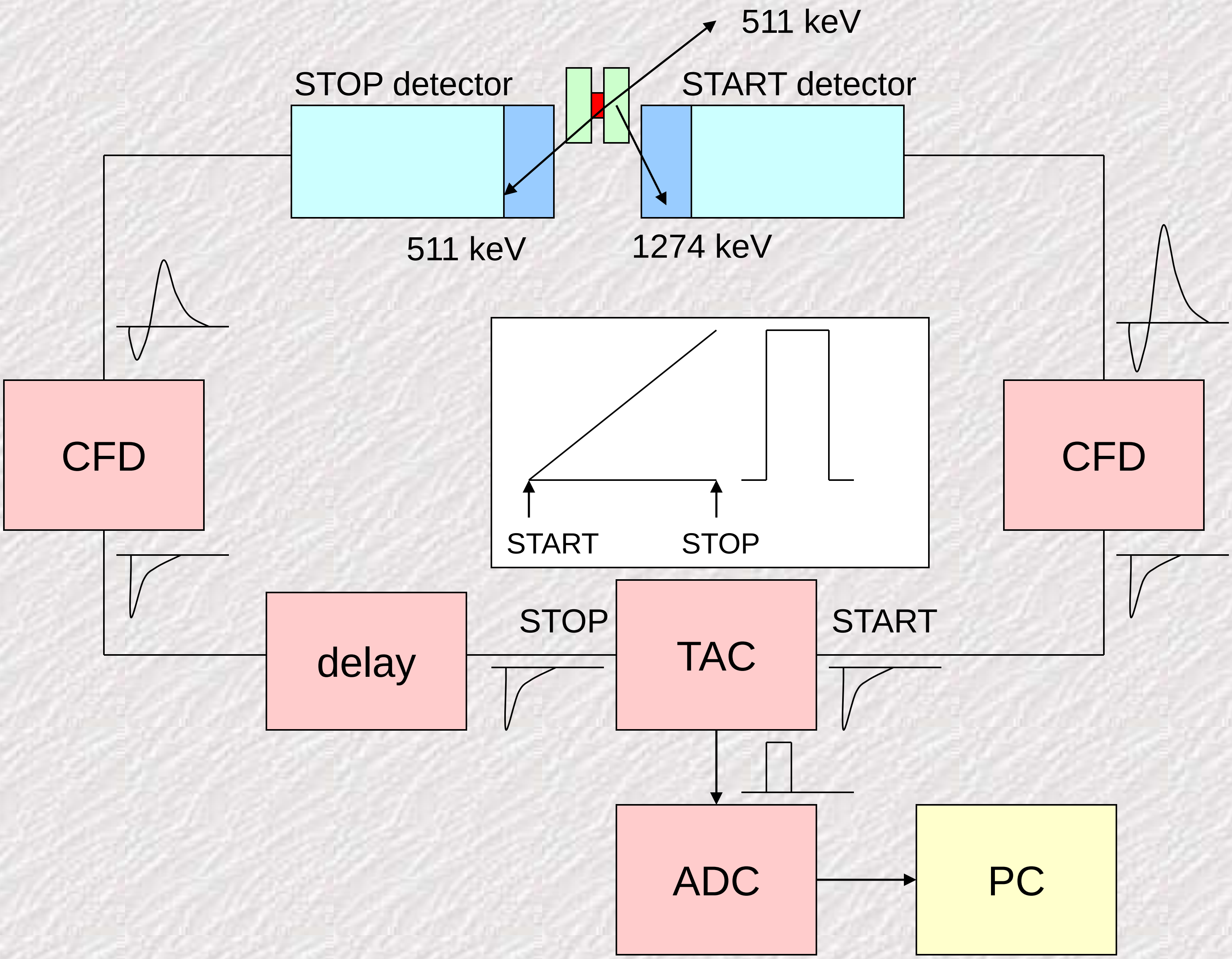


Linearly focused PMT

Positron – lifetime spectrometer



Positron – lifetime spectrometer

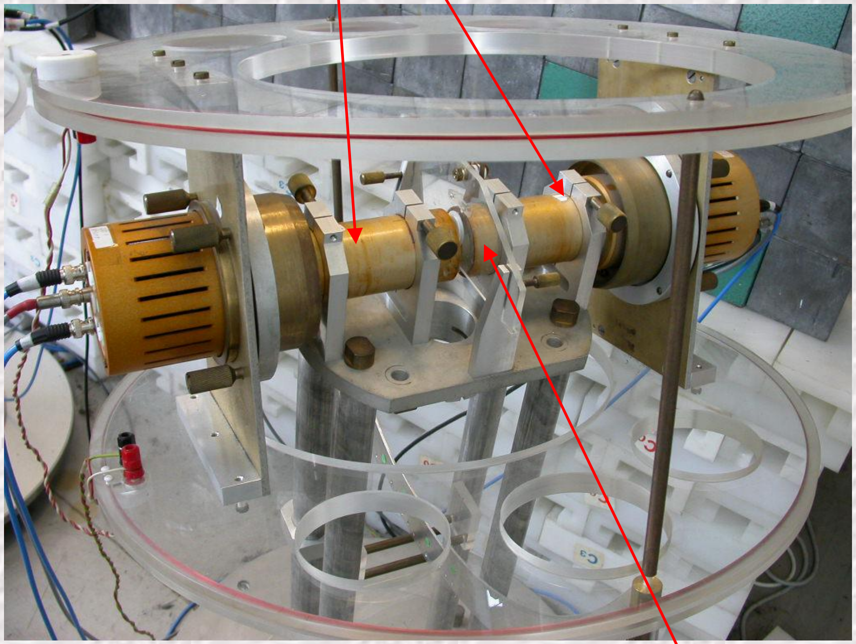


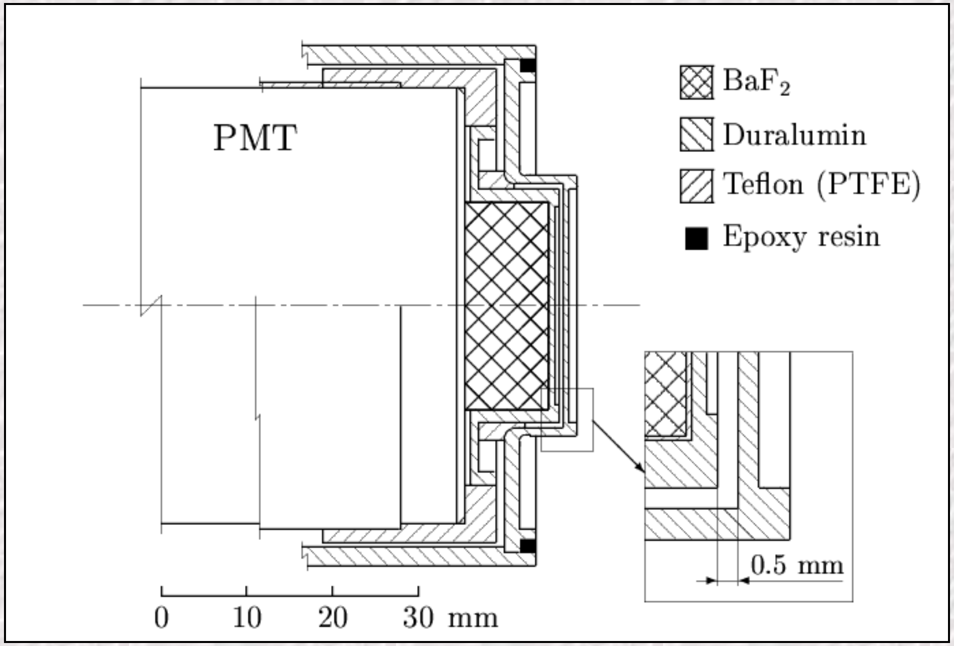
Positron – lifetime spectrometer

- fast-fast PL spectrometer
- timing resolution 160 ps (FWHM ^{22}Na)
- coincidence count rate 100 s^{-1}
- 10^{7} counts in spectrum

F. Bečvář et al., Nucl. Instr. Meth. A ***443****, 557 (2000)*

detectors

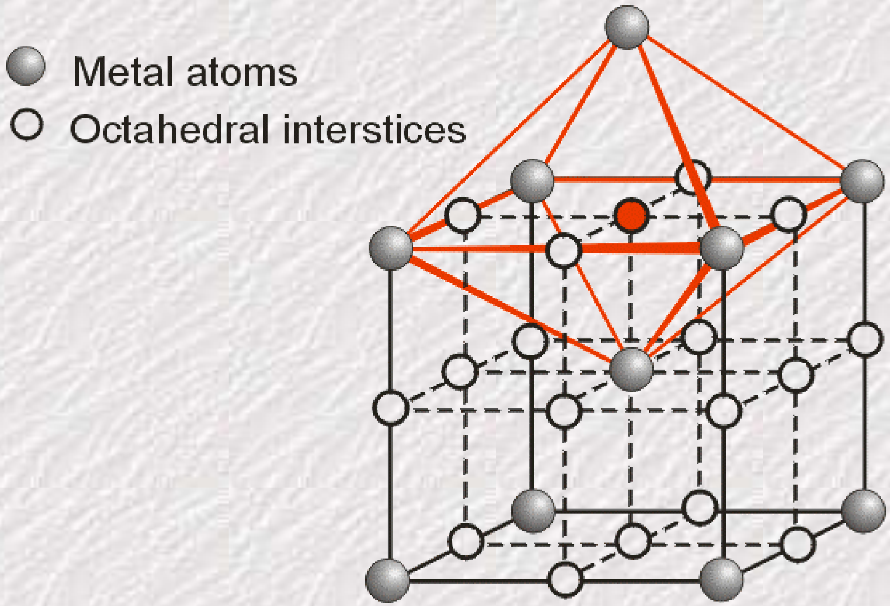


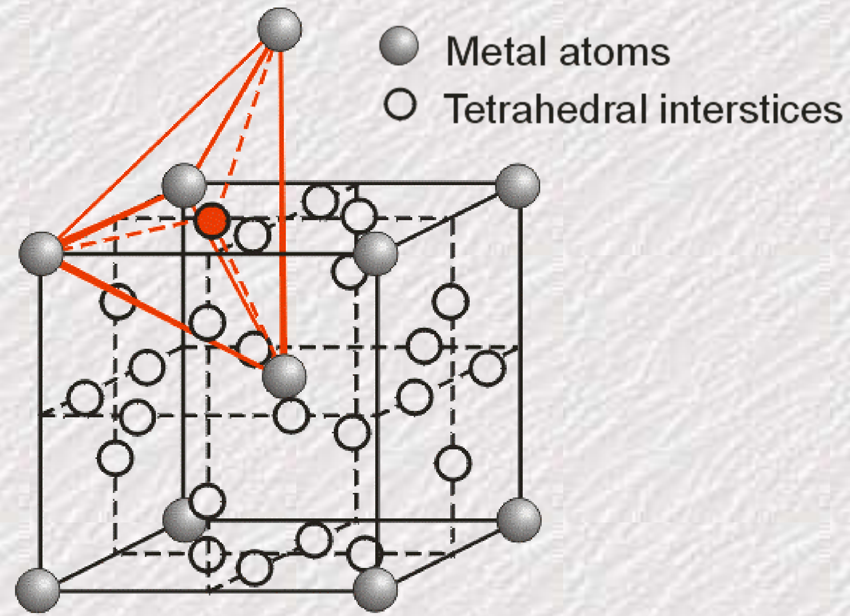


source-sample sandwich

Hydrogen in Niobium

Nb: bcc structure a = 3.3033(1) Å [PDF-2]
H in Nb – interstitial solid solution





H ≈0.35

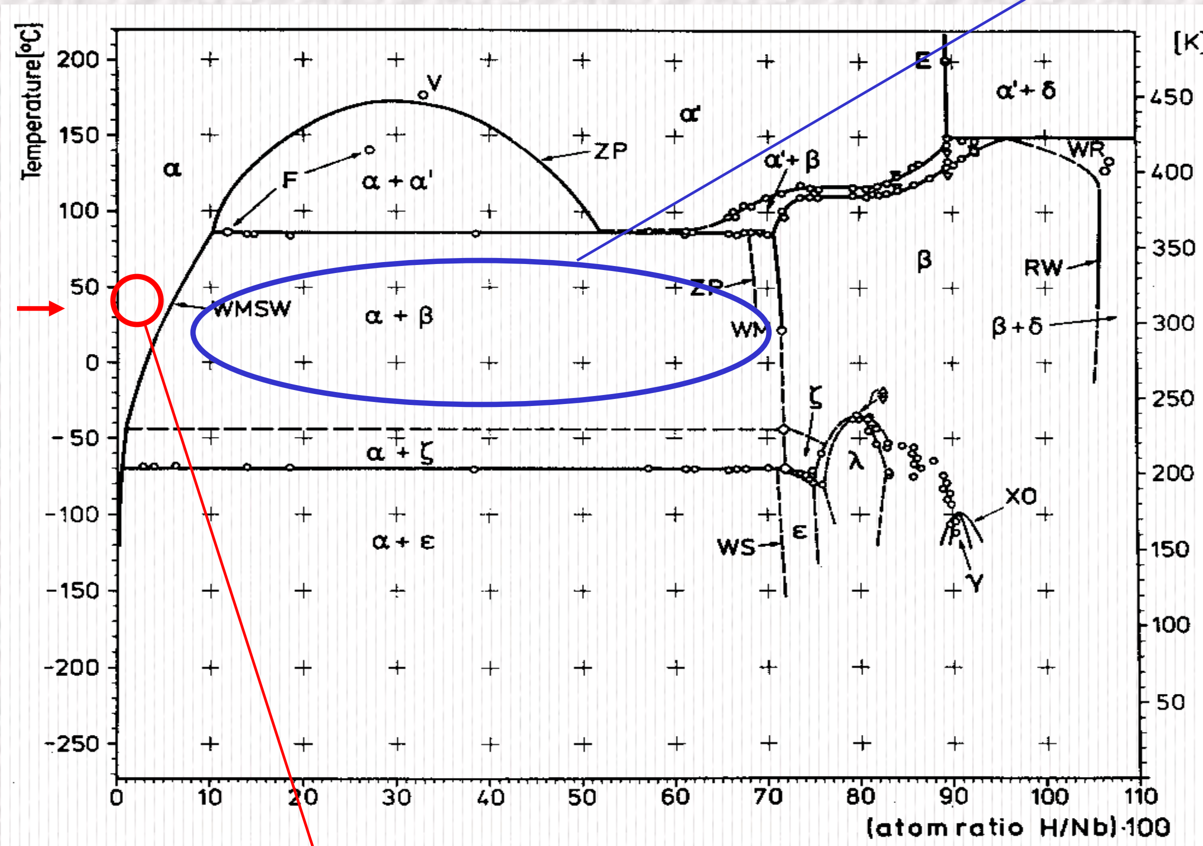
size (r_{Nb}):	0.155	0.291
N_i/cell	6	12
N_i/M	3	6

