Structure, Neutron Scattering Cross Sections, and Applications of Fluorine-Intercalated Graphite

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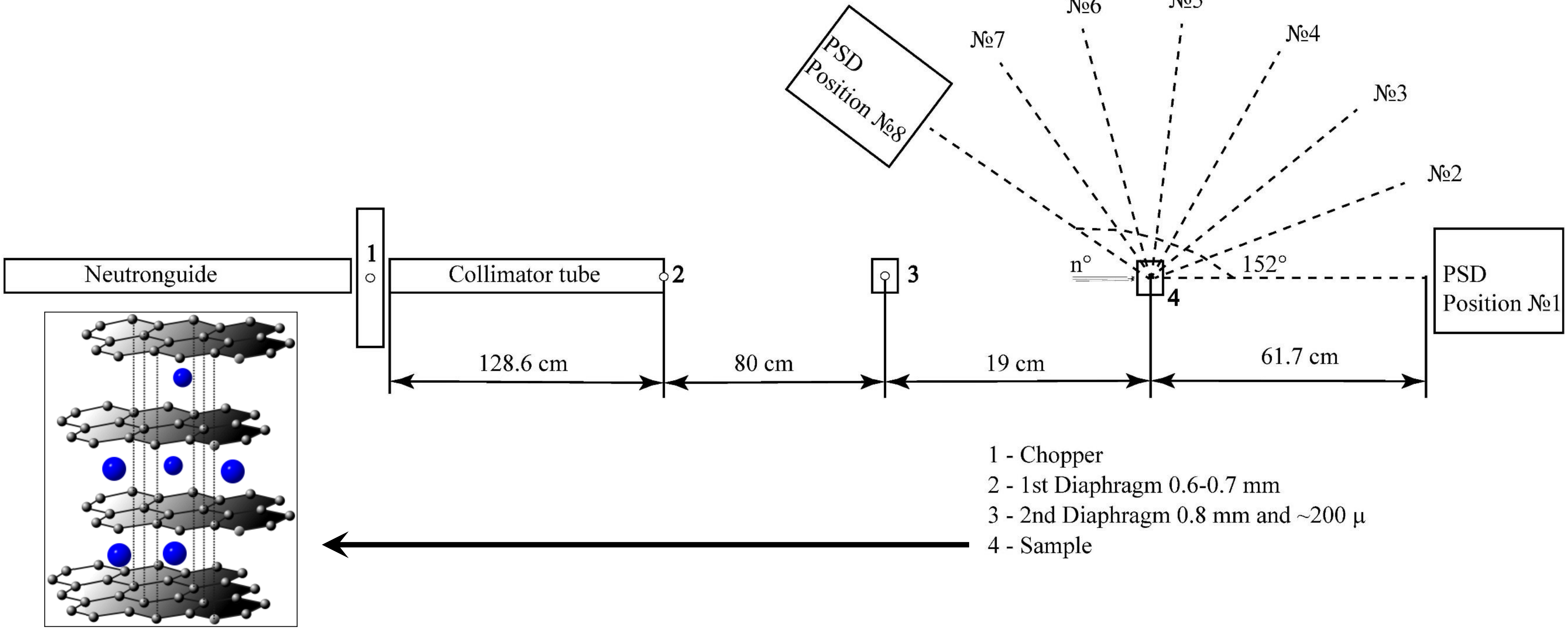
