Positron annihilation spectroscopy in material research

Dzelepov Laboratory of Nuclear Problems
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Introduction

Aim of the project:

Determine the type and concentration of structural defects induced in different samples by sandblasting and pressing, using positron annihilation spectroscopy (PAS).

β^+ decay

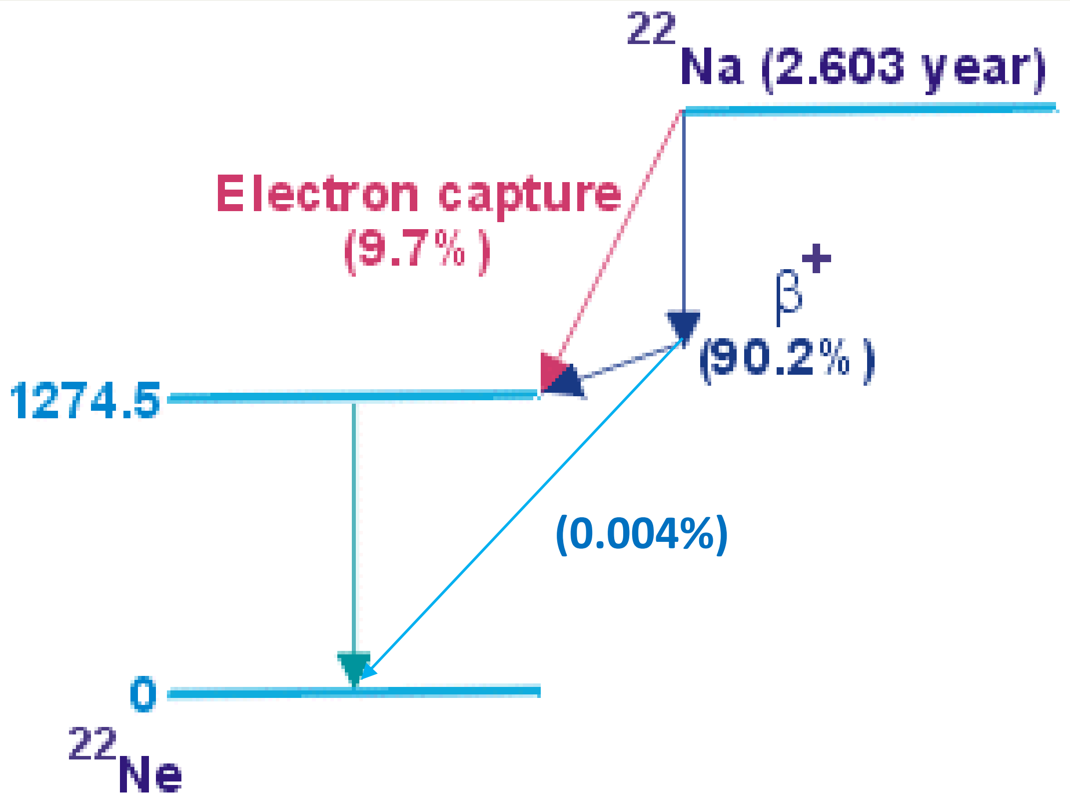


Fig. 1. β^+ decay schema

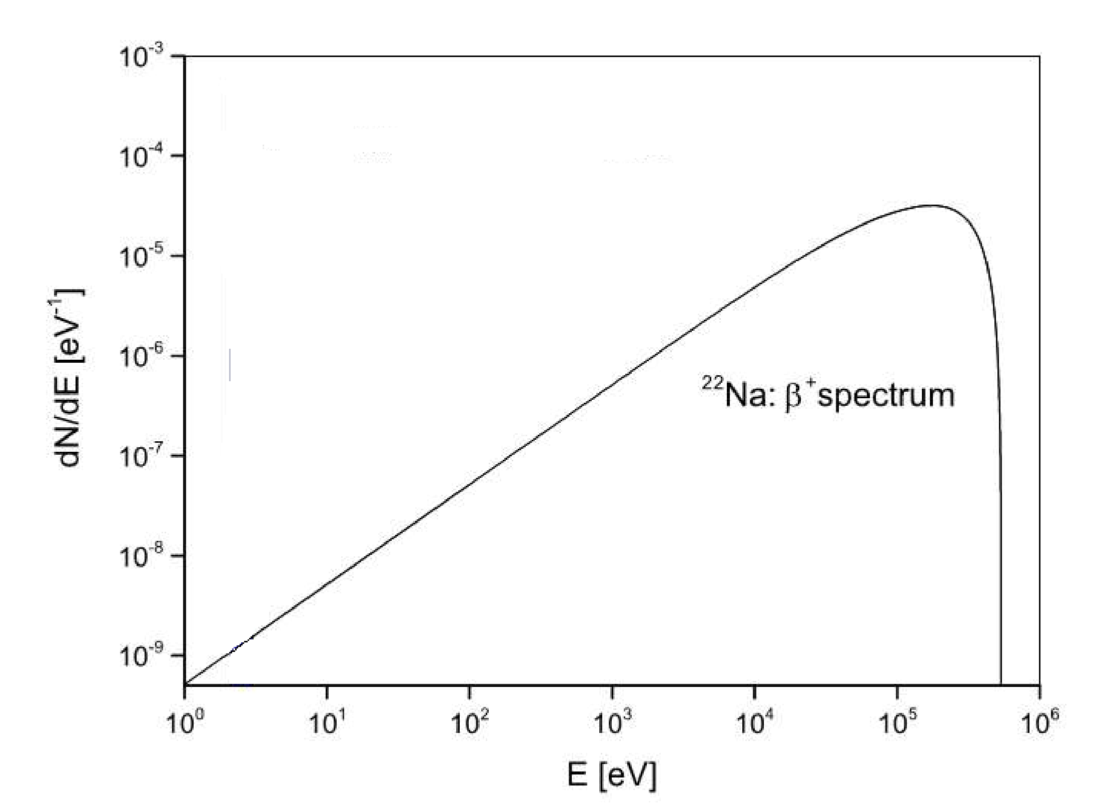


Fig. 2. Energy spectrum of positrons emitted from ^{22}Na

Interaction with matter and annihilation

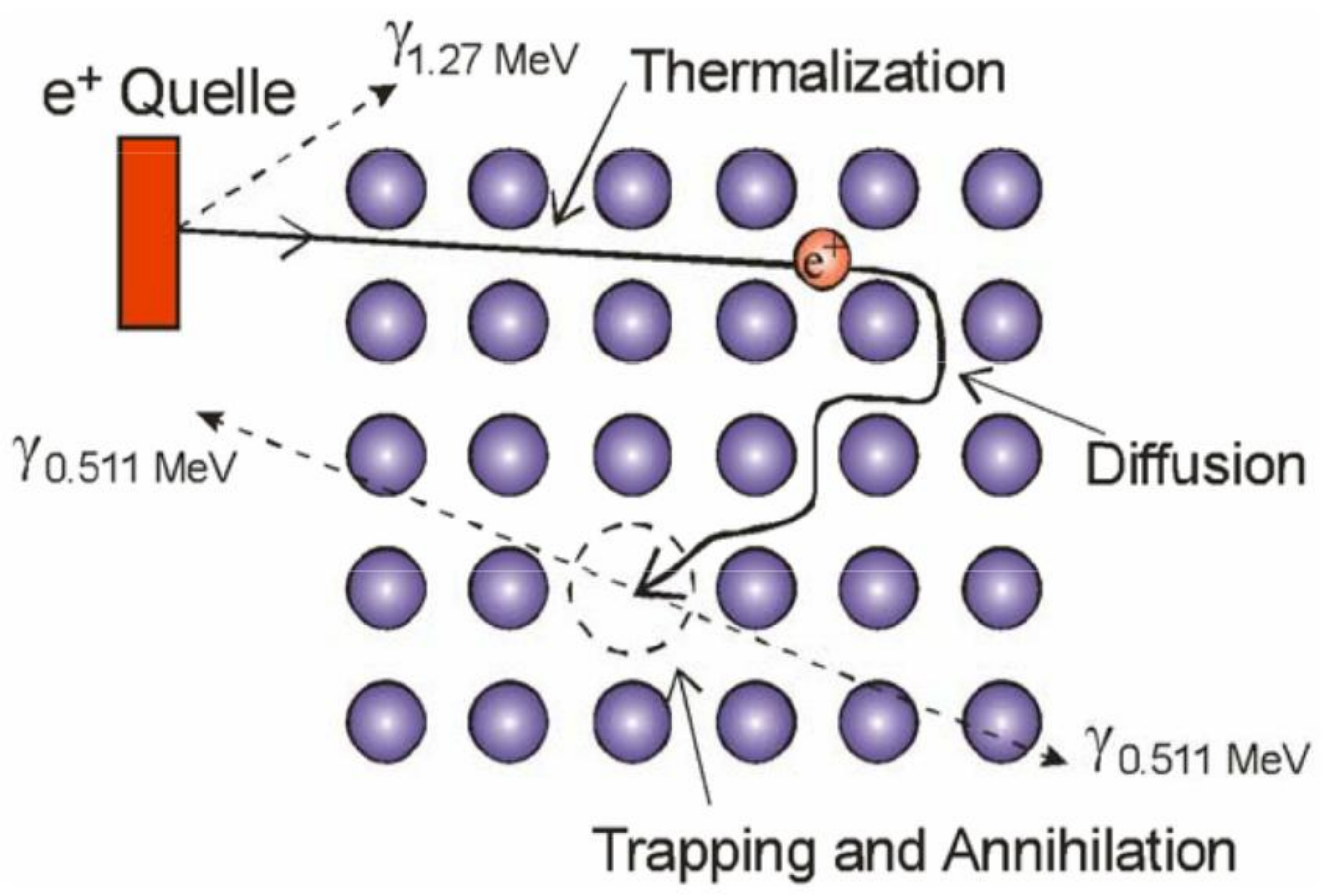
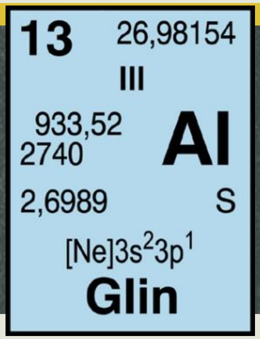