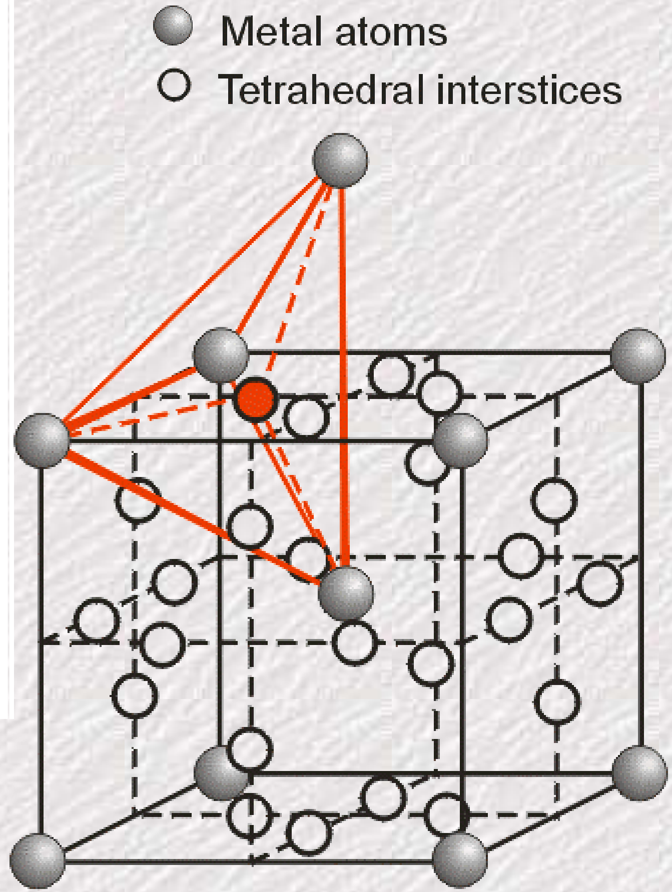
$x_H = N_H/M$ – number of hydrogen atoms per metal atoms

Hydrogen in Niobium

two-phase field (α + β)

Equilibrium phase diagram of Nb-H system



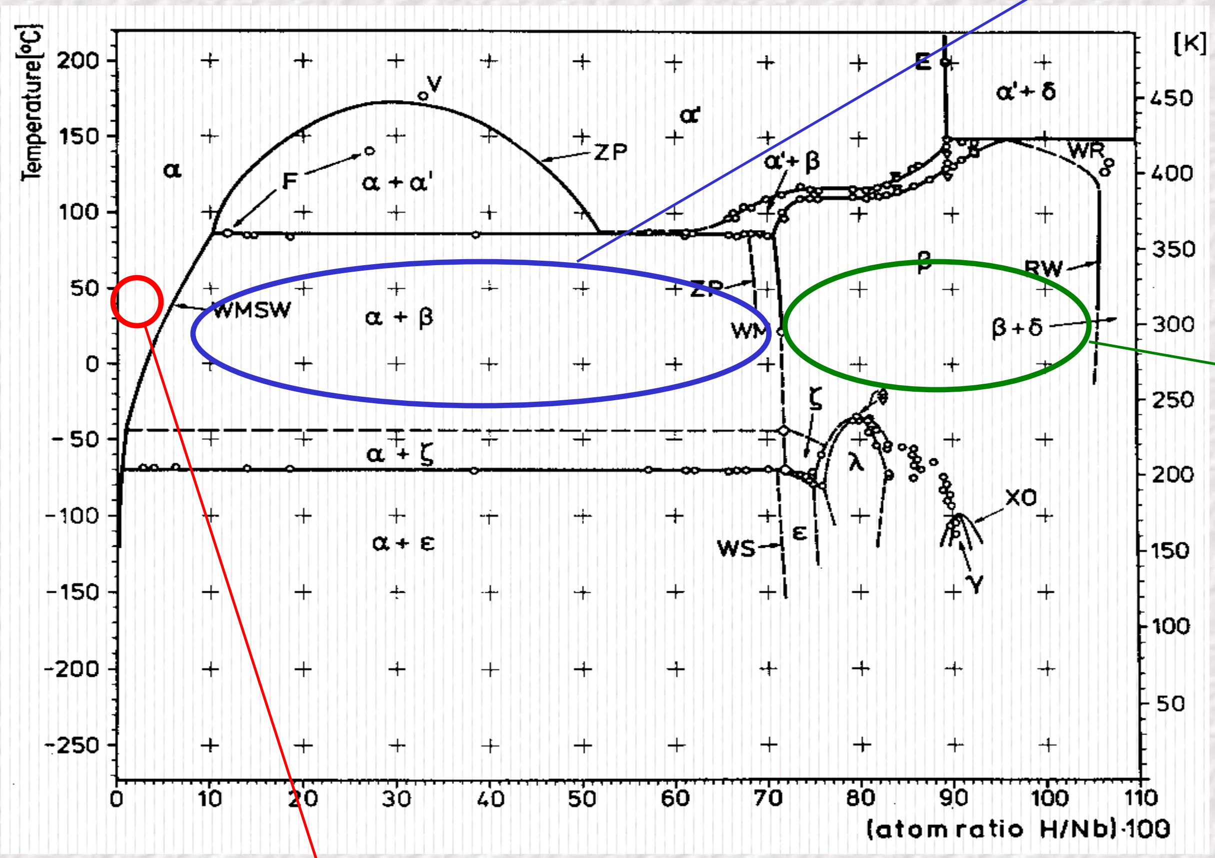


x_H = 0 - 0.06 (atom ratio H/Nb):
single phase solid solution (α-phase), bcc
H fills tetrahedral interstitial positions

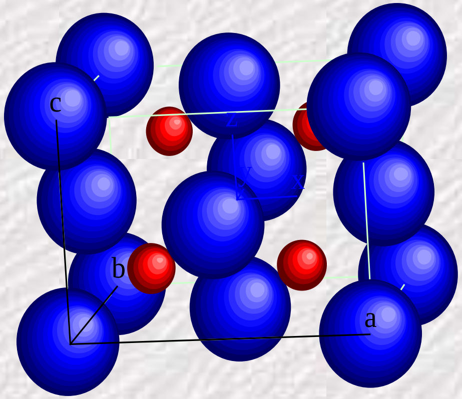
Hydrogen in Niobium

two-phase field ($\alpha + \beta$)

Equilibrium phase diagram of Nb-H system



β-phase (NbH)
orthorhombic
a = 4.859 Å
b = 4.878 Å
c = 3.453 Å



x_H = 0 - 0.06 (atom ratio H/Nb):
single phase solid solution (α-phase), bcc
H fills tetrahedral interstitial positions

Samples

- **defect-free Nb**
  - bulk Nb (99.9%)
  - annealing 1000 ^oC / 1h to anneal out all existing defects
- **electron irradiated Nb**
  - bulk Nb (99.9%)
  - annealing 1000 ^oC / 1h to anneal out all existing defects
  - 10 MeV electron irradiation, $F = 2 \times 10^{21}$ m^{-2}, $T_{irr} \leq 100^oC$

all samples:

Pd cap (thickness 30 nm) ⟶ prevent oxidation

⟶ facilitate H absorption

R. Kircheim et al., Acta Metall. ***30****, 1059 (1982)*

Hydrogen loading

Electrochemical H loading

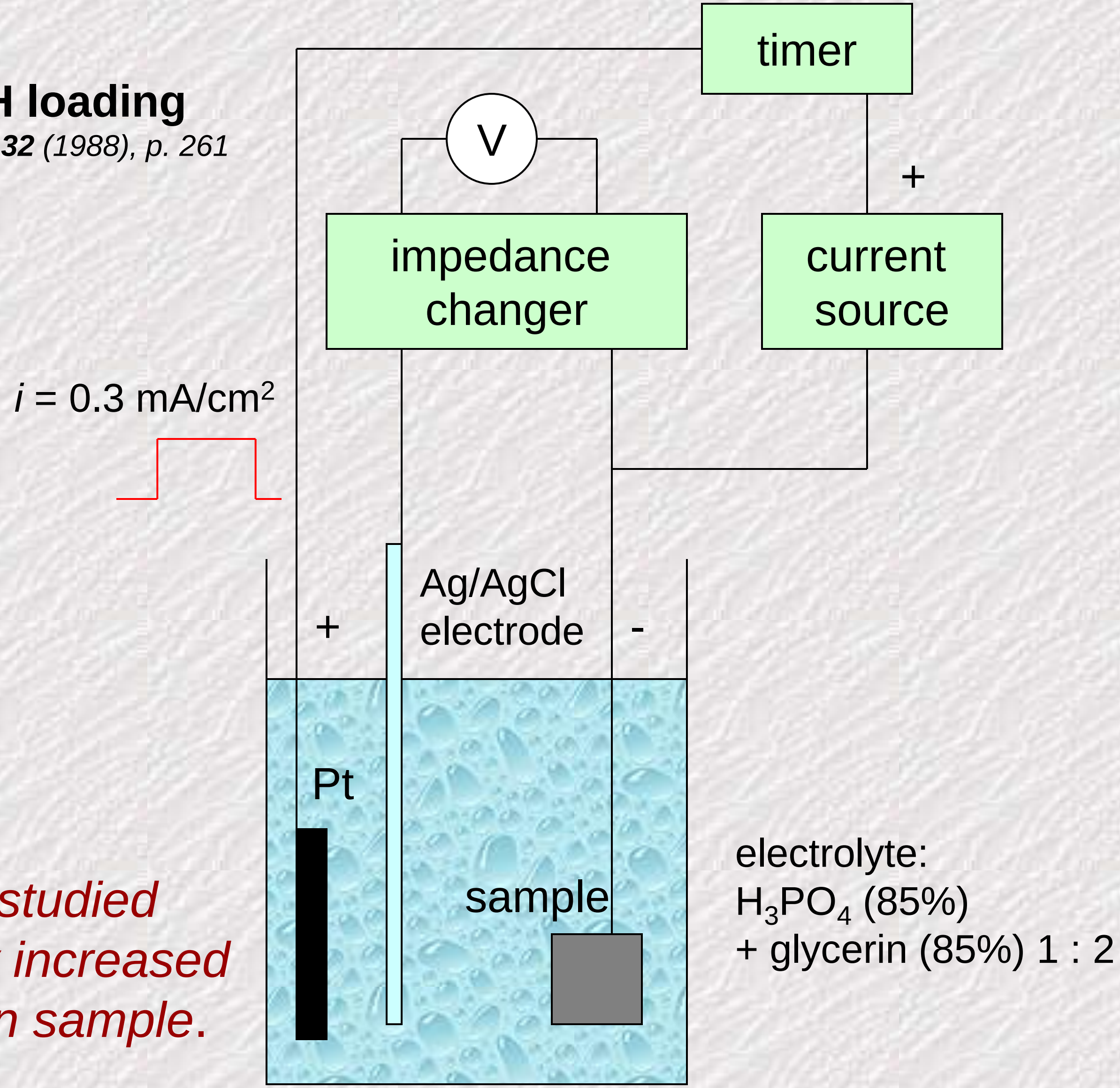
R. Kircheim, Prog. Mat. Sci. ***32*** *(1988), p. 261*

hydrogen concentration

↓

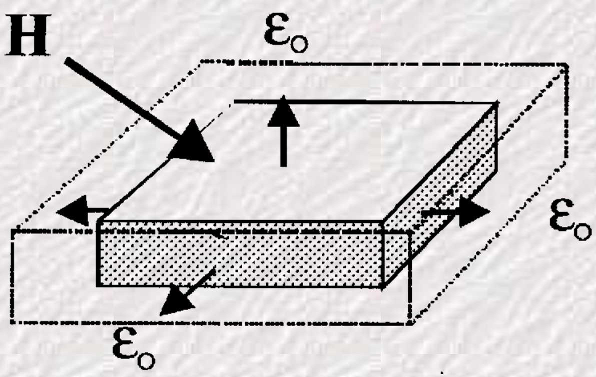
Faraday‘s law

$$x_H = \frac{It}{F}\frac{Vm, Nb}{V}$$



Evolution of defects was studied as a function of gradually increased hydrogen concentration in sample.

H-induced lattice expansion: X-ray diffraction



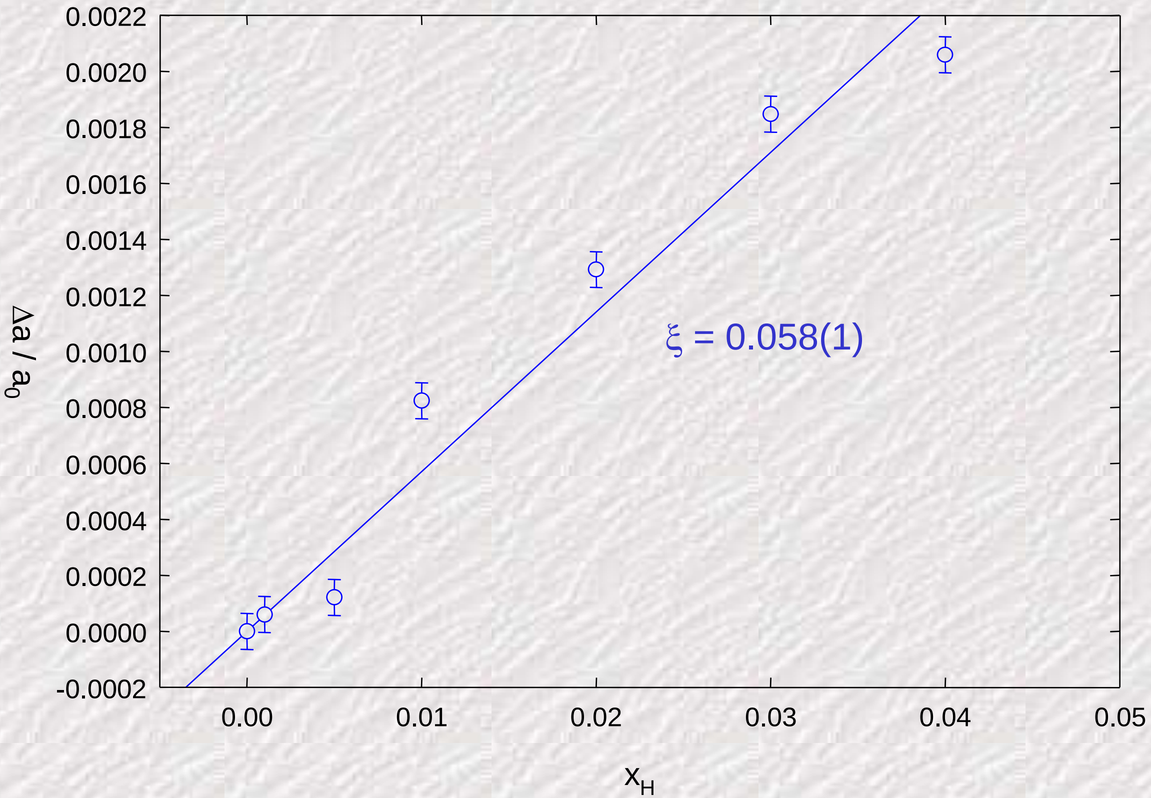
relative lattice expansion: $\frac{a - a_0}{a_0} = \xi \, x_H$

a_0 – lattice constant for virgin sample

a – lattice constant for hydrogen-loaded sample

for Nb : $\xi = 0.058$

H. Peisl, in:. Hydrogen in Metals I, Springer-Verlag, Berlin (1978), p. 53



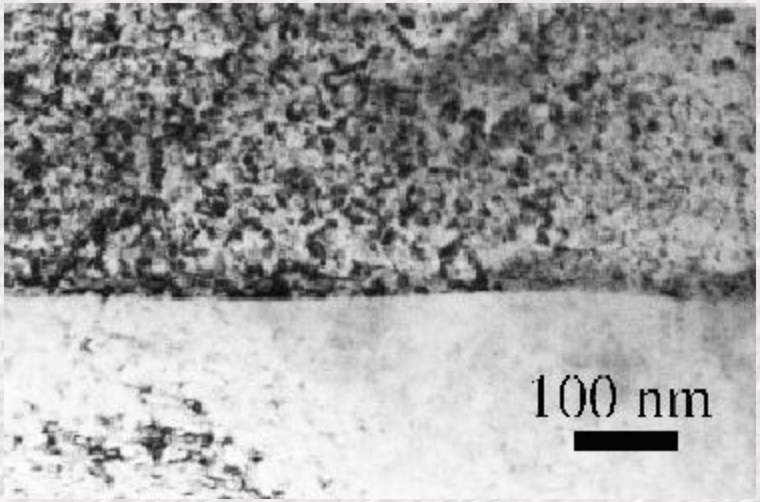
Hydrogen-induced vacancies

well annealed Nb (1000°C / 1h):