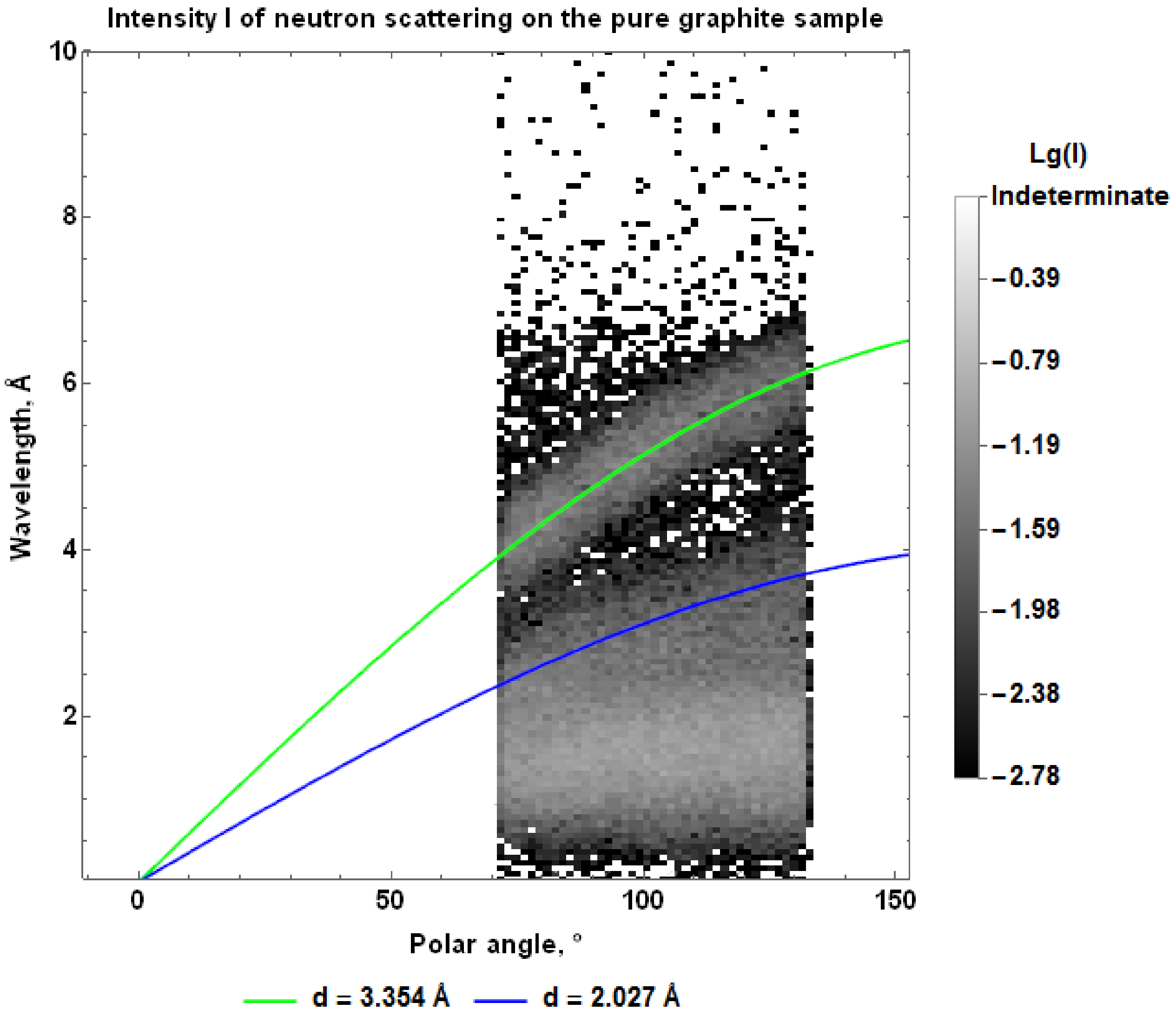
XXVII International Scientific Conference of Young Scientists and Specialists
October 30 – November 3, 2023
Dubna, Russia