Fig. 3. Positron movement in the metal structure

Interaction processes:

- Elastic scattering
- Inelastic scattering
- Ionizations
- Bremsstrahlung

Aluminium Crystalline Structure (^{27}Al)



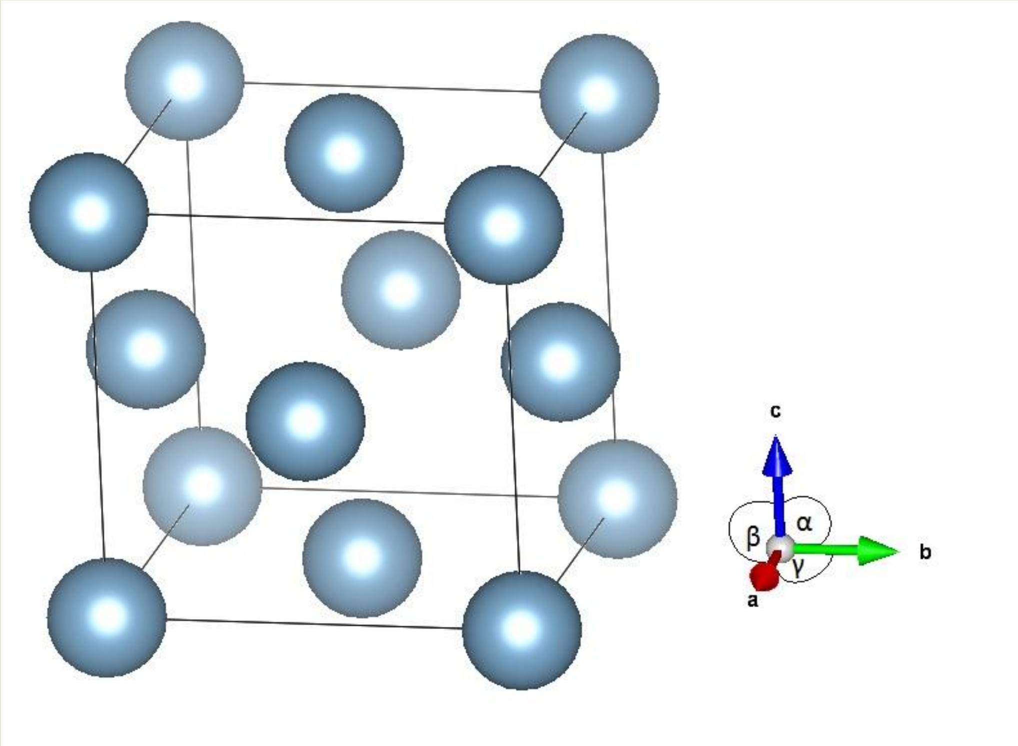


Fig. 4. Aluminium crystalline structure

Coordination numer: **12**
Space group: **Fm-3m**
Space group number: **225**
Structure: **fcc, cubic close-packed**
Cell parameters:

- *a*: 404.95 pm
- *b*: 404.95 pm
- *c*: 404.95 pm
- α: 90.000°
- β: 90.000°
- γ: 90.000°