- single component PL spectrum τ_1 = (128.3 $\pm$ 0.4) ps
- calculated bulk Nb lifetime (ATSUP): τ_B = (126 $\pm$ 1) ps
- “defect-free” material

TEM

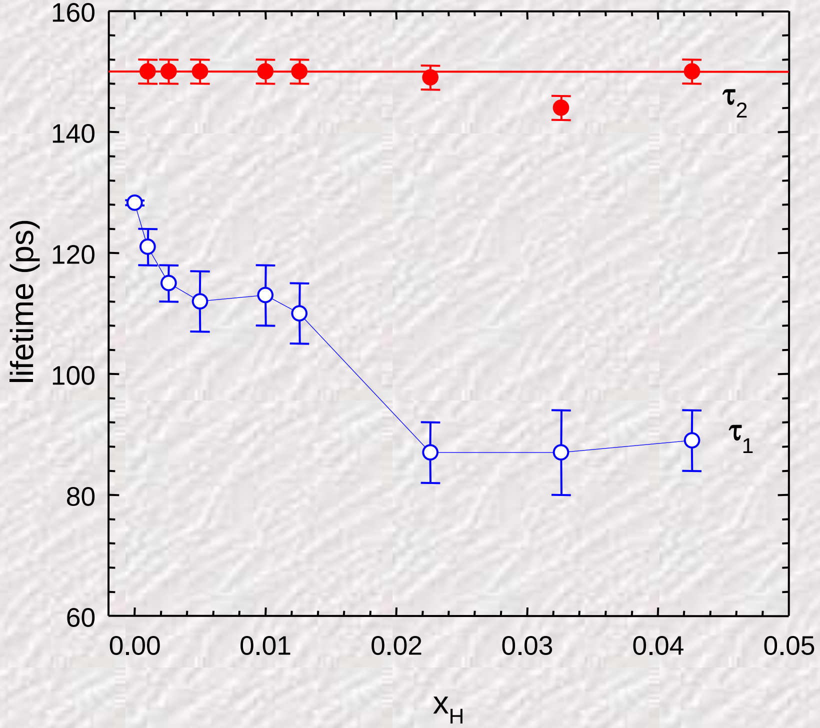
no dislocations observed, grain size > 10 μm

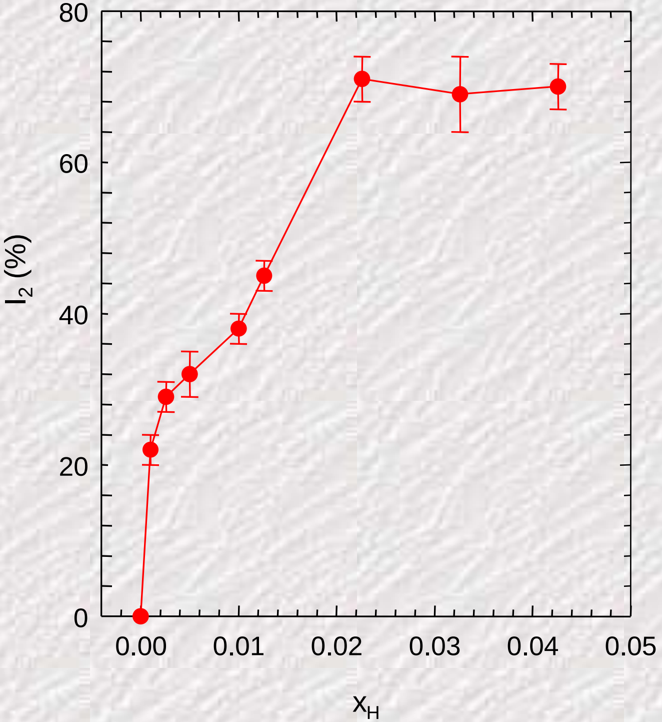


Hydrogen-induced vacancies

well annealed Nb (1000ºC / 1h) – hydrogen loading

- hydrogen induced defects τ_2 = (150 ± 0.5) ps
- hydrogen-induced volume expansion → elastic process → dislocations
- calculated lifetime for Nb vacancy (ATSUP): τ_V = (222 ± 1) ps
- vacancies surrounded by hydrogen → shortening of positron lifetime

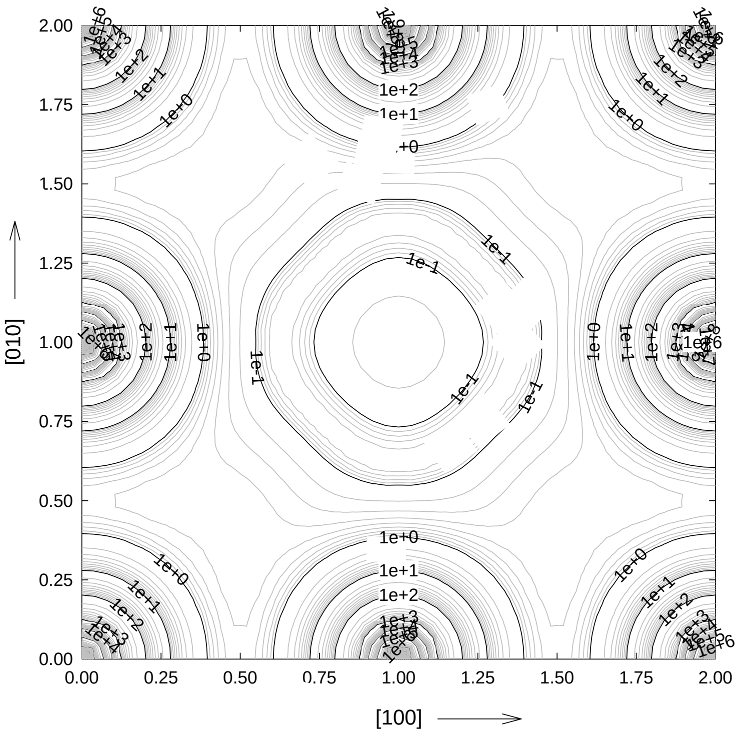


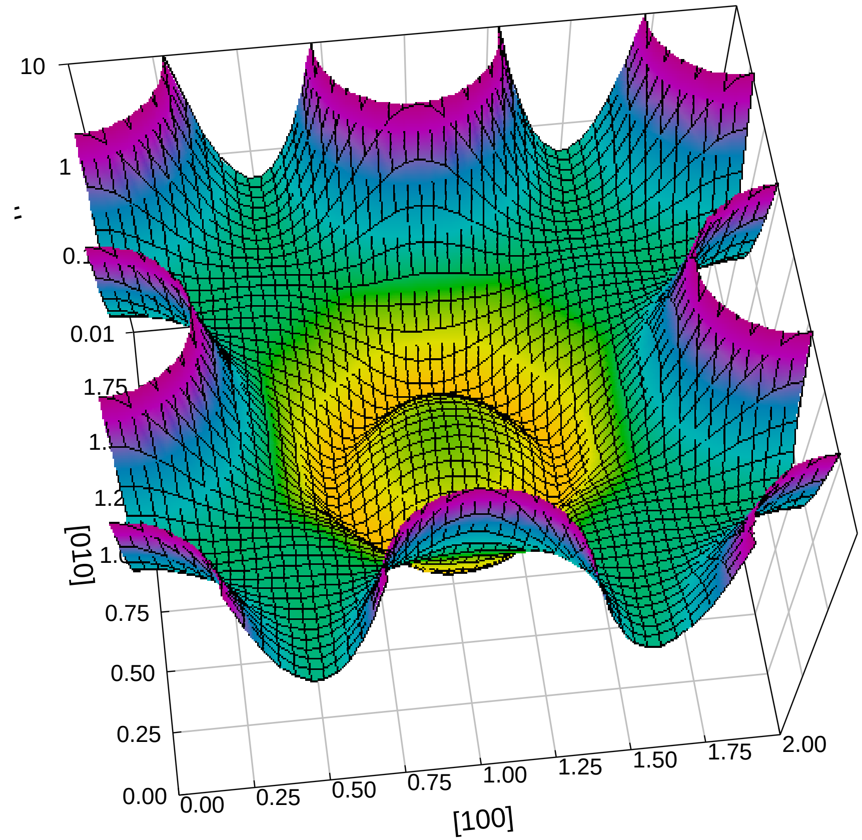


Hydrogen-induced vacancies

Effective medium theory
J. Nørskov, Phys. Rev. B ***26****, 2875 (1982)*

$\Delta E^{hom}(\mathbf{r})$ in (001) plane
vacancy in 1,1,0

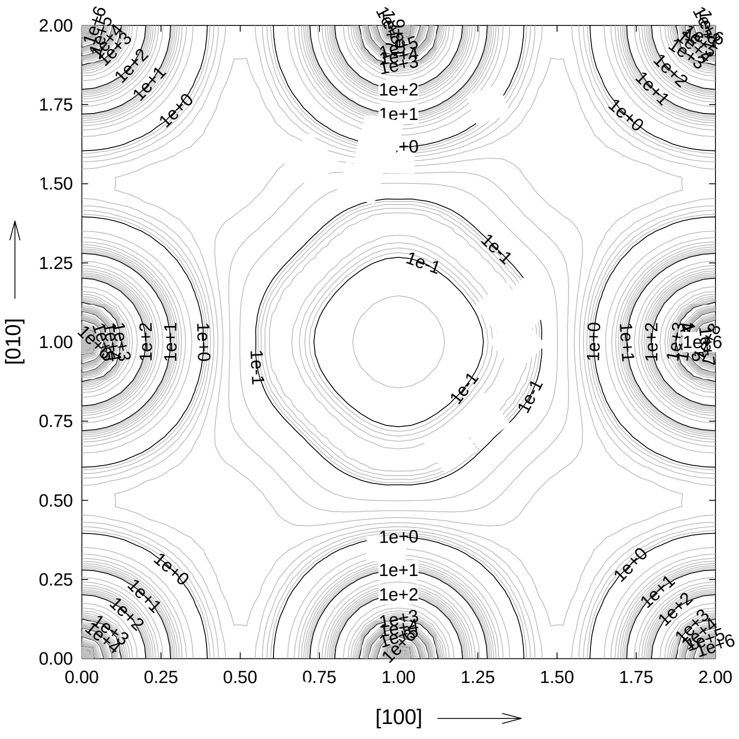


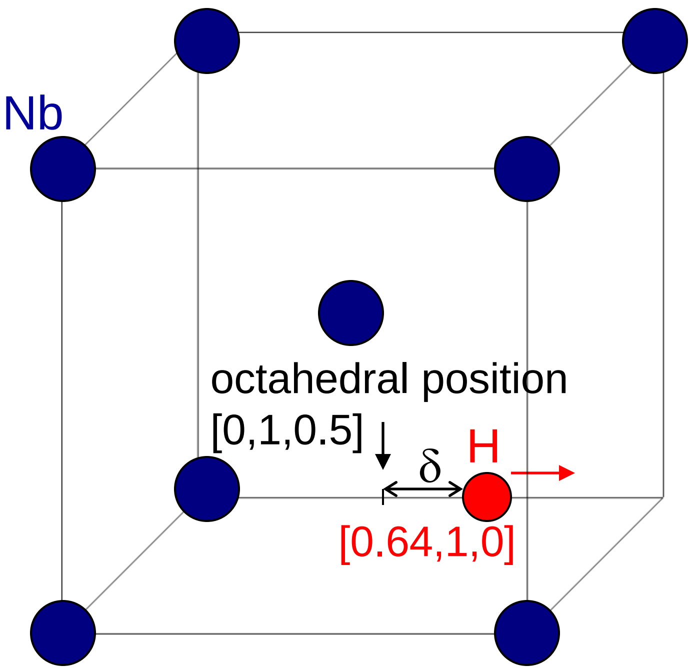


H positions: [0.64,1,0], [1,0.64,0], [1,1,0.36]
[1.36,1,0], [1,1.36,0], [1,1,-0.36]

Hydrogen-induced vacancies

Effective medium theory
Stott, Zaremba, Nørskov, Lang 1980

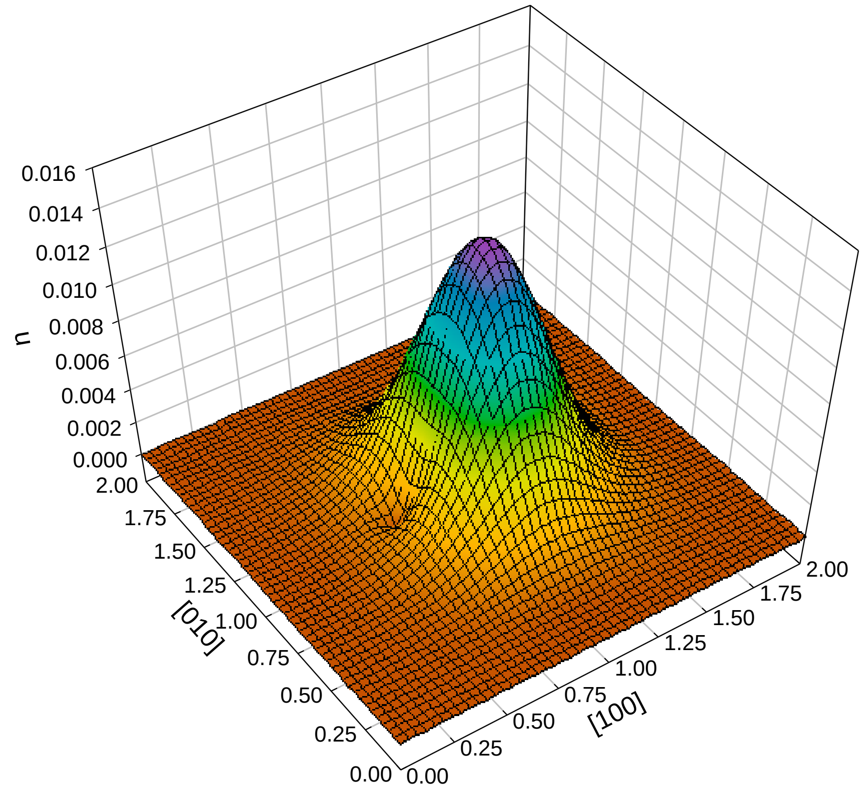


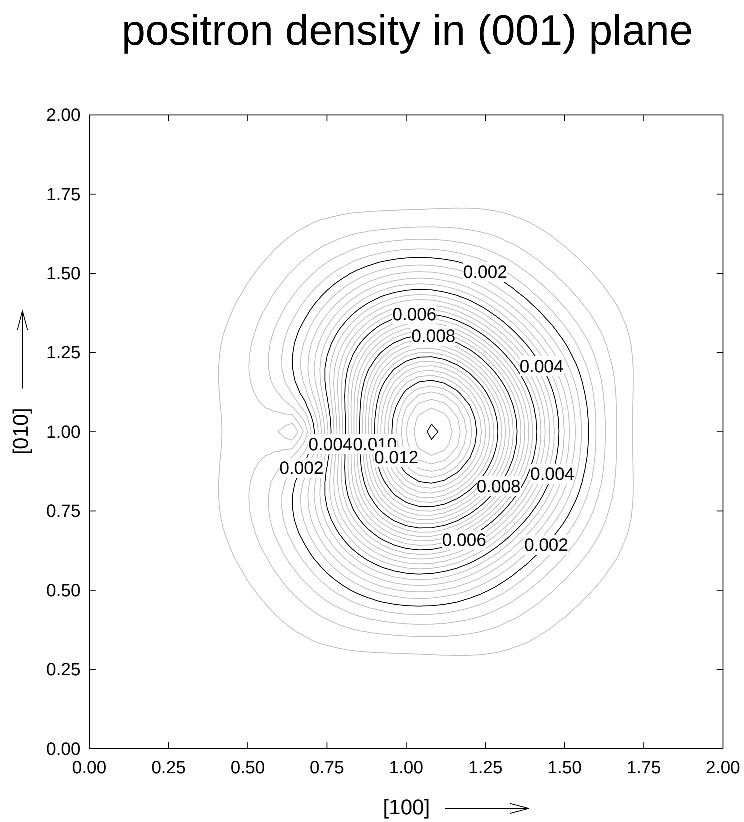


• displacement $\delta = 0.46(7)$ Å

H positions: [0.64,1,0], [1,0.64,0], [1,1,0.36]
[1.36,1,0], [1,1.36,0], [1,1,-0.36]