Experiment Scheme



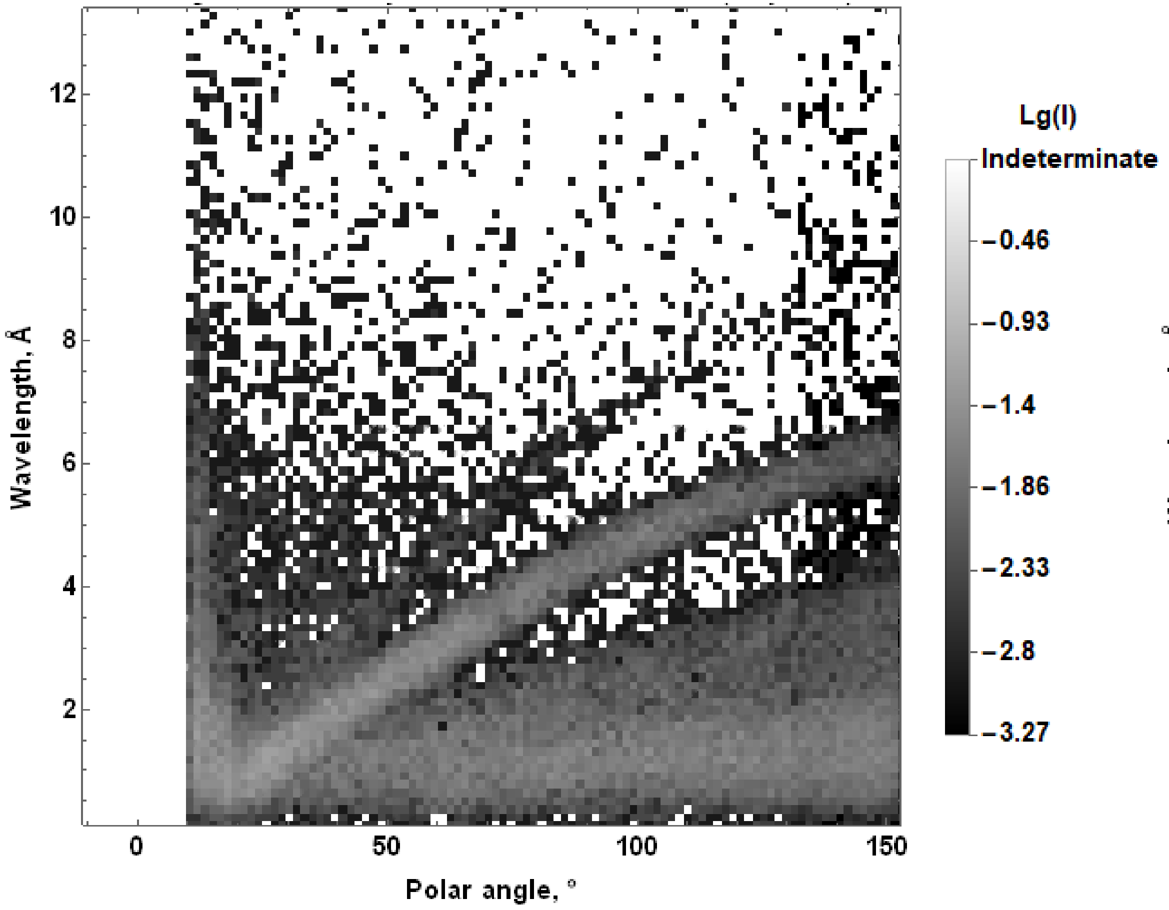
1 - Chopper
2 - 1st Diaphragm 0.6-0.7 mm
3 - 2nd Diaphragm 0.8 mm and ~200 μ
4 - Sample