Examples of vacancies in Aluminium

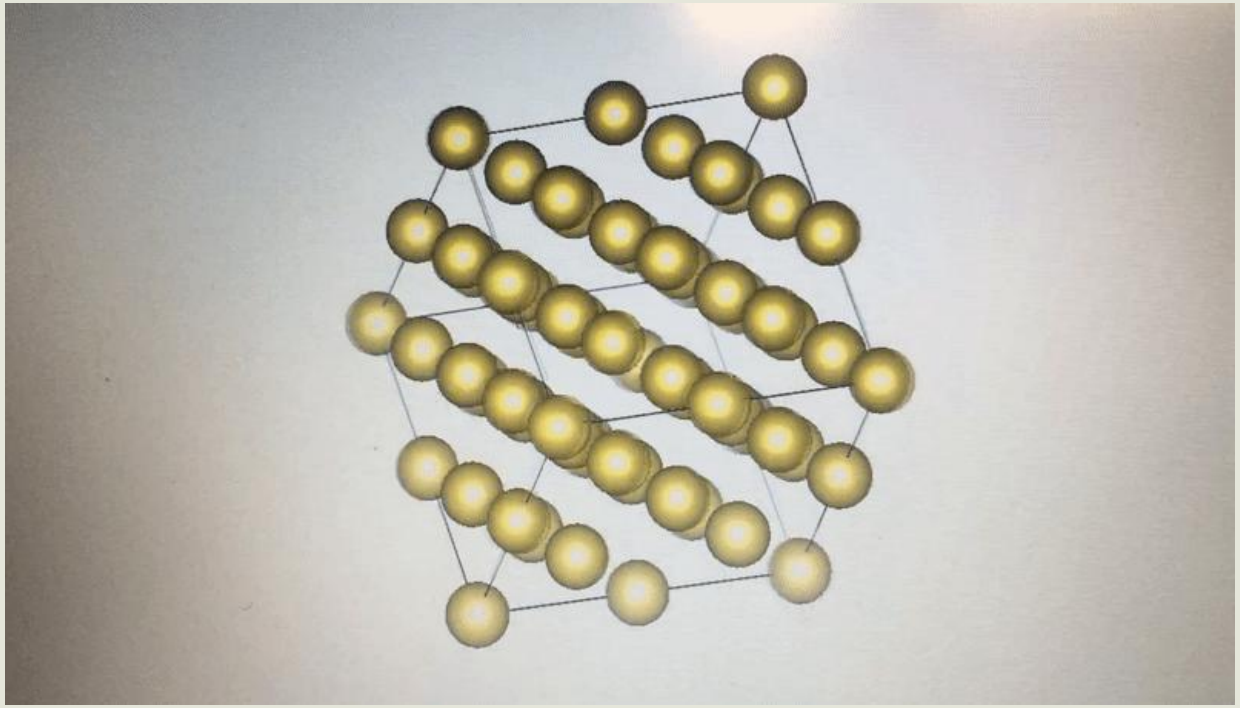


Fig. 5. Crystalline structure Al with one vacancy

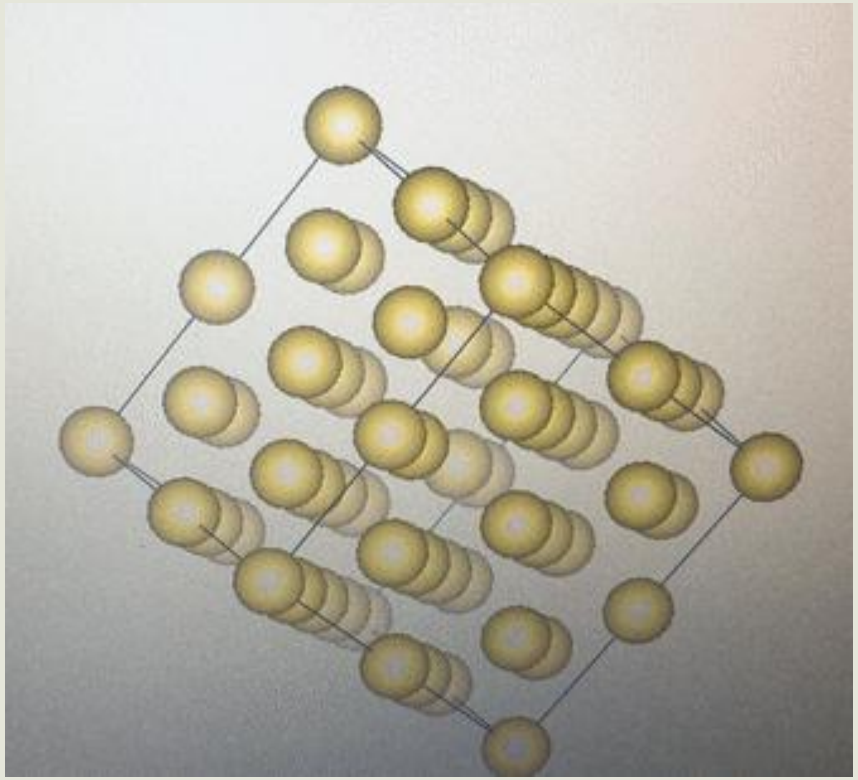


Fig. 6. Crystalline structure Al with two vacancies

Examples of vacancies in Aluminium

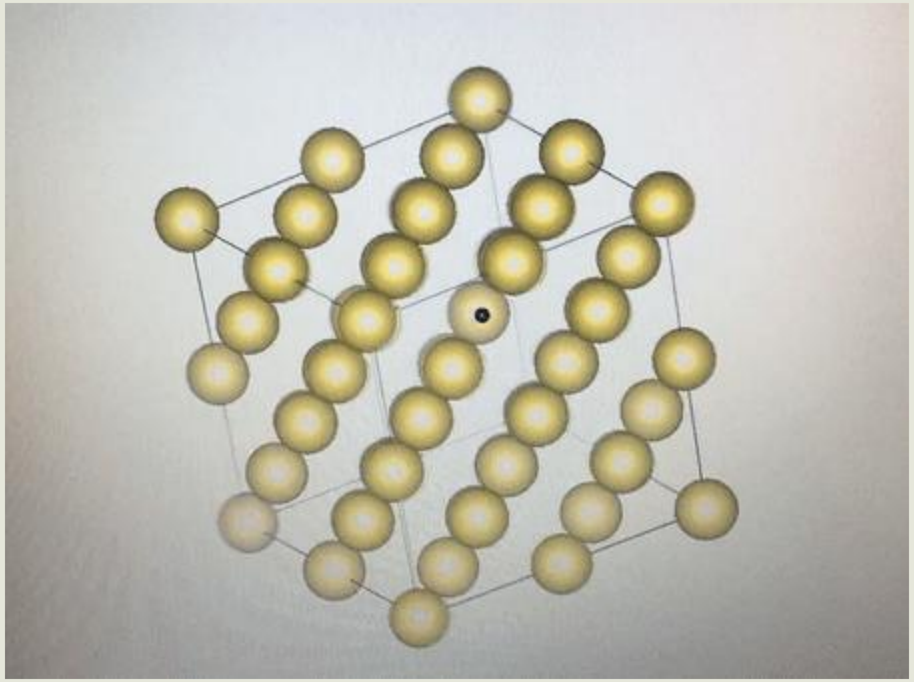


Fig. 7. Crystalline structure Al with three vacancies

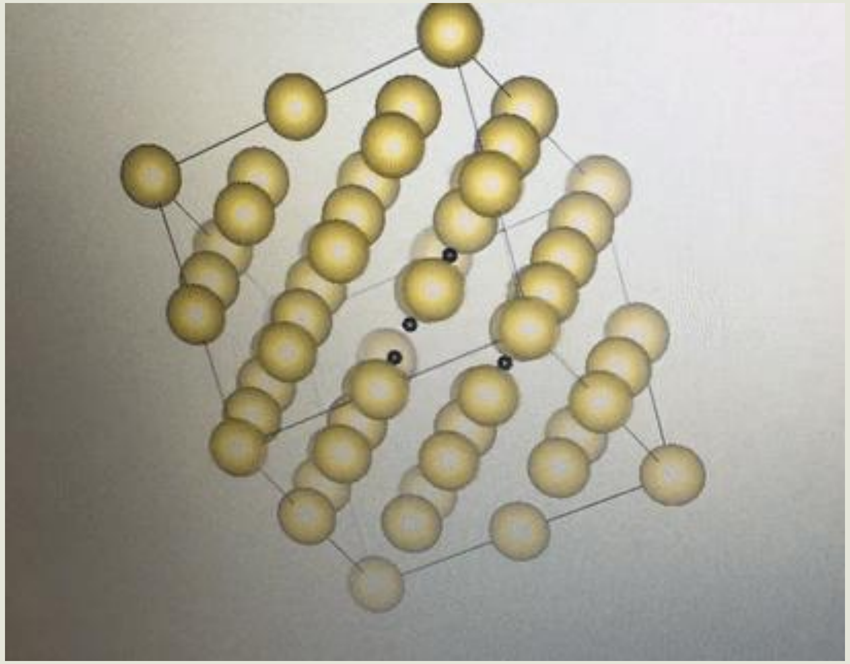
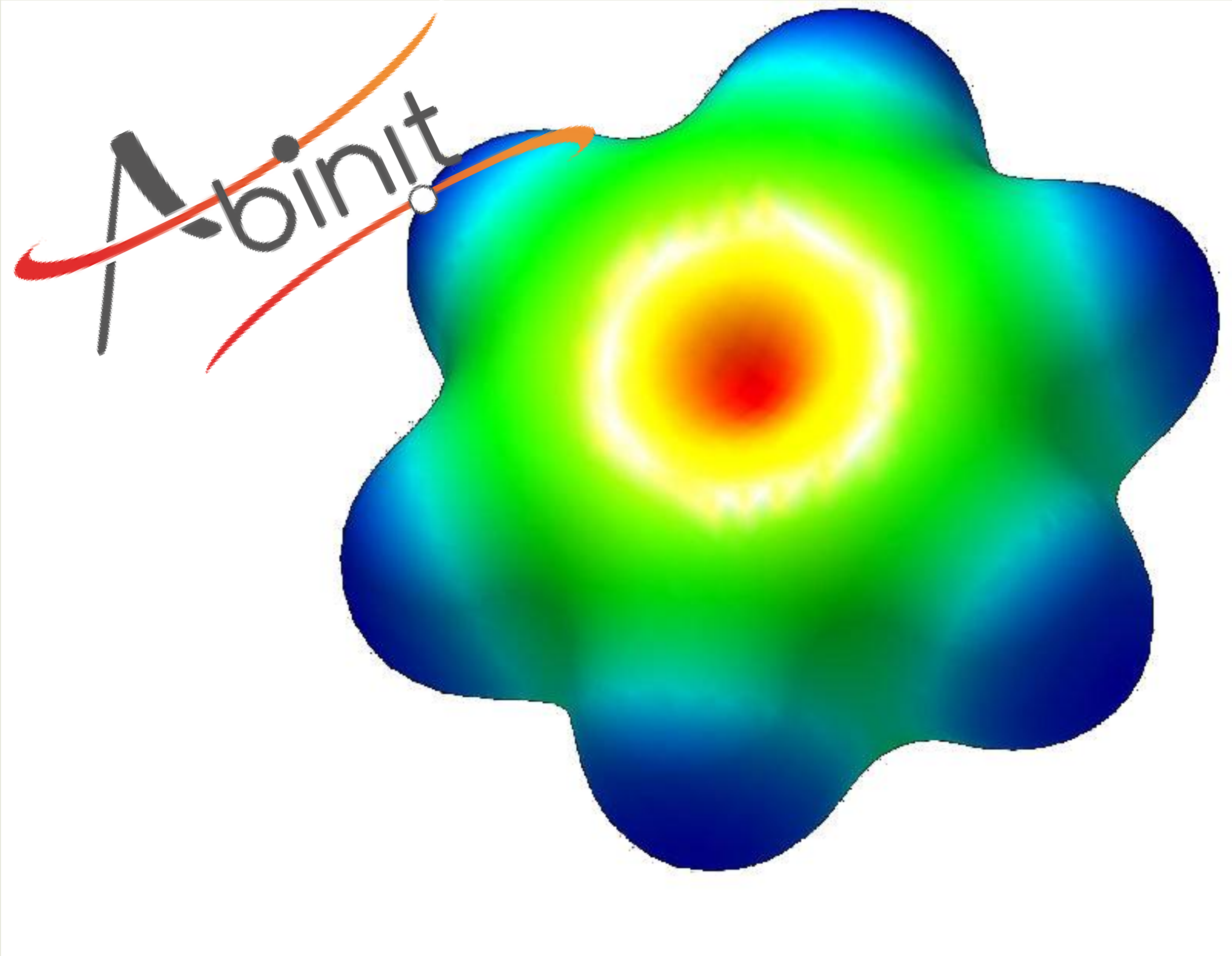


Fig. 8. Crystalline structure Al with four vacancies

Abinit



- Calculate the total energy, charge density, positron lifetime and electronic structure of systems made of electrons and nuclei
- Optimize the geometry according to the DFT forces and stresses
- Perform molecular dynamics simulations using these forces or generate phonons, Born effective charges, and dielectric tensors
- And many more properties

Calculated positron lifetime

Number of vacancies (per unit cel)	Positrons lifetime [ps]	Positron lifetime (after structure optimization)
0	162	162
1	242	237
2	266	253
3	294	283
4	331	320

Fig. 9. Table of calculated positron lifetime.