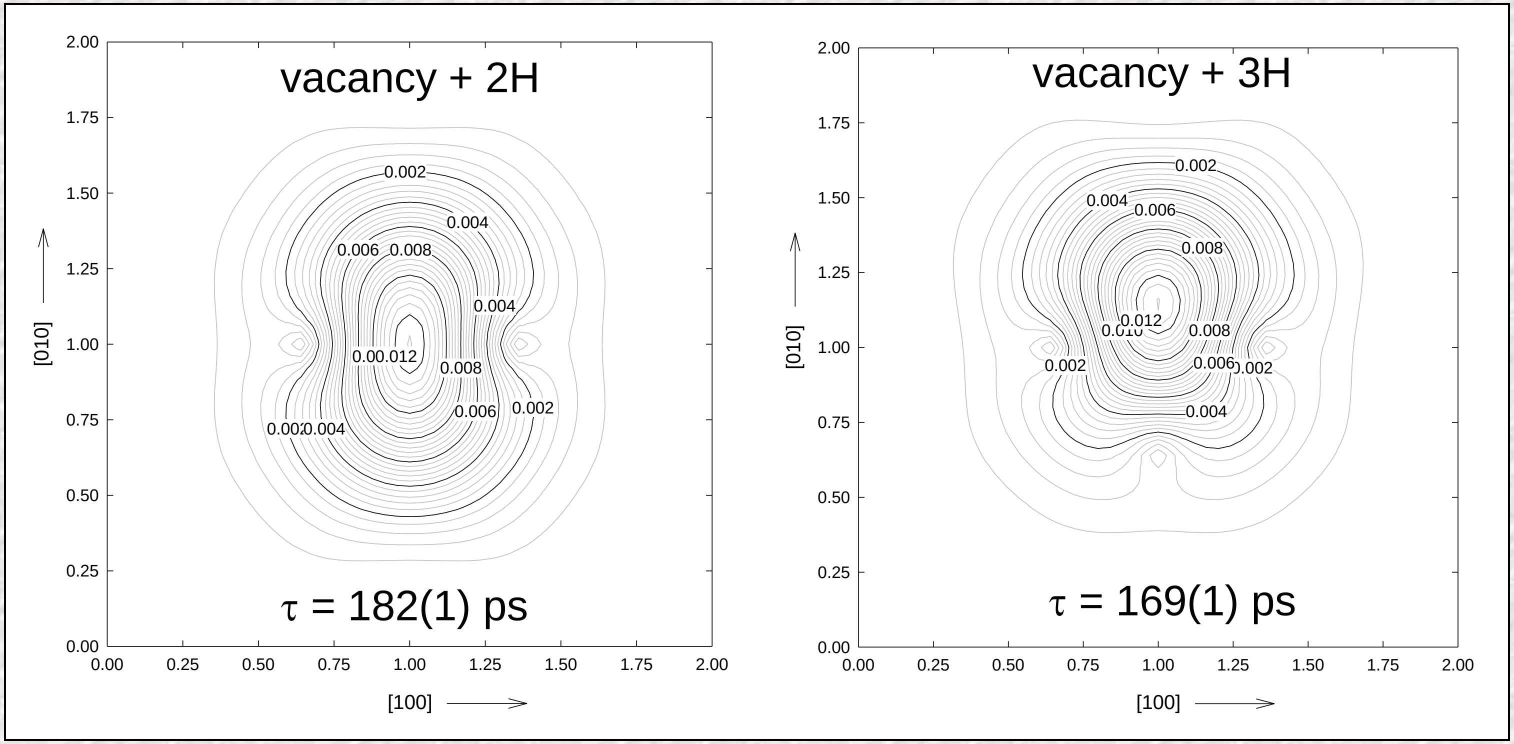
ATSUP calculations – Nb vacancy in [1,1,0] and H in [0.64,1,0]



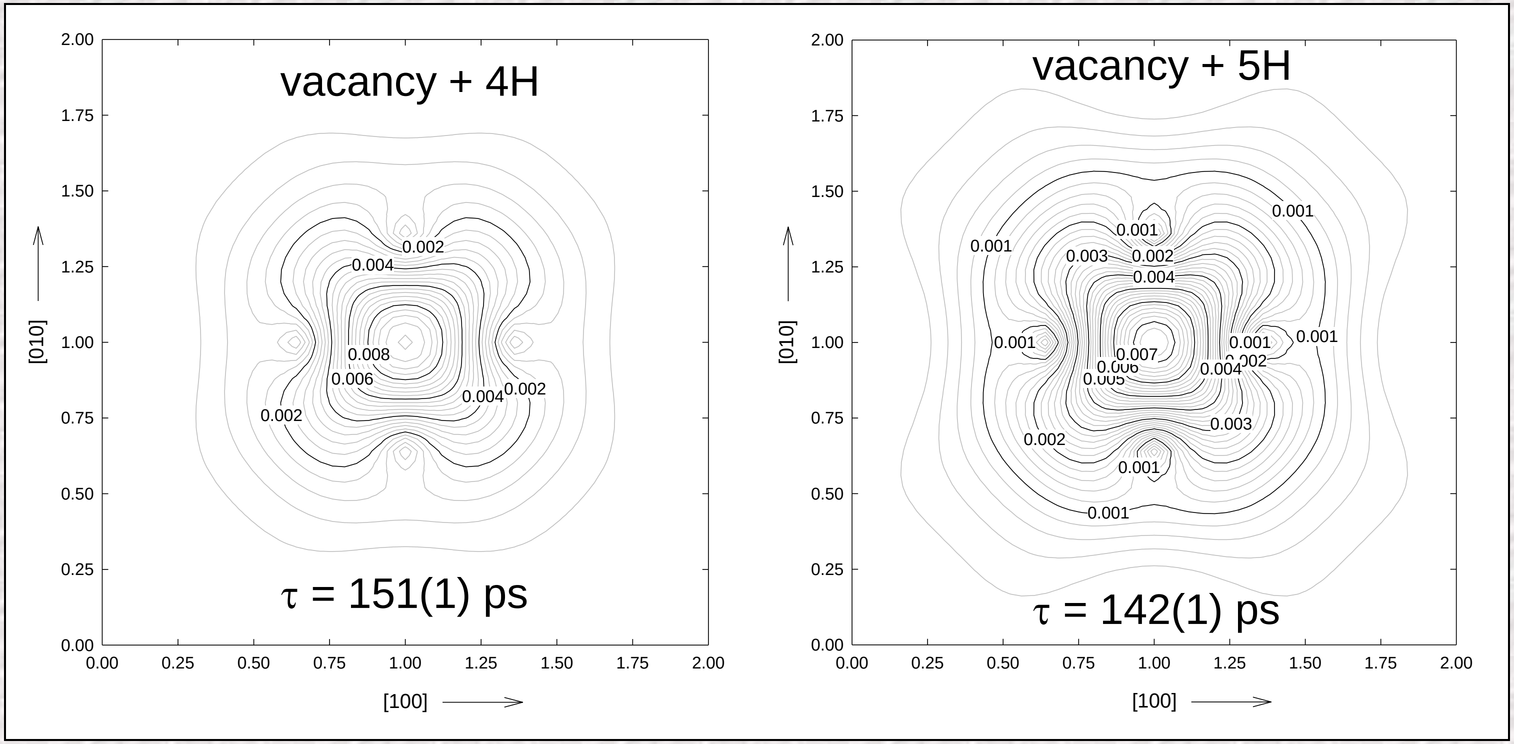


positron lifetime $\tau_{v\text{-}H}$ = 204(1) ps

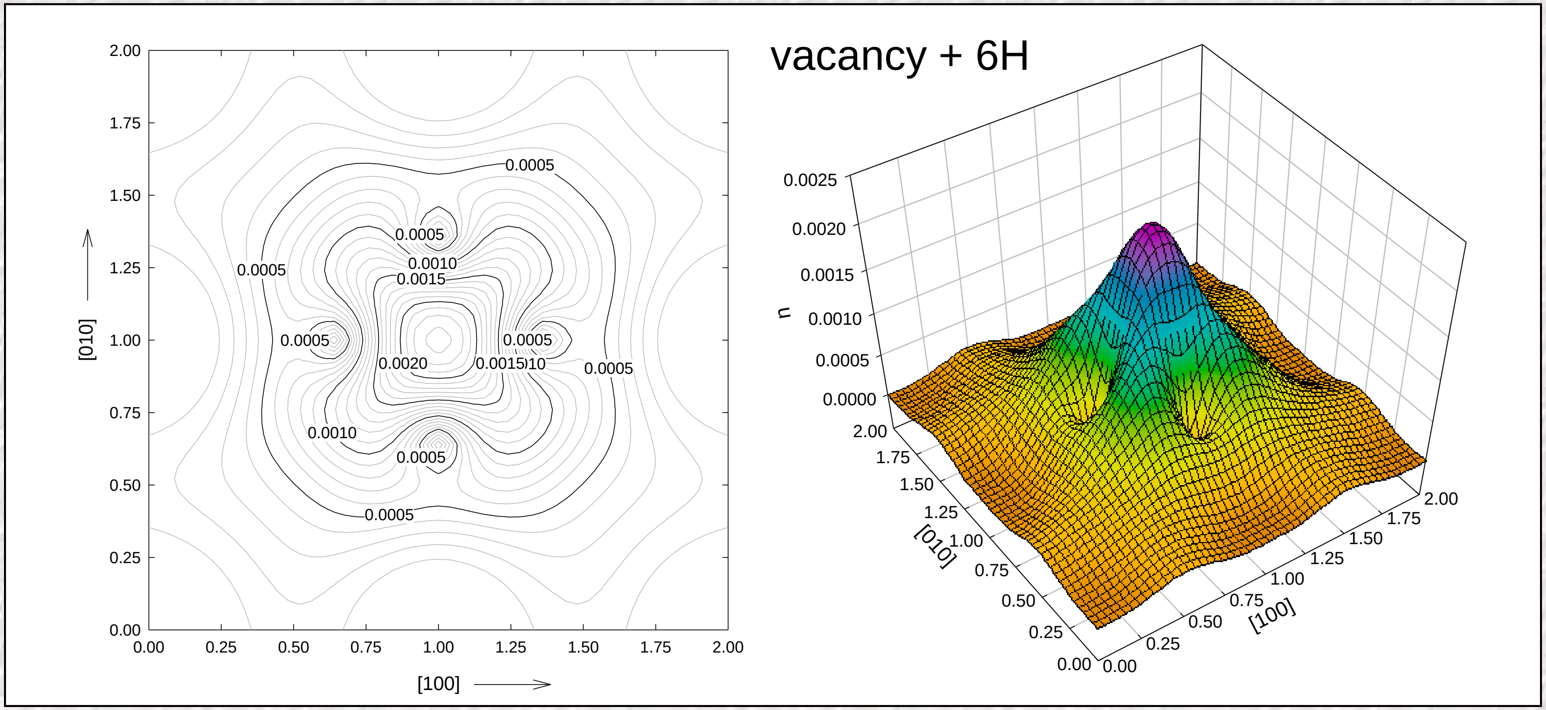
ATSUP calculations – complexes (vacancy – H)



ATSUP calculations – complexes (vacancy – H)



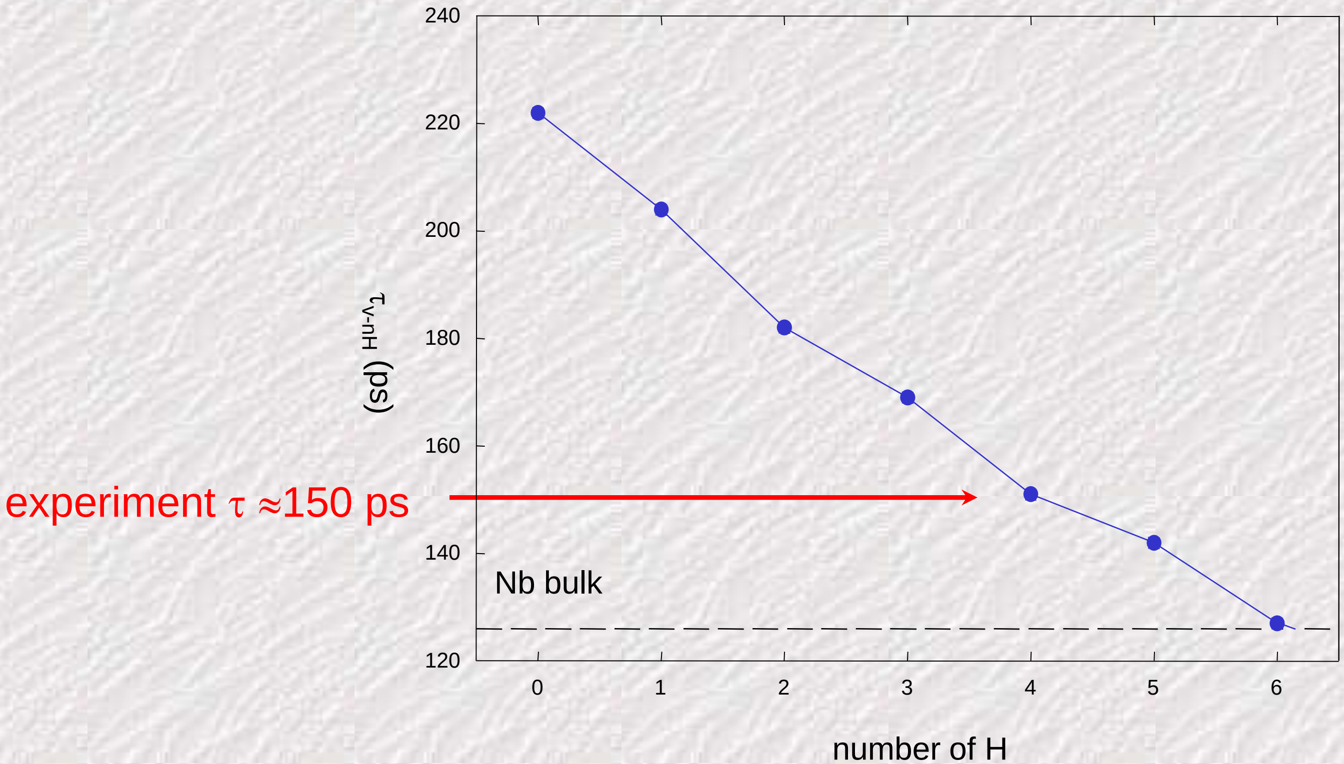
ATSUP calculations – complexes (vacancy – H)