Calibration Using the Pure Graphite Sample

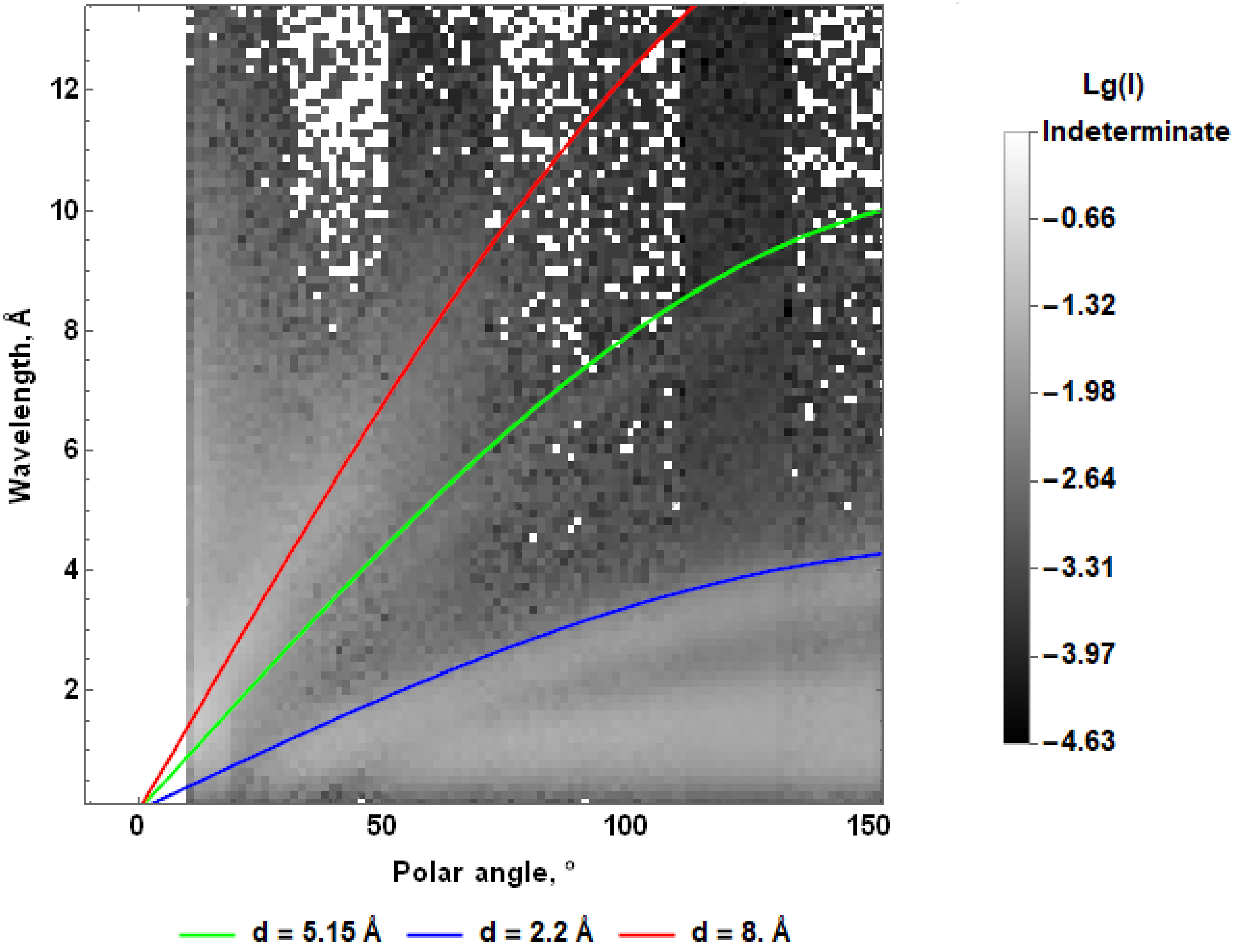


- The direct beam was restored using the pair of monitor/detector spectrums.
- TOF delay time determined from the direct beam data on different sample-monitor distances.