Metal	τ_v (ps)	τ_{exp} (ps)	E_b (eV)
Al	240	248	1.59
Zn	266	222	1.53
Cd	323	250	1.23
Mg	317	253	1.35

Fig. 10. Table of positron lifetime and Binding energy located in single vacancy.

[J.Dryzek, Charakterystyka procesu anihilacji pozytonów w fazie skondensowanej, Kraków 2005]

Preparation of the samples for lifetime spectroscopy

Fig. 11. The sample after cutting

Fig. 12. The sample after polishing

Fig. 13. Annealing

Fig. 14. The sample after annealing

Preparation of the samples for lifetime spectroscopy

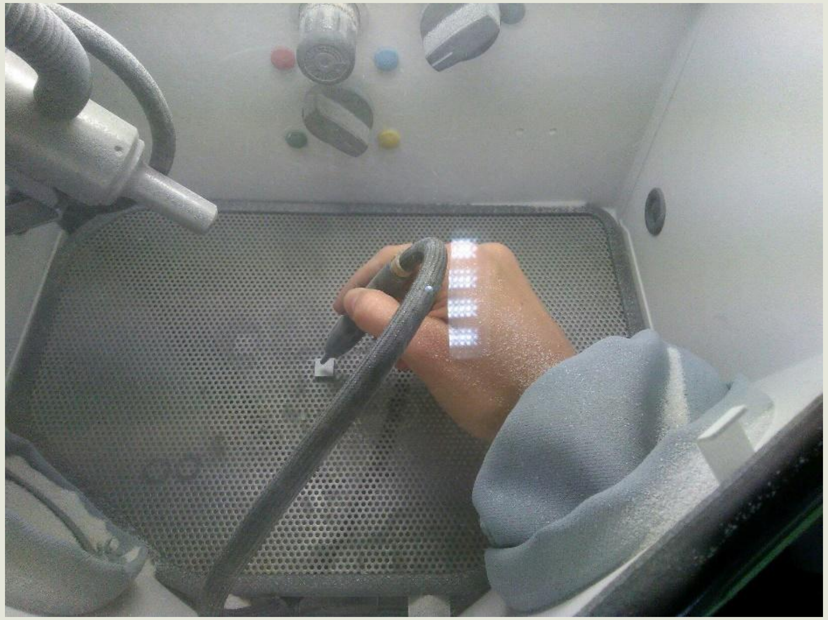


Fig. 15. Sandblasting

Fig. 16. The sample after sandblasting

Positron Annihilation Lifetime Spectroscopy (PALS)

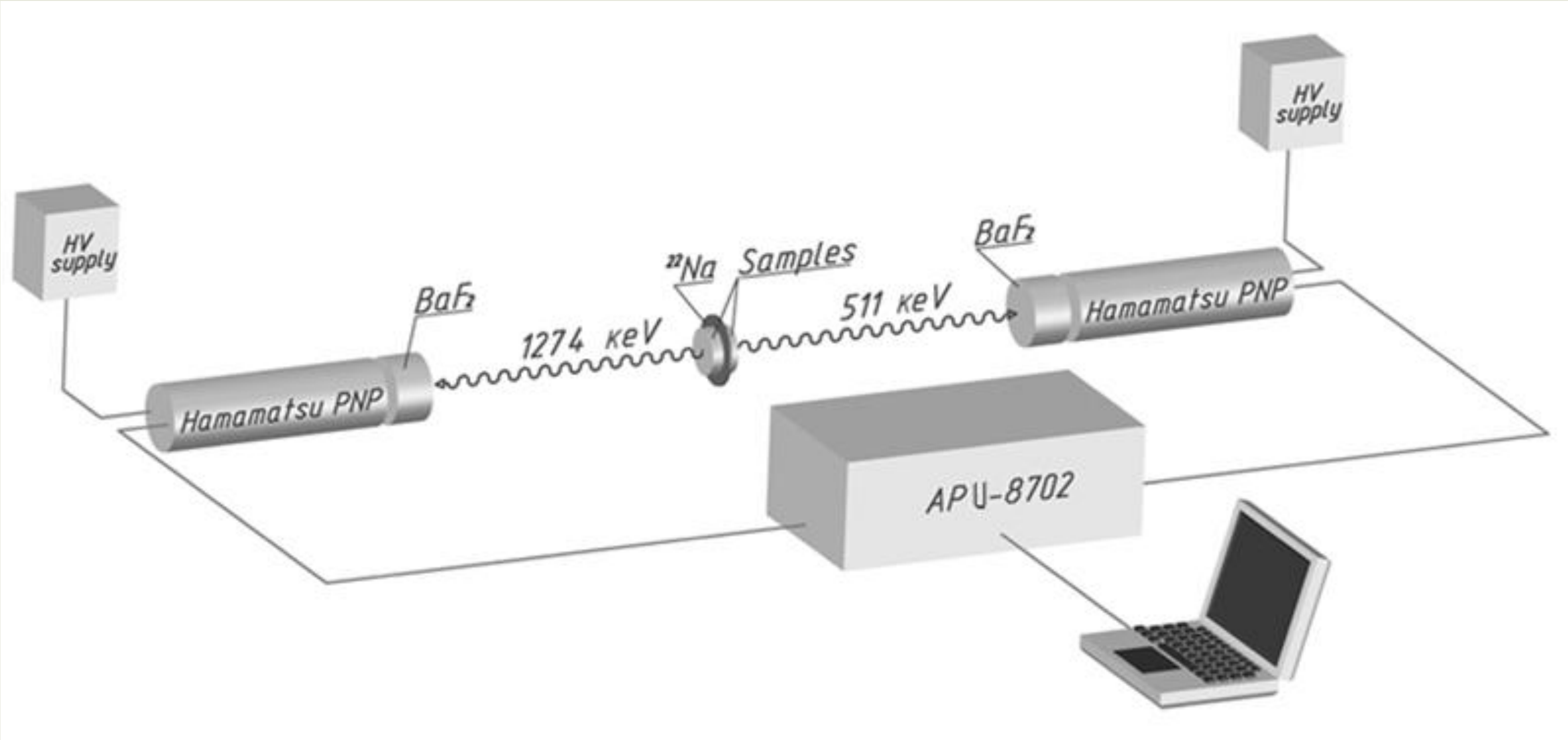
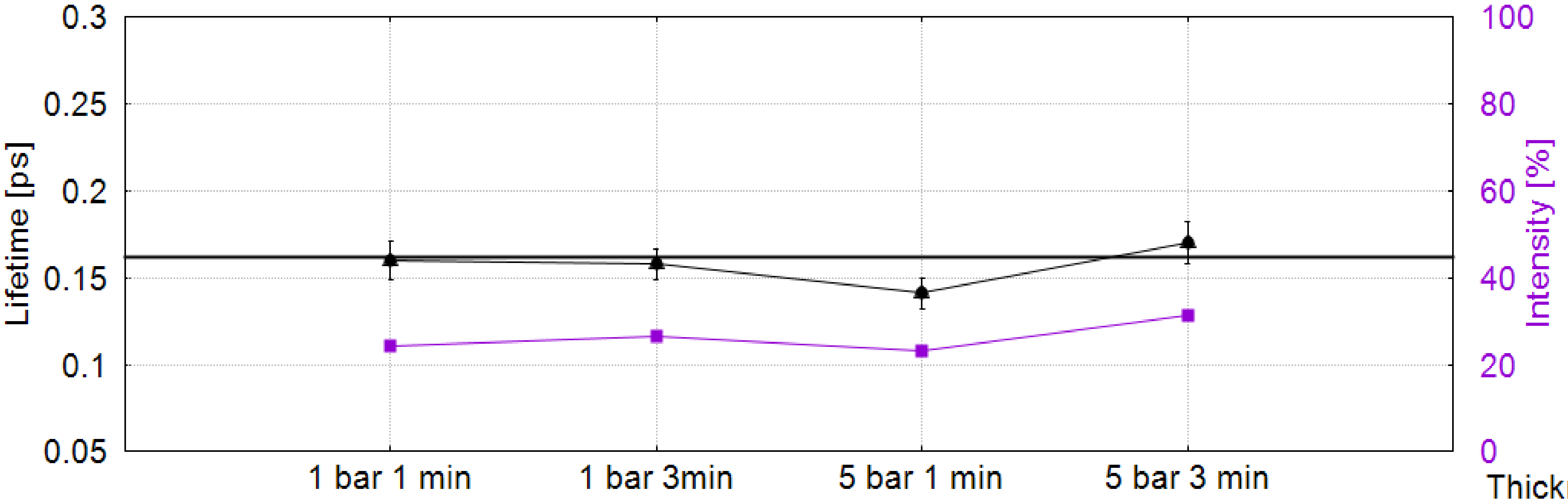
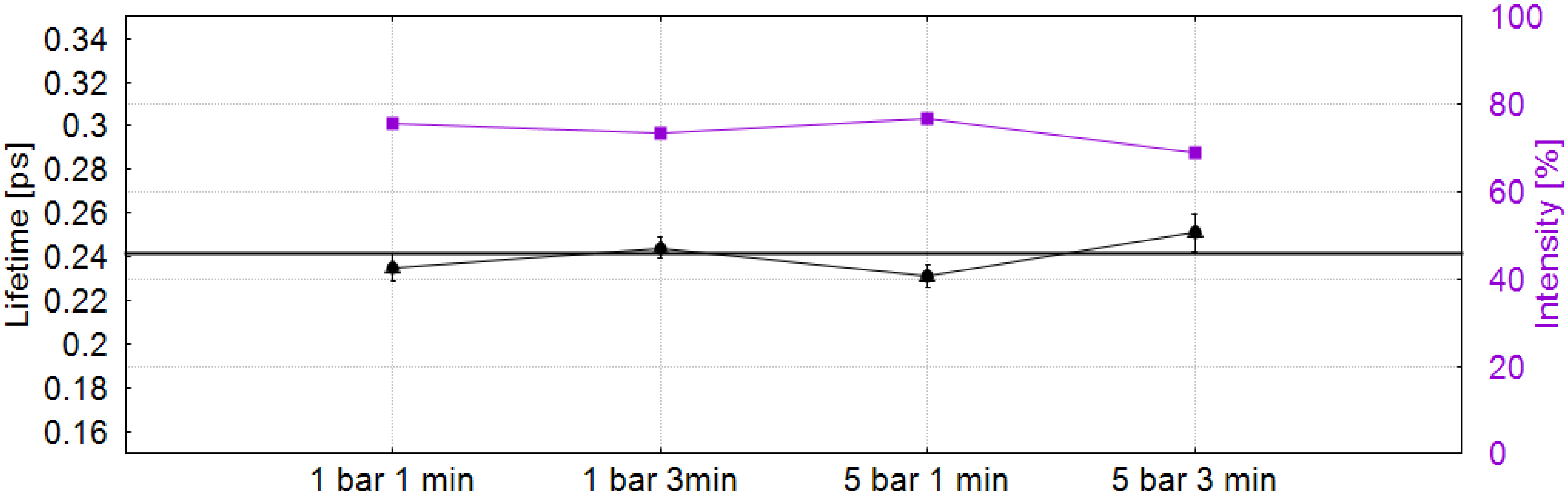