τ = 127(1) ps

Hydrogen-induced vacancies

calculated positron lifetime for vacancy is surrounded by several H atoms



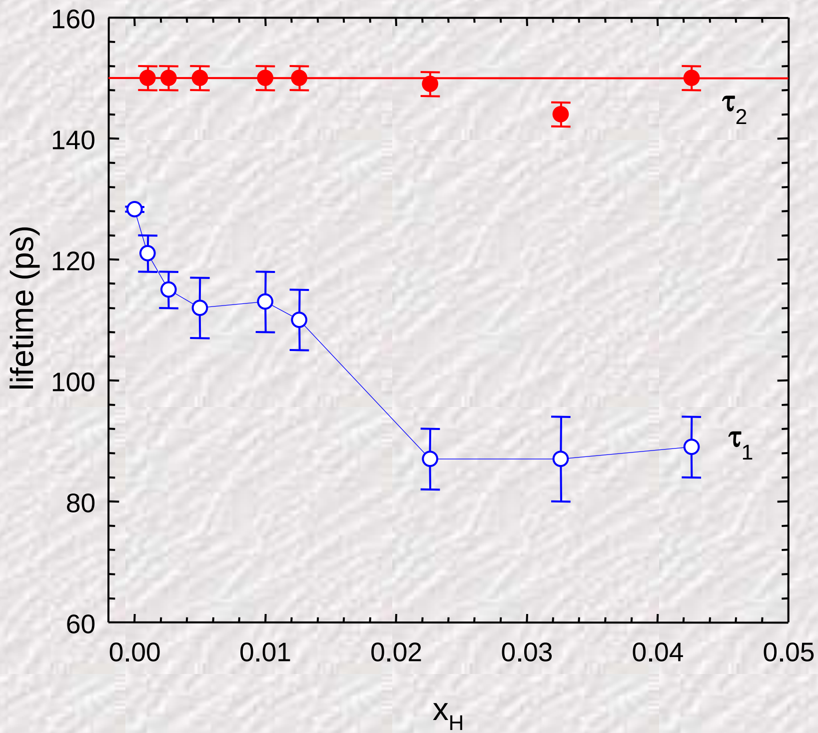
Hydrogen loading → creation of vacancies surrounded for 4 hydrogen atoms

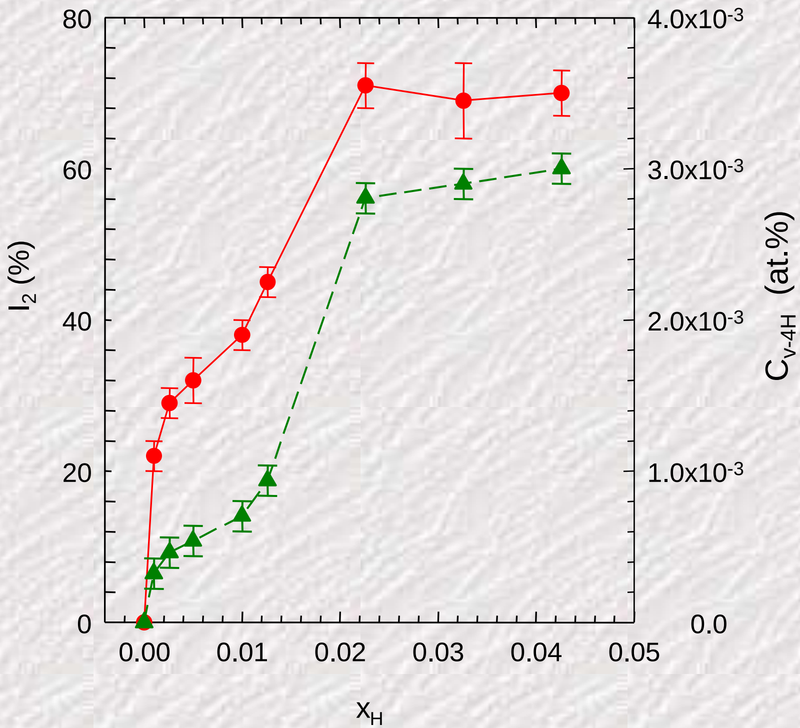
Hydrogen-induced vacancies

well annealed Nb (1000^{o}C / 1h) – hydrogen loading

- hydrogen induced defects τ_2 = (150 $\pm$ 0.5) ps
- hydrogen-induced volume expansion $\rightarrow$ elastic process $\rightarrow$ dislocations
- calculated lifetime for Nb vacancy (ATSUP): τ_V = (222 $\pm$ 1) ps
- vacancies surrounded by hydrogen $\rightarrow$ shortening of positron lifetime

$c_v \approx 3 \times 10^{-3}$ at.% $\Leftrightarrow$ T $\approx$ 1850^{o}C (0.8 Tm)





H-induced defects – bulk Nb – mechanism of formation

- effective medium theory: $E_b^{H-v} = 0.50\ \mathrm{eV}$
- vacancy formation energy: $E_f = 2.32\ \mathrm{eV}$

P. Korzhavyi et al. PRB 59, 11693 (1999)

- vacancy – 4H: $E_f - 4E_b^{H-v} = 0.32\ \mathrm{eV}$

equilibrium concentration of vacancy – 4H complexes:

$$c \approx p\, e^{S_k/k} e^{-\left(E_f - 4E_b^{H-v}\right)/kT}$$

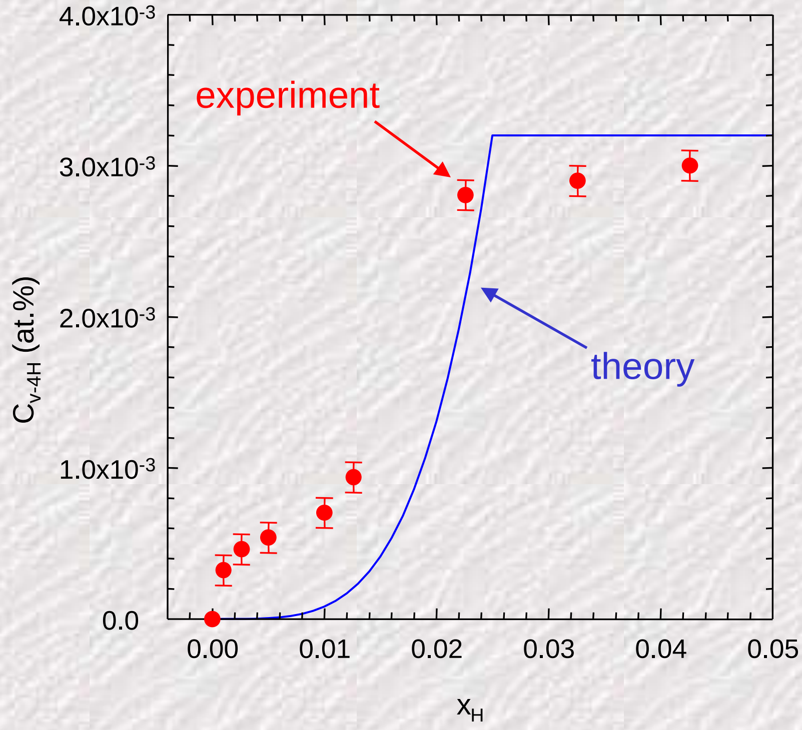
- 4 H in nearest neighbor positions required

$$p \sim c_H^4 \quad \rightarrow \quad c \approx 7\times10^{-9}\ \text{at.\%}$$

- 4 H in active volume V_0

$$V_0 = 2.9\ \mathrm{nm}^3 \quad \leftrightarrow \quad 80\ \text{unit cells of Nb}$$

*J. Čížek et al. PRB **69**, 224106 (2004)*



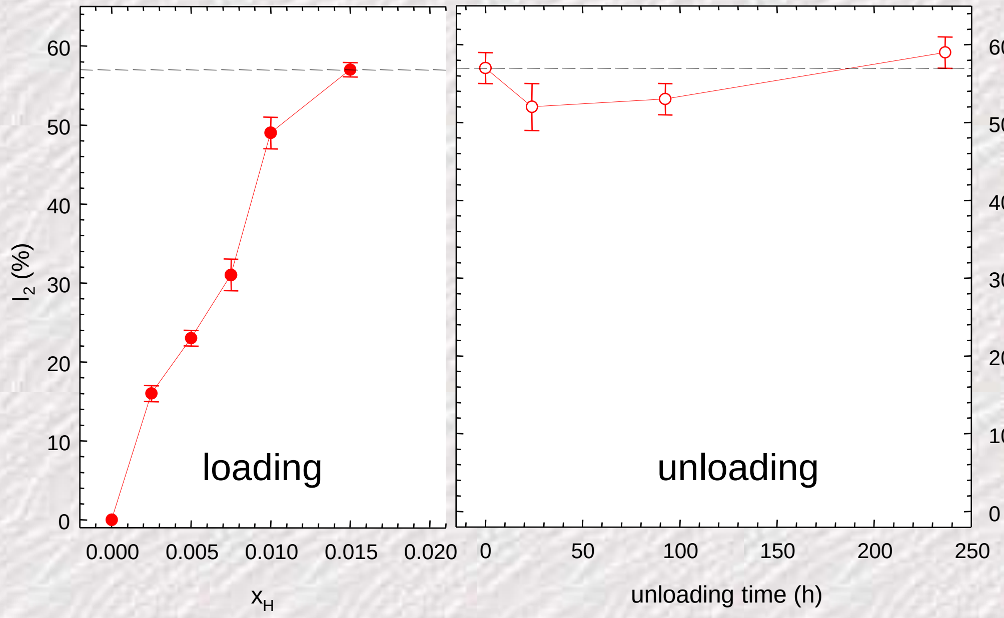
Hydrogen-induced vacancies

Loading – unloading experiment

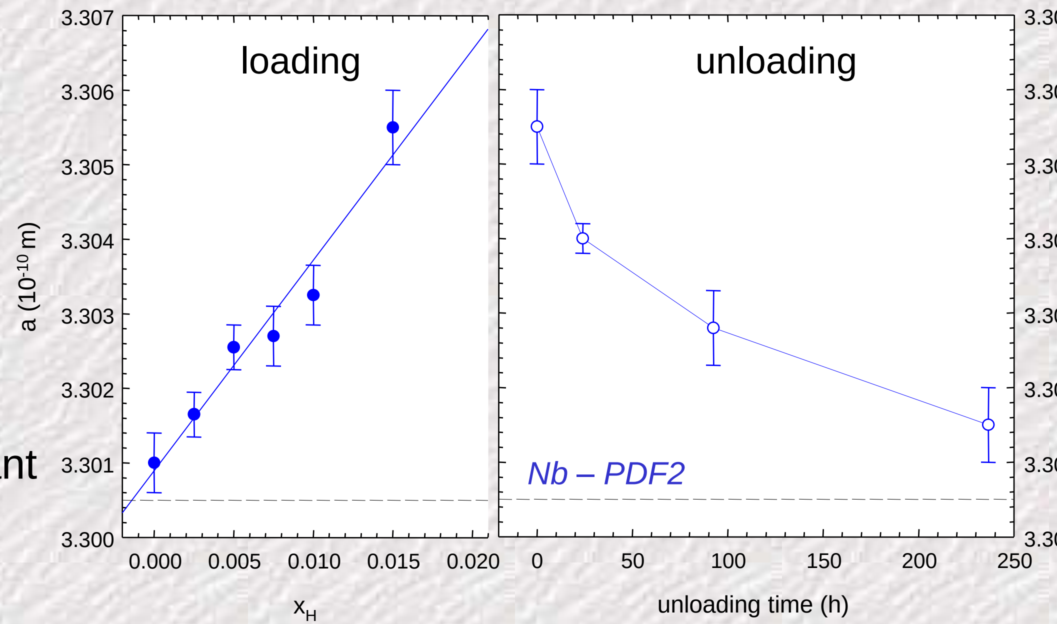
- loading: constant current 0.3 mA
- unloading: constant voltage 0.8 V

τ_2 = 150 ps

PL – intensity of trapped positrons



XRD – lattice constant



Electron irradiated bulk Nb

sample 1

- bare Nb electron irradiated (10 MeV e^-, F = 2×10^{21} m^{-2}, $T_{irr} \leq 100^oC$)
- Pd cap sputtered after irradiation

sample 2

- Nb with Pd cap electron irradiated (10 MeV e^-, F = 2×10^{21} m^{-2}, $T_{irr} \leq 100^oC$)

Sample	τ_1 (ps)	I_1 (%)	τ_2 (ps)	I_2 (%)
bare Nb electron irradiated	47 ± 6	15 ± 1	190.6 ± 0.5	85 ± 1
…. + Pd cap	47 ± 9	15 ± 2	190.0 ± 0.8	85 ± 2
Nb electron irradiated with Pd cap	57 ± 7	17.0 ± 0.8	185.8 ± 0.8	83.0 ± 0.8

vacancy-H complexes

- mixture of v-H ($\tau_{v\text{-}H}$ = 204 ps) and v-2H ($\tau_{v\text{-}2H}$ = 182 ps) complexes