Experimental Data



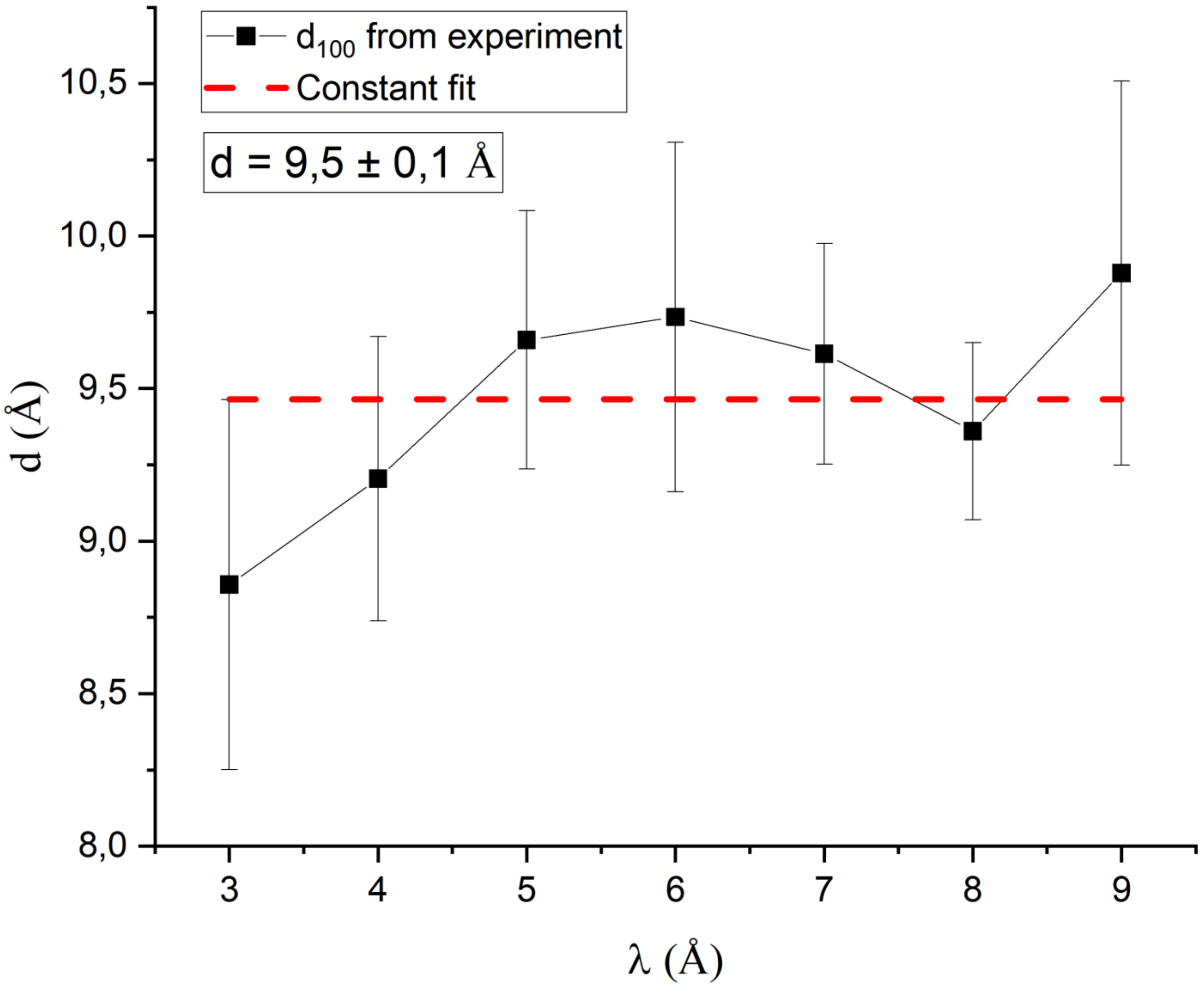
Original graphite powder



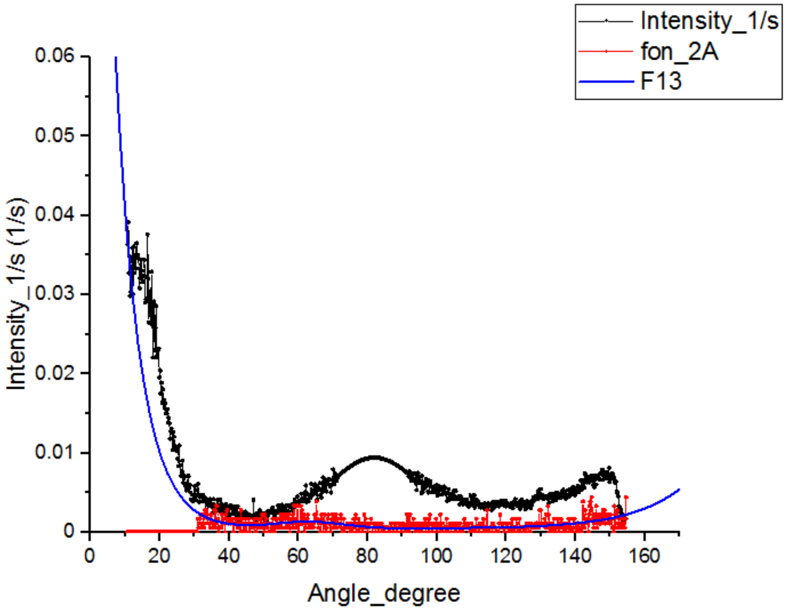
Graphite intercalated with fluorine

Interplanar Spacing of Intercalated Graphite

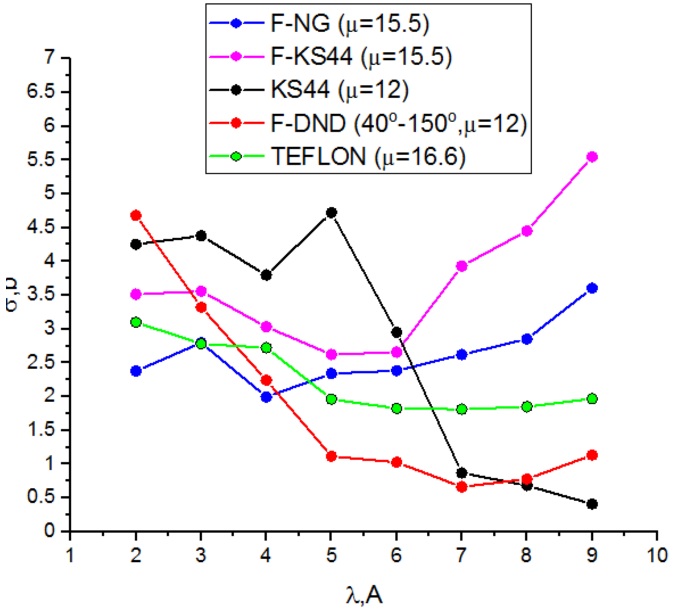