Fig. 17. Experimental setup for PALS



Thickness reduction: 19.7%

Lifetime : 0.231 [ps]



Doppler spectroscopy

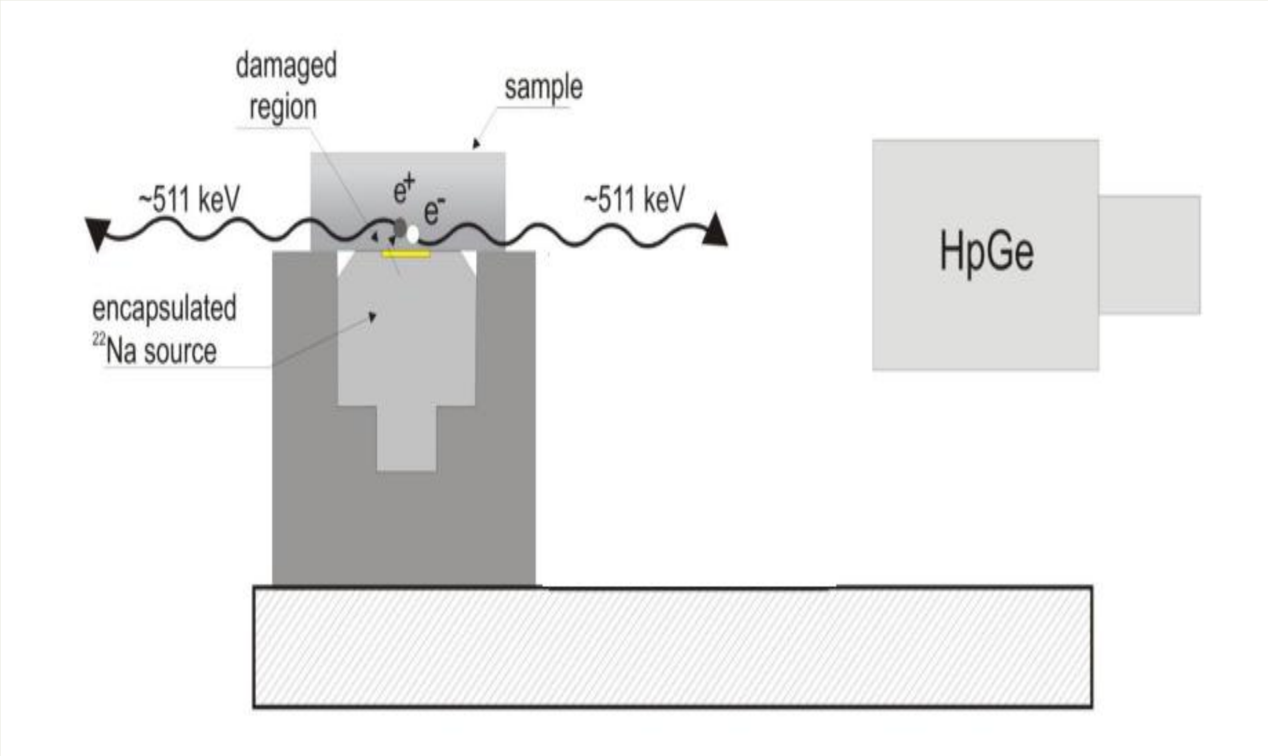


Fig. 18. The geometry of experiment with an encapsulated positron source

Annihilation lines

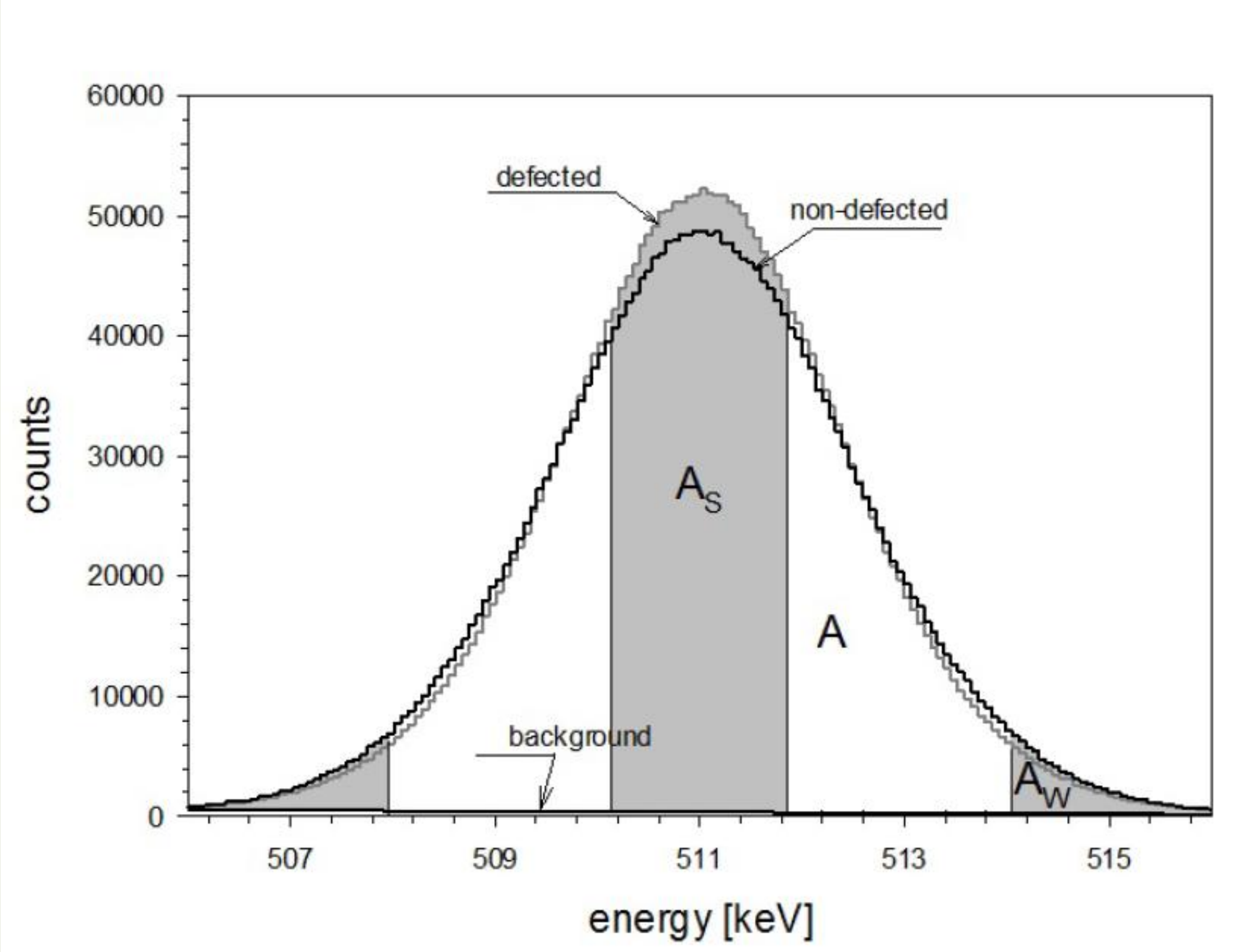


Fig.19. Annihilation lines measured for defected and non-defected samples

S- shape parameter

$$S = \frac{A_s}{A}$$

W-wing parameter

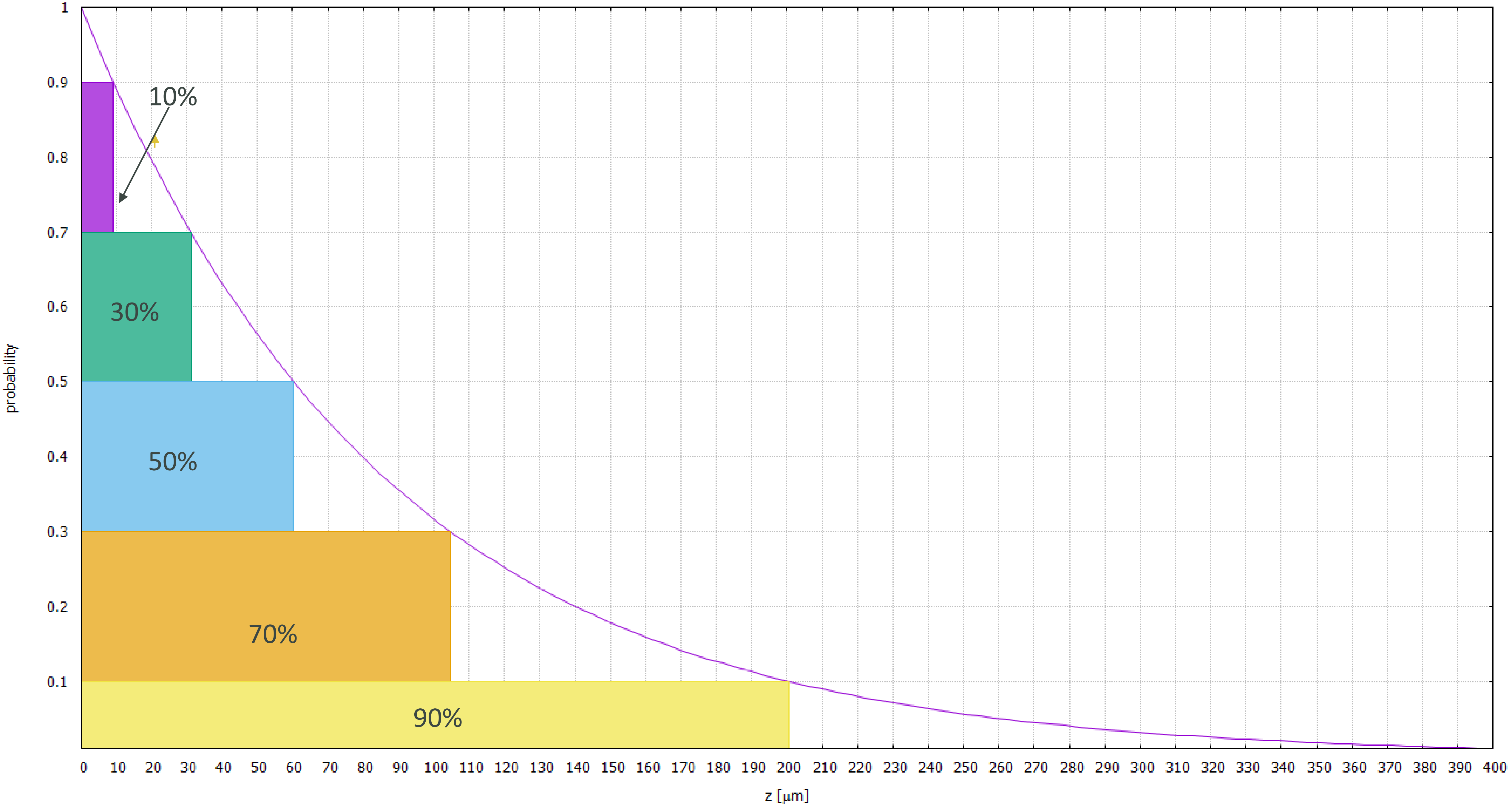
$$W = \frac{A_W}{A}$$

Energy of the annihilation quantum:

$$E_\gamma \cong mc^2 + E_B \pm \frac{p_{||}c}{2}$$

E_γ- energy of the annihilation quantum
m-rest mass of the electron
c- speed of light in vacuum
E_B- energy of bond positron-electron pair
$p_{||}$- projection of the positron momentum

Probability of annihilation with low momentum electrons is bigger when positron is trapped in vacancy. High momentum electrons make the energy E_γ lower or bigger and in results that make annihilation line broadener.