Electron irradiated bulk Nb

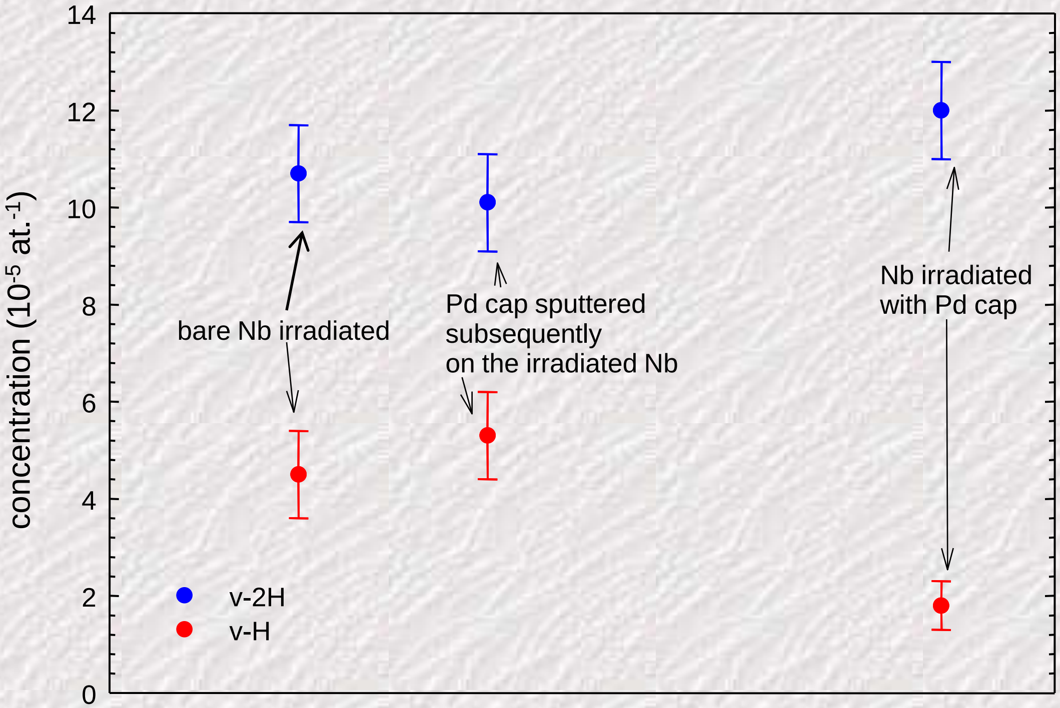
3-component fit

Sample	τ_1 (ps)	I_1 (%)	τ_2 (ps)	I_2 (%)	τ_3 (ps)	I_3 (%)
bare Nb electron irradiated	43 ± 8	14 ± 2	182 Fix	61 ± 2	204 Fix	25 ± 3
…. + Pd cap	44 ± 9	14 ± 2	182 Fix	57 ± 2	204 Fix	29 ± 4
Nb electron irradiated with Pd cap	48 ± 5	15 ± 2	182 Fix	74 ± 1	204 Fix	11 ± 3

v-2H complexes (τ_2, I_2)   v-H complexes (τ_3, I_3)

Electron irradiated bulk Nb

application of 3-state trapping model
(trapping coefficient: $\nu = 1 \times 10^{14}$ at. s^{-1})

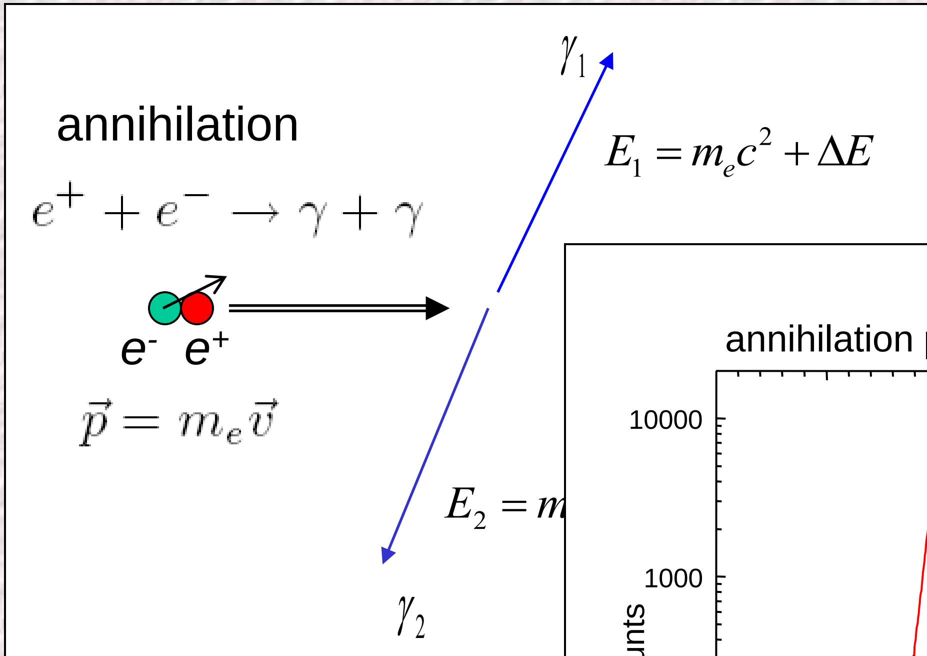


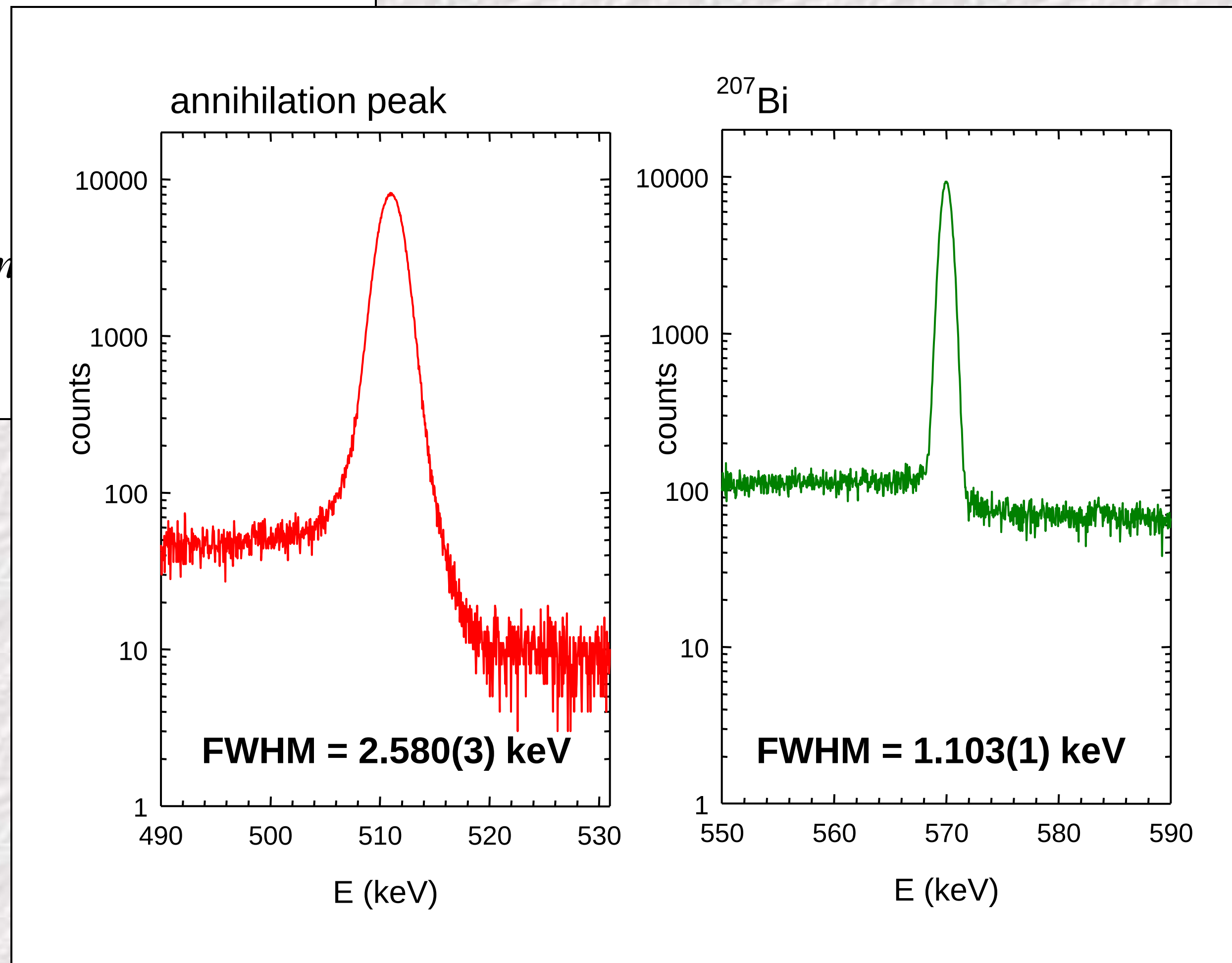
catalytic effect of Pd cap

⇓

v-H transforms into v-2H

Doppler Broadening

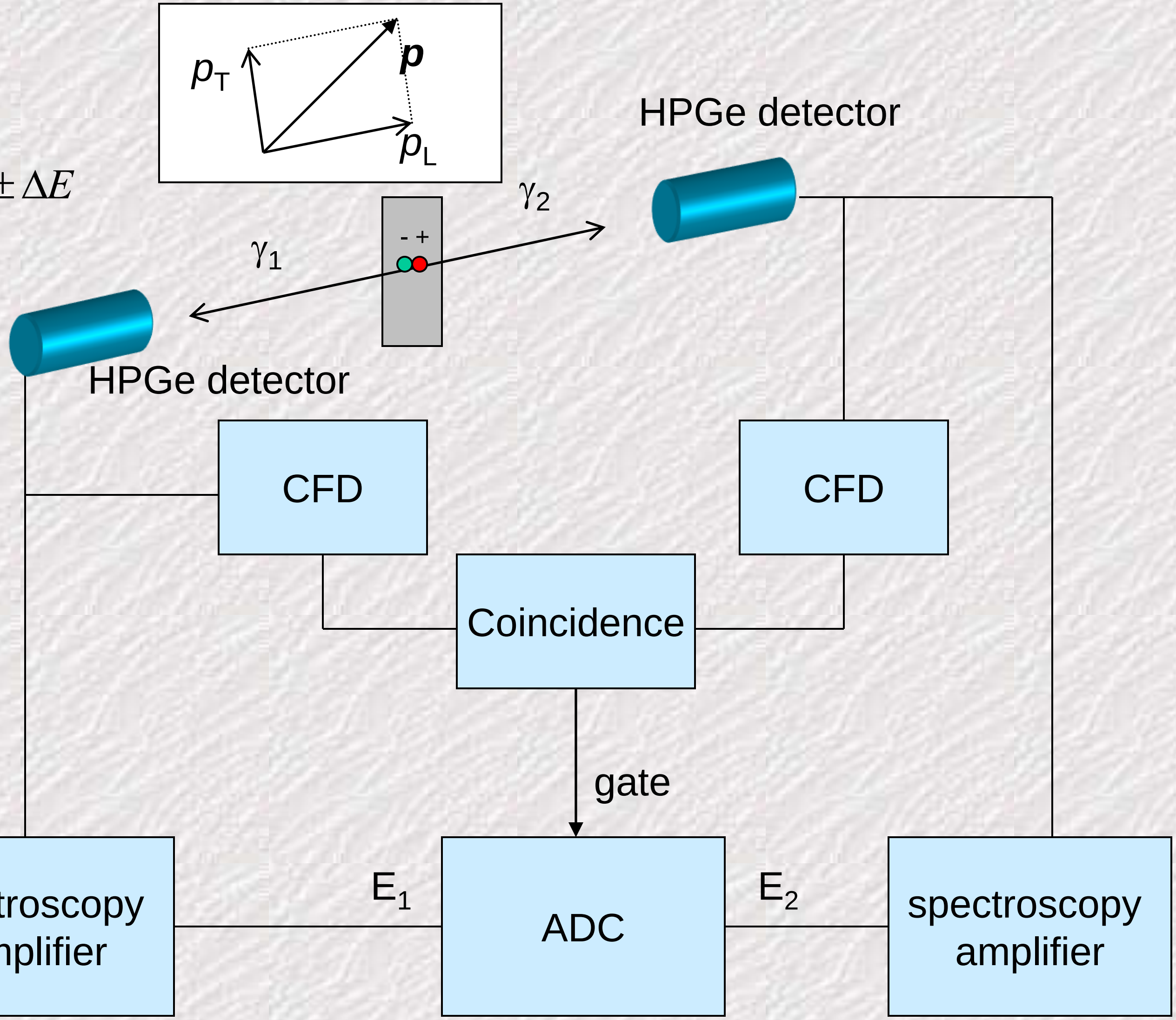




Coincidence Doppler Broadening spectroscopy (CDB)