- (100) plane of ICG
- $\lambda = \{3, 4, 5, 6, 7, 8, 9\}$ Å
- $\Delta\lambda = 0{,}2$ Å
- Peak positions θ from Pseudo-Voigt fit of experimental data
- d from $2d \sin\theta = \lambda$



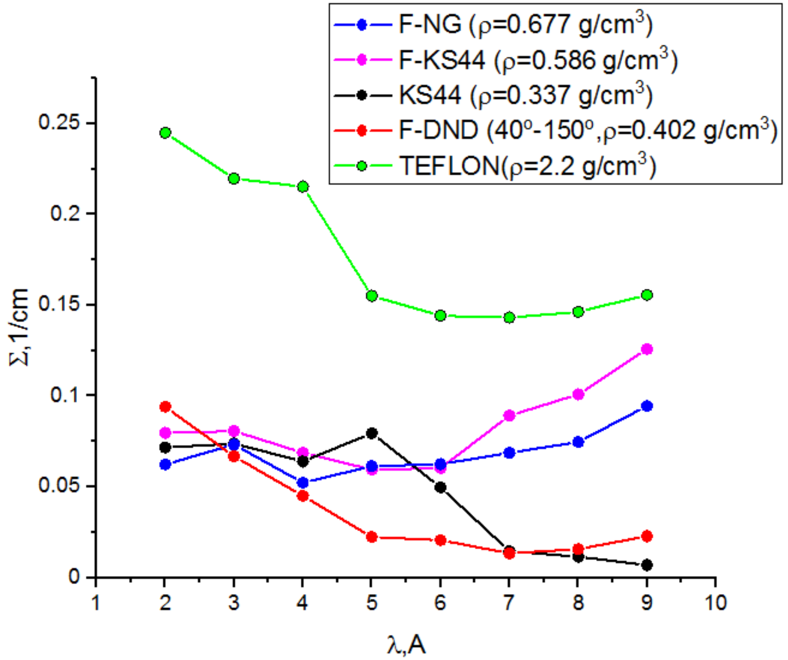
Estimating the Diffraction Cross-Sections