probability
z [µm]
10%
30%
50%
70%
90%

Single trapping model

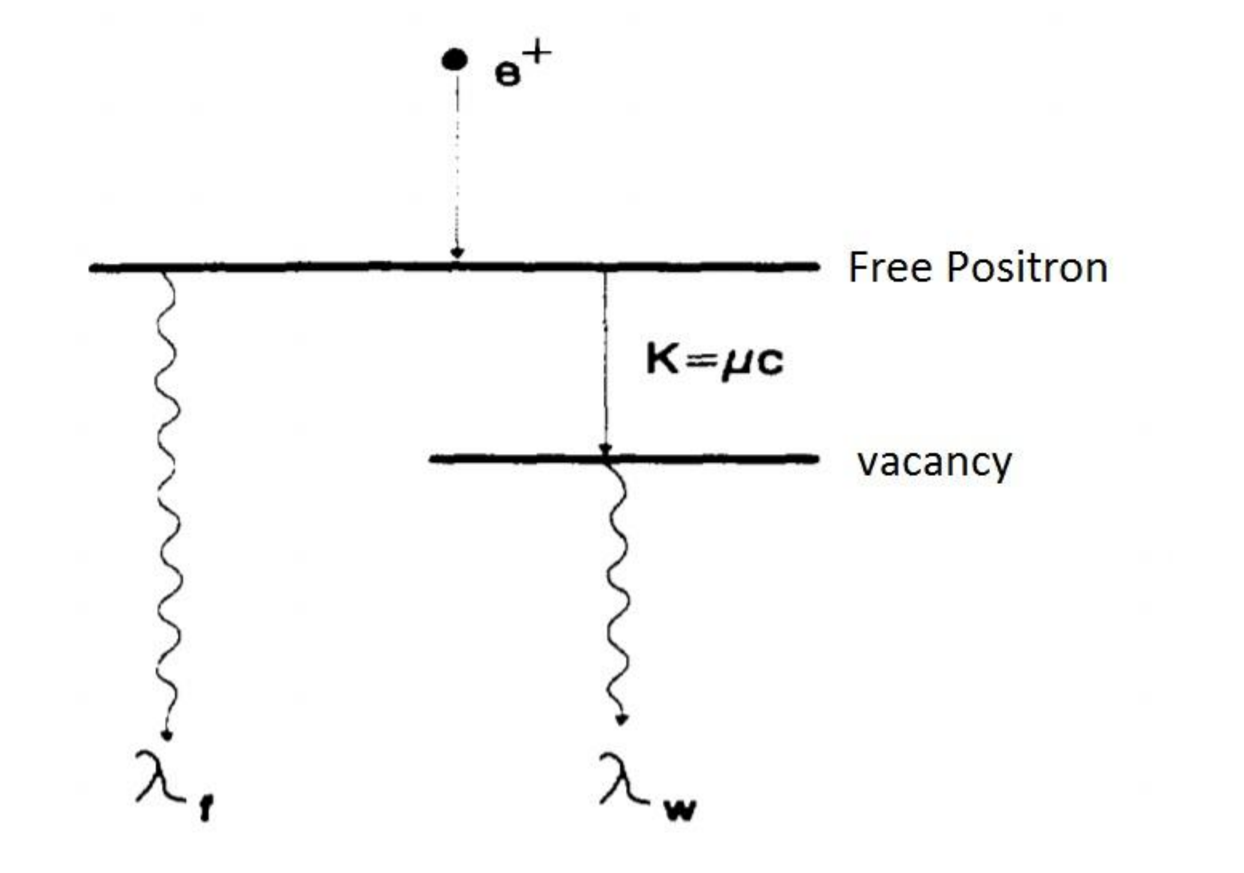


Fig.20. Single trapping model

$$S = \frac{\lambda_f S_f + K S_w}{\lambda_f + K}$$

Where:

$\lambda_f = \frac{1}{\tau_f}$ - positron annihilation rate in bulk material

K – positron trapping rate

c - concentration of vacancies

$\mu = 1{,}2 * 10^{14}\ s^{-1}$ - positron trapping coefficient

S_f - S-parameter for positrons annihilating in bulk material

S_w - S-parameter for positrons trapped in vacancies

Pressing experiment

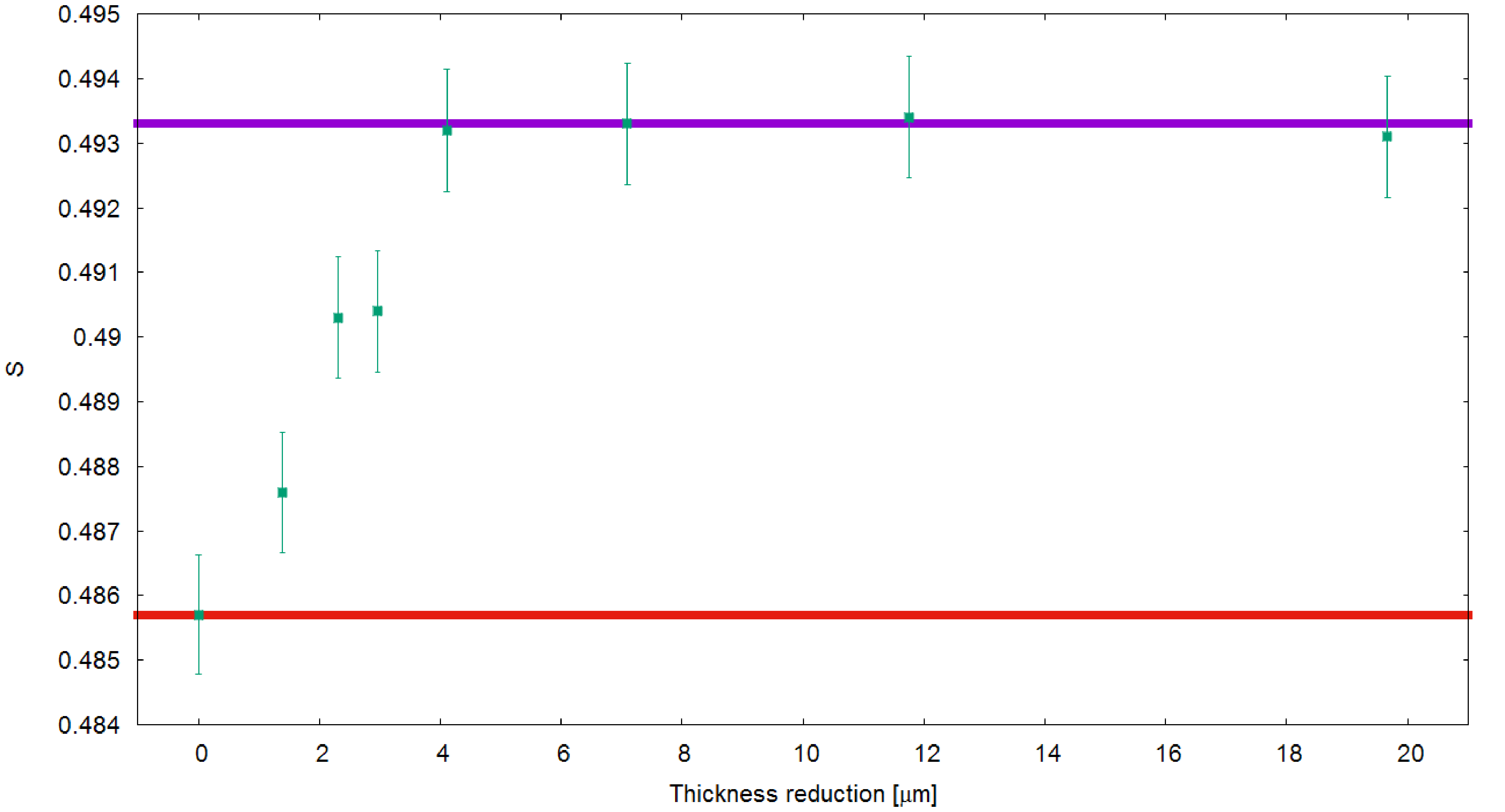
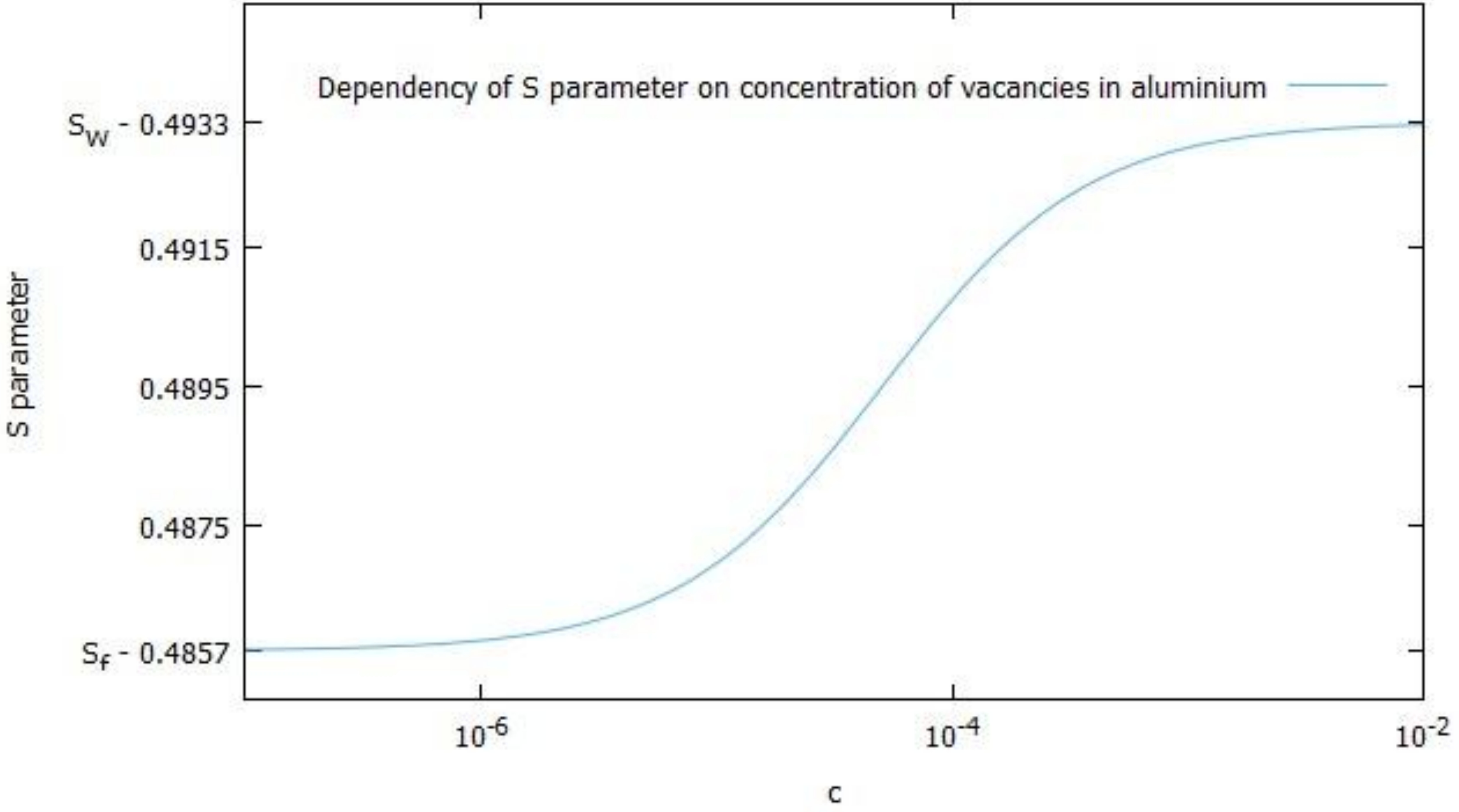