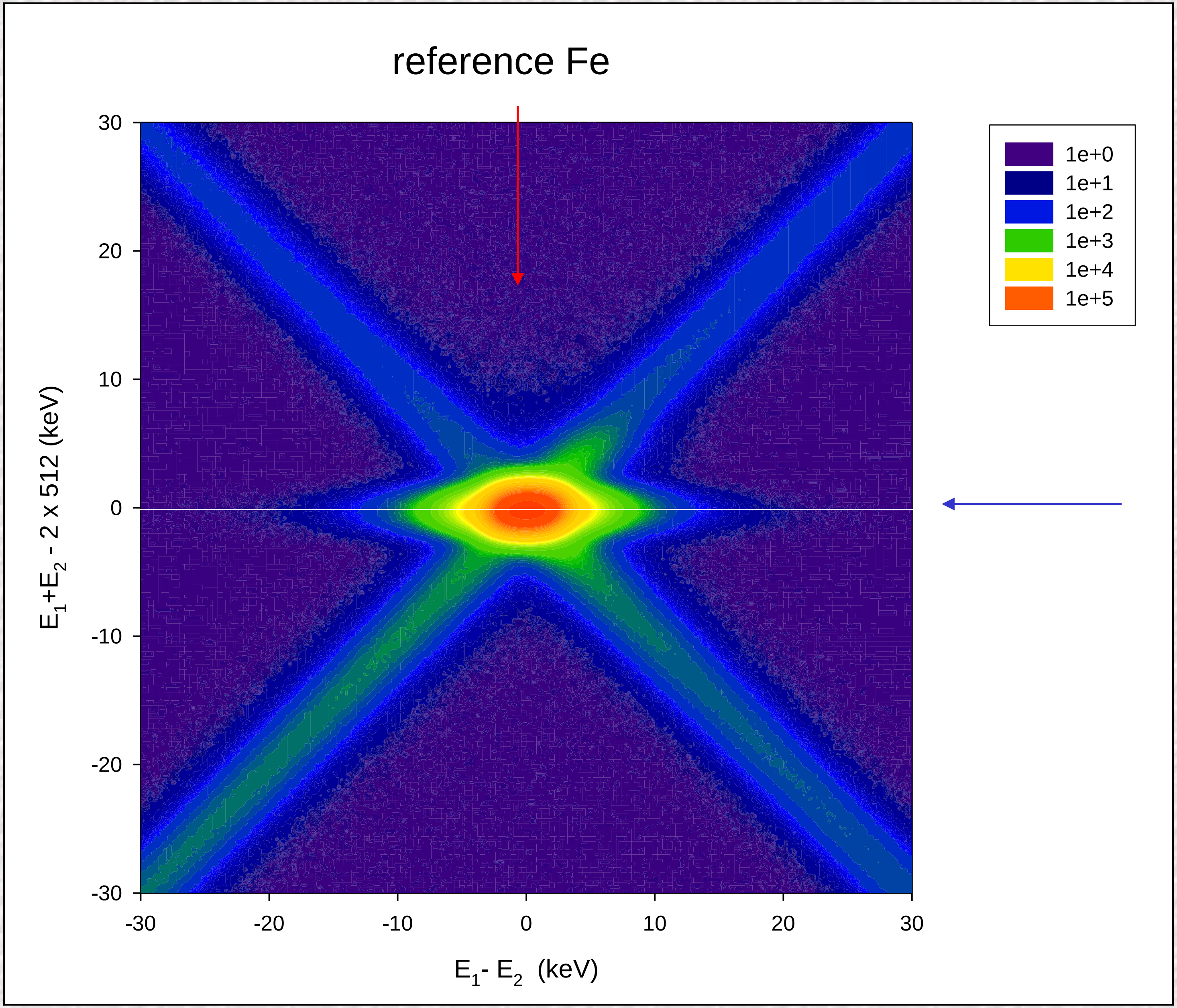
$$E_1 = m_e c^2 \pm \Delta E$$

$$\Delta E = \frac{c p_L}{2}$$

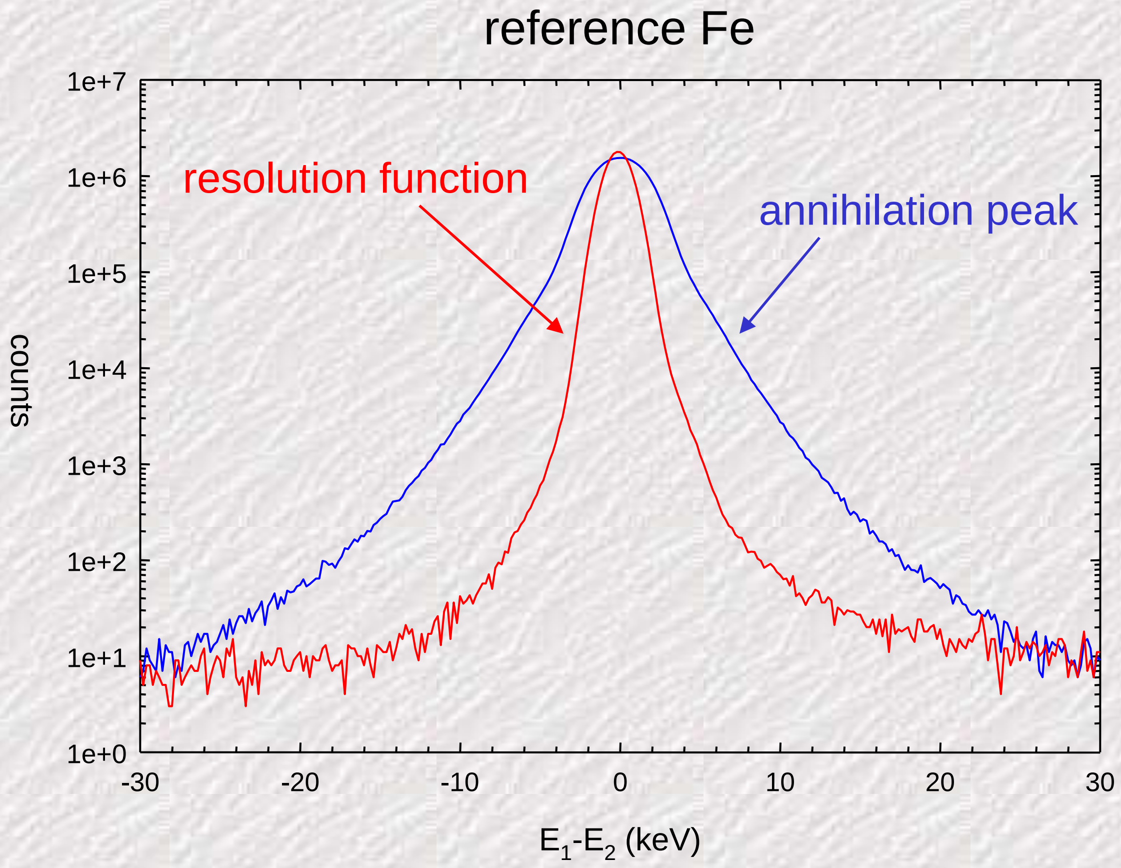


$$E_1 - E_2 = 2\Delta E = c p_L$$

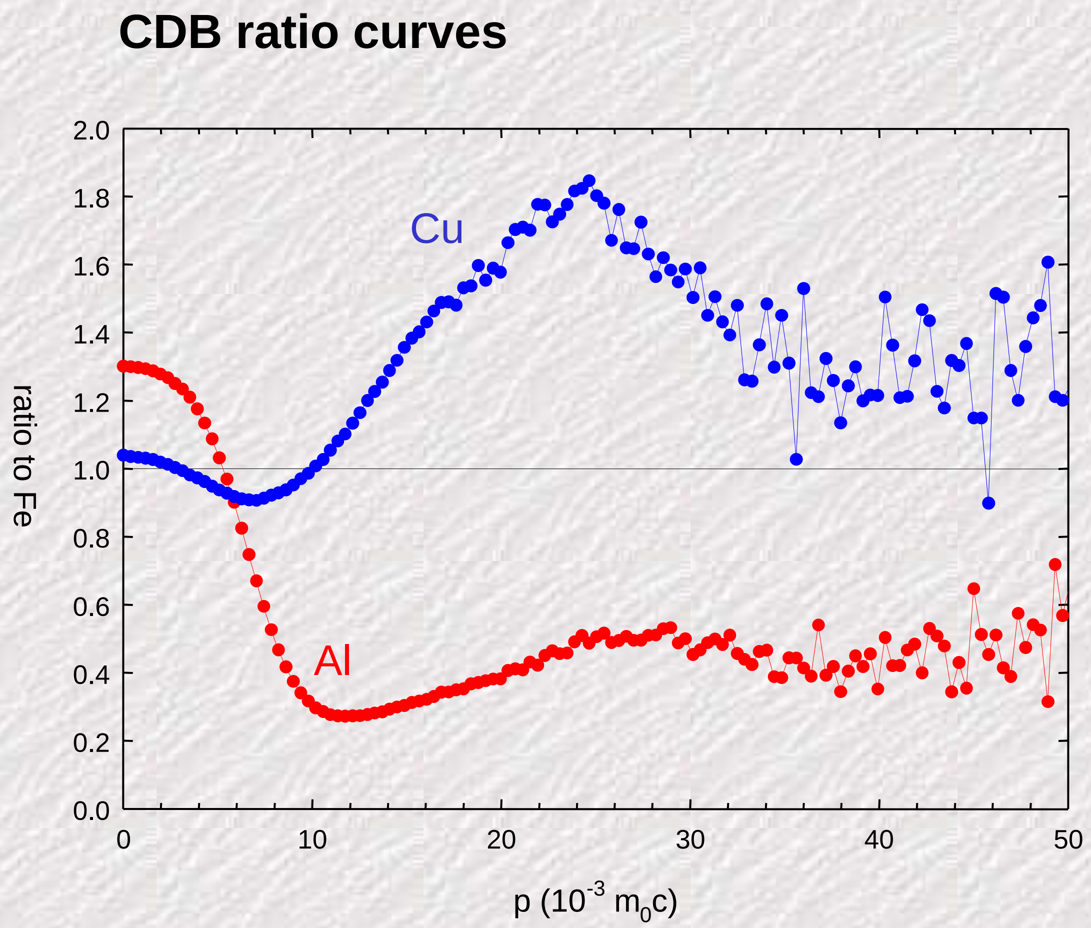
Coincidence Doppler Broadening spectroscopy (CDB)



Coincidence Doppler Broadening spectroscopy (CDB)



Coincidence Doppler Broadening spectroscopy (CDB)



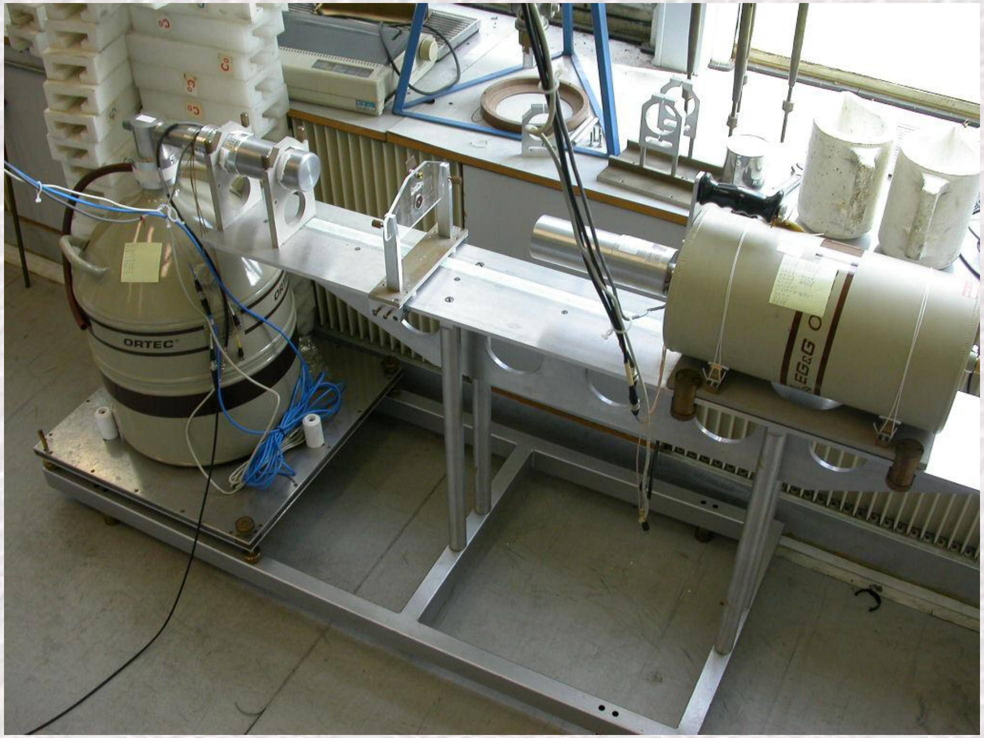
element sensitivity

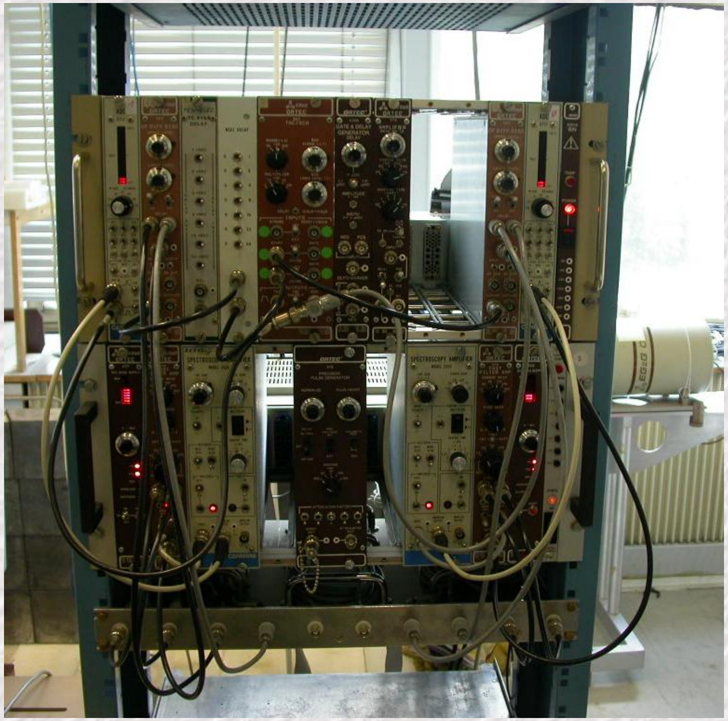
Coincidence Doppler Broadening spectroscopy (CDB)

Chemical environment of defects → CDB measurements

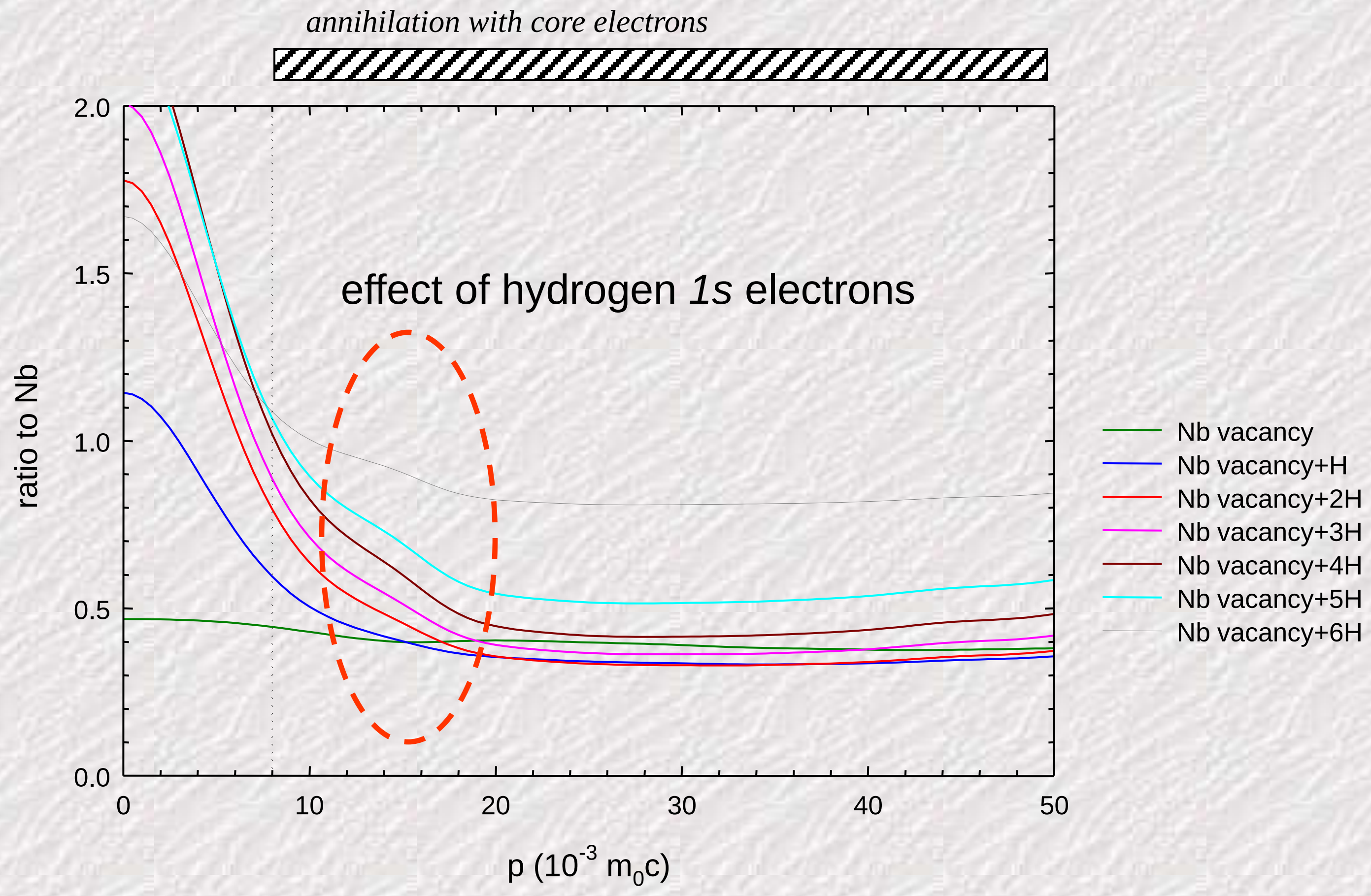
- two HPGe detectors
- energy resolution 1.05 keV (FWHM, E = 512 keV)
- coincidence count rate 550 s^{-1}
- 10^8 counts in spectrum