Analysis of the peak

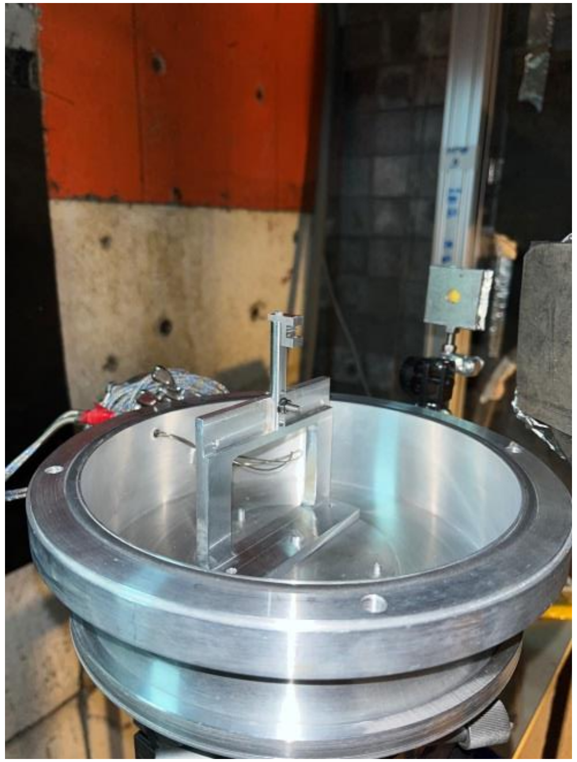


Microscopic cross-section

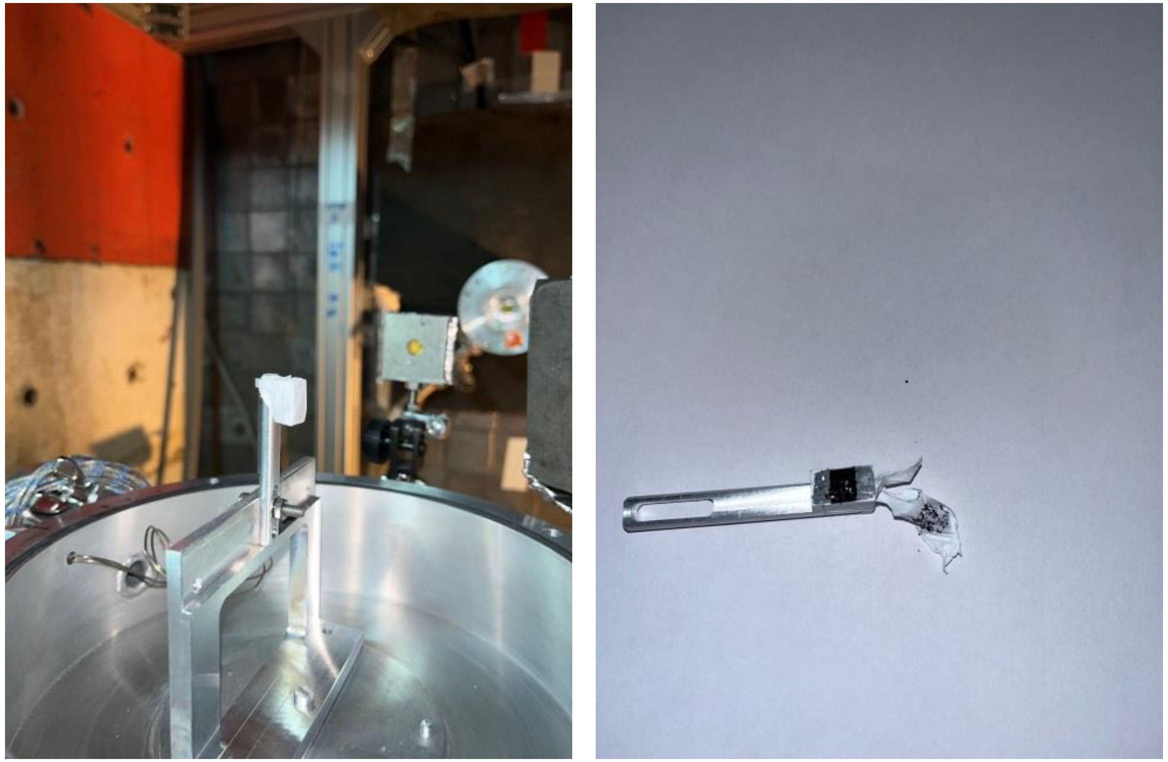


Macroscopic cross-section

Some Photos from the Experiments



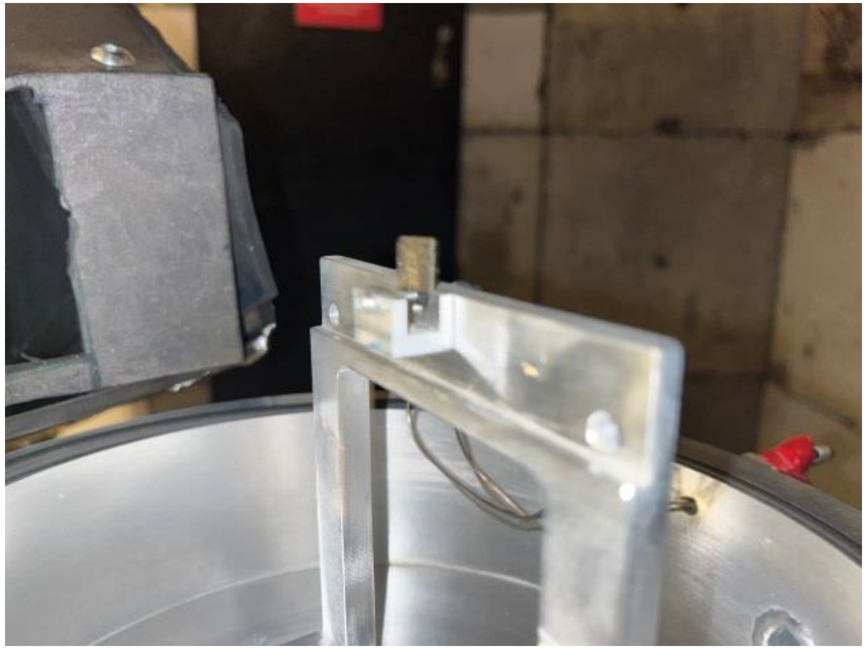
Sample Environment



The sample and sample holder

Graphite Foils

Some Photos from the Experiments

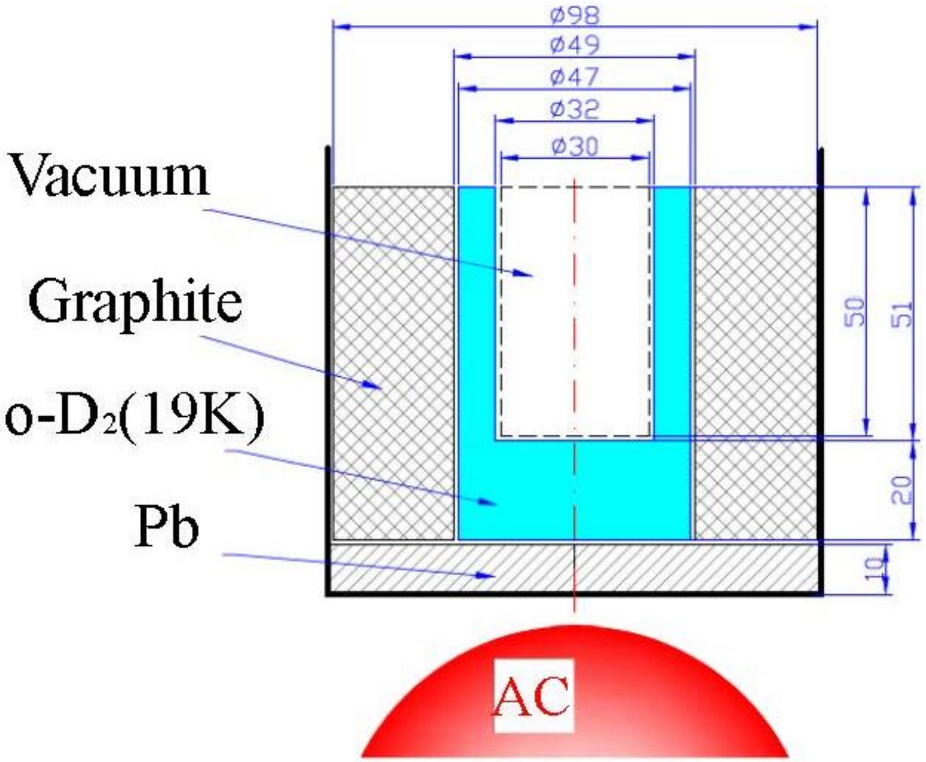