Fig.21. Dependency of S-parameter on thickness reduction



Dependency of S parameter on concentration of vacancies in aluminium
S parameter
S_W - 0.4933
0.4915
0.4895
0.4875
S_f - 0.4857
10^-6
10^-4
10^-2
c

Etching and measuring the samples

Fig. 21. Etching solutions

- Purpose: determine how deep the vacancies were created after sandblasting.
- Etchant: NaOH solution with high concentration.
- Etched thickness: ≈ 100 μm before every measurement
- Etching was performed until we reached bulk material.

Comparison of results

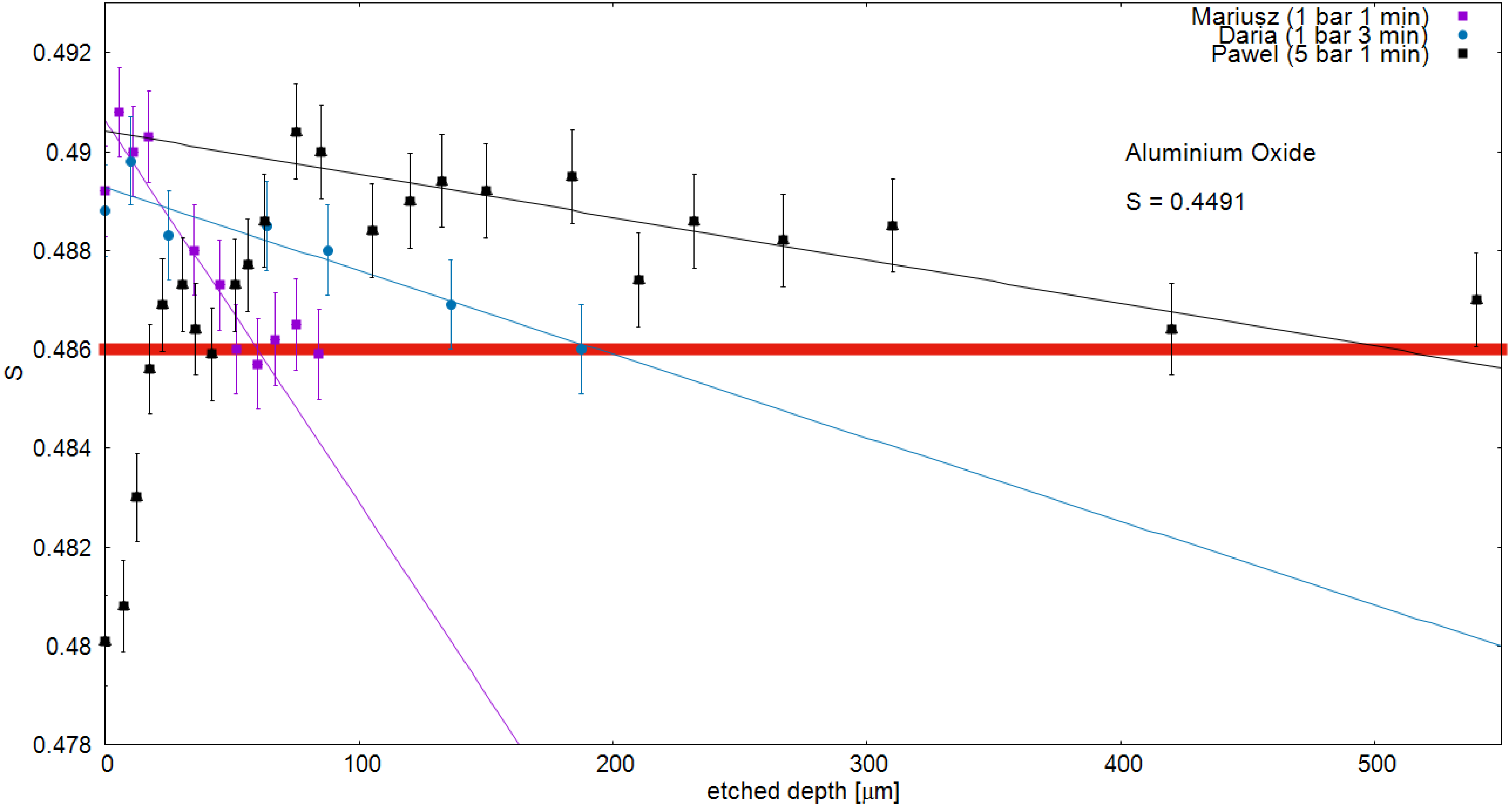
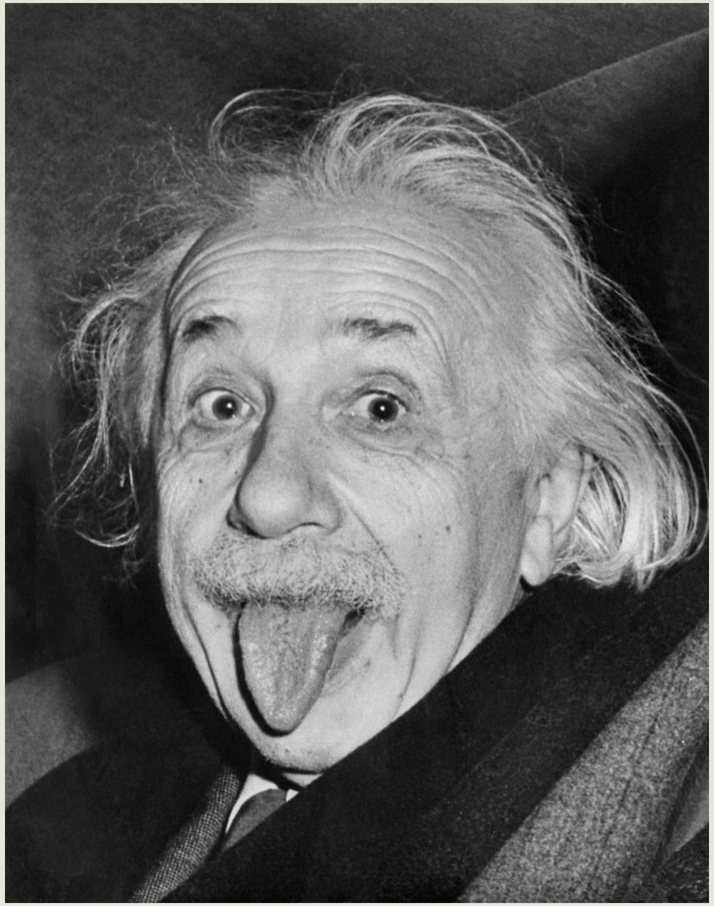


Fig. 22. Results comparison for sandblasted samples

Conclusions

- After analysing the aluminium samples using PALS we have concluded that only one type of defects were produced (monovacancies) after sandblasting and pressing.
- The Doppler broadening of the positron annihilation line method was successfully used to determine the size of defected zone in sandblasted aluminium samples.
- By calculating the defect concentration using the single trapping model and the numerical experimental values, for example for sample sandblasted 1min under the pressure 1bar we obtained $c = 1{,}52 \cdot 10^{-3}$ and it is linearly decreasing with the depth.



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THANK YOU FOR YOUR ATTENTION! ☺