J. Čížek et al., Mat. Sci. Forum. ***445-446****, 63 (2004)*

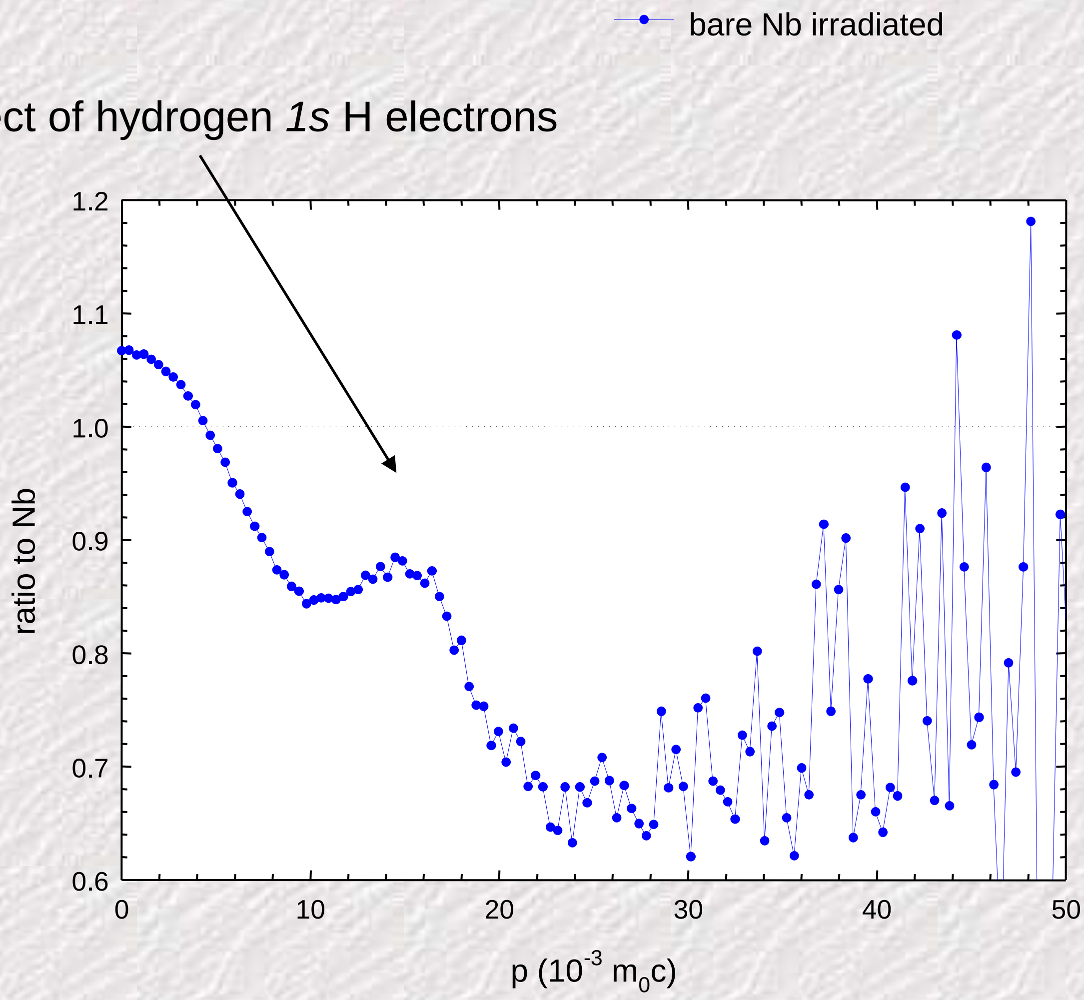




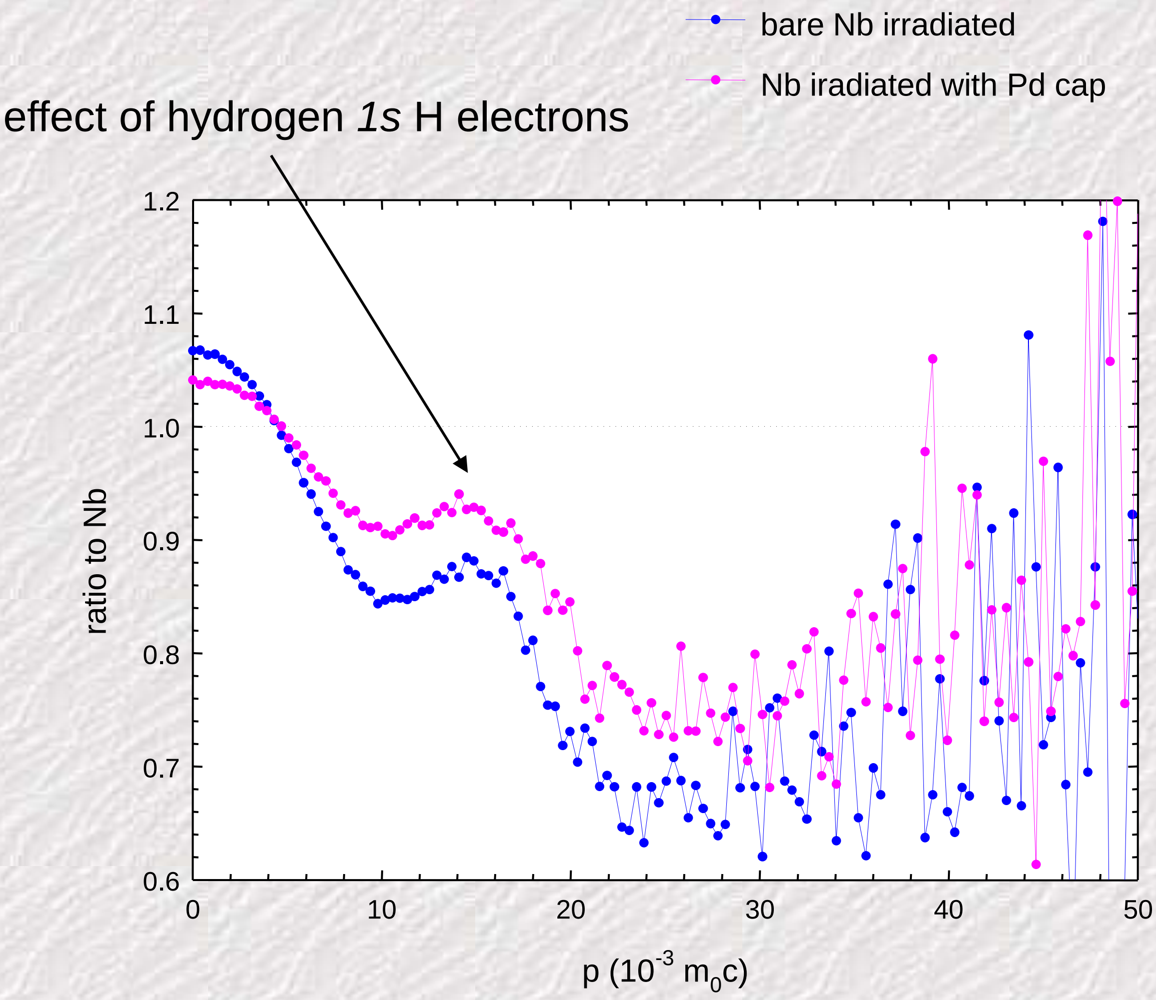
Vacancy-H complexes – calculated HMP's



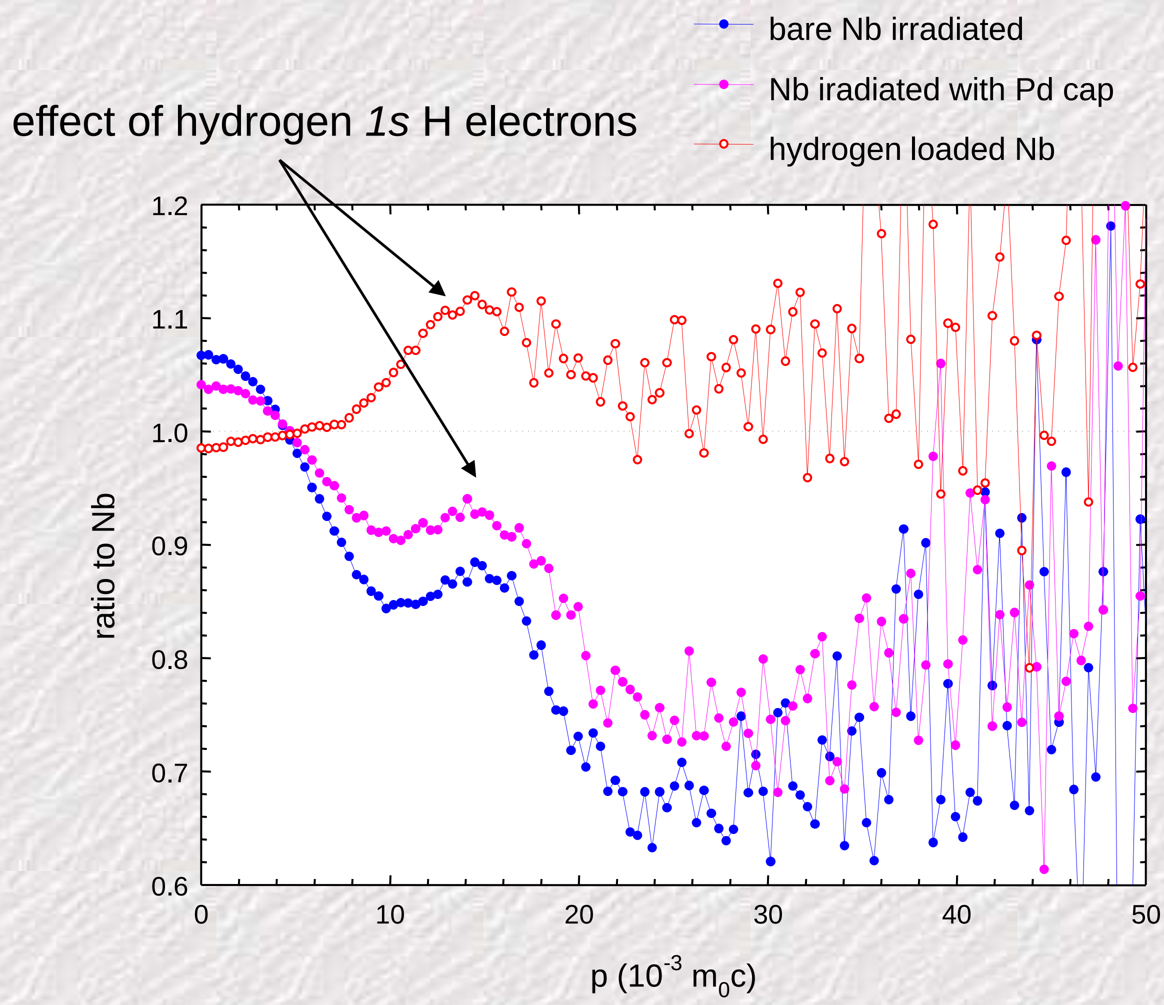
Electron irradiated Nb – experimental high momentum profiles



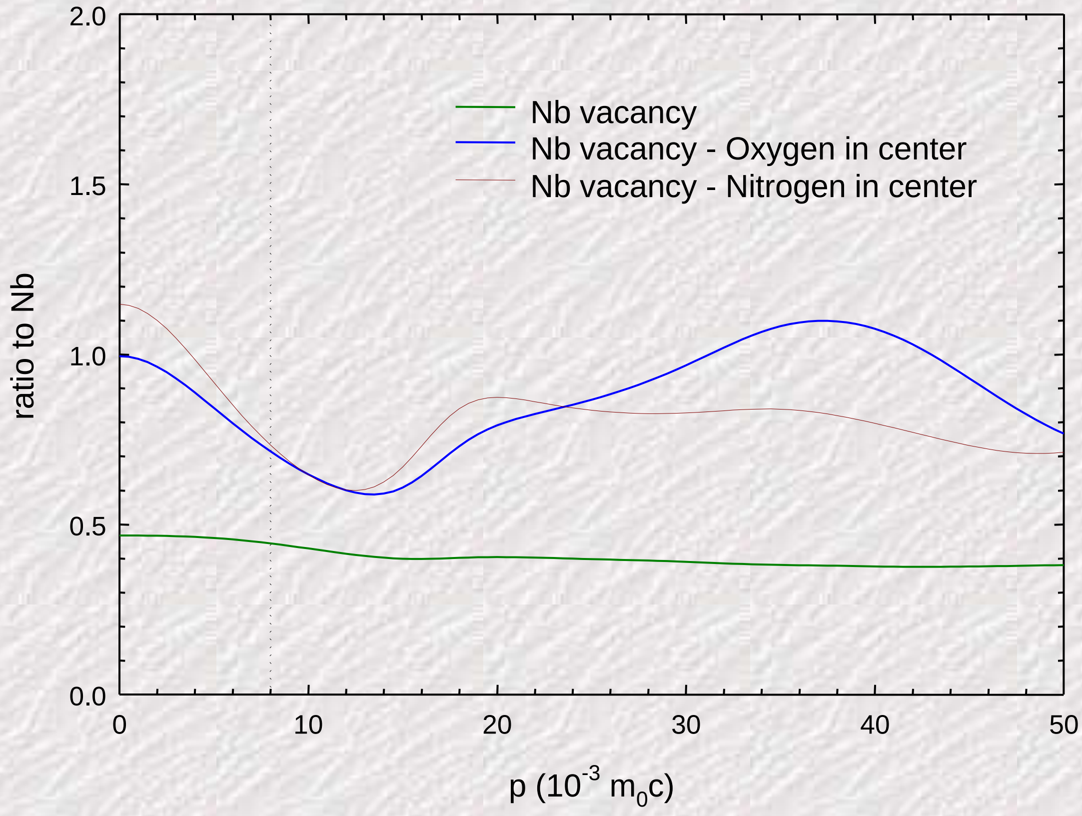
Electron irradiated Nb – experimental high momentum profiles



Electron irradiated Nb – experimental high momentum profiles



Other gas impurities – calculated HMP's



Další informace o anihilaci pozitronů

- přednáška anihilace pozitronů v pevných látkách NFPL 103

https://physics.mff.cuni.cz/kfnt/vyuka/anihilace/index.html

Anihilace pozitronů v pevných látkách

NFPL103, ZS 2020

Jakub Čížek

V zimním semestru 2020 probíhá přednáška distanční formou

Studijní literatura:

- P. Hautojärvi: Positrons in Solids
- M.J. Puska, R.M. Nieminen: Theory of positrons in solids and on solid surfaces Rev. Mod. Phys. 66 (1994) 841-897
- P.J. Schultz, K.G. Lynn: Interaction of positron beams with surfaces, thin films, and interfaces Rev. Mod. Phys. 60 (1988) 701-779

- **1. přednáška** , *základní charakteristiky pozitronu, zdroje pozitronů*
  - **prezentace**
  - **videozáznam přednášky**
  - **videozáznam on-line diskuze**
- **2. přednáška** , *dozimetrické jednotky, interakce pozitronů s pevnou látkou*
  - **prezentace**
  - **videozáznam přednášky**
  - **videozáznam on-line diskuze**
- **3. přednáška** , *termalizace pozitronu, anihilace pozitronu, pozorovatelné*
  - **prezentace**
  - **videozáznam přednášky**

Další informace o anihilaci pozitronů

- Den s experimentální fyzikou 2020

  https://www.youtube.com/watch?v=_Jp-_eg1uAs

  (nejdřív přednáška o atmosféře, pak nanomateriály, experiment COMPASS a potom anihilace pozitronů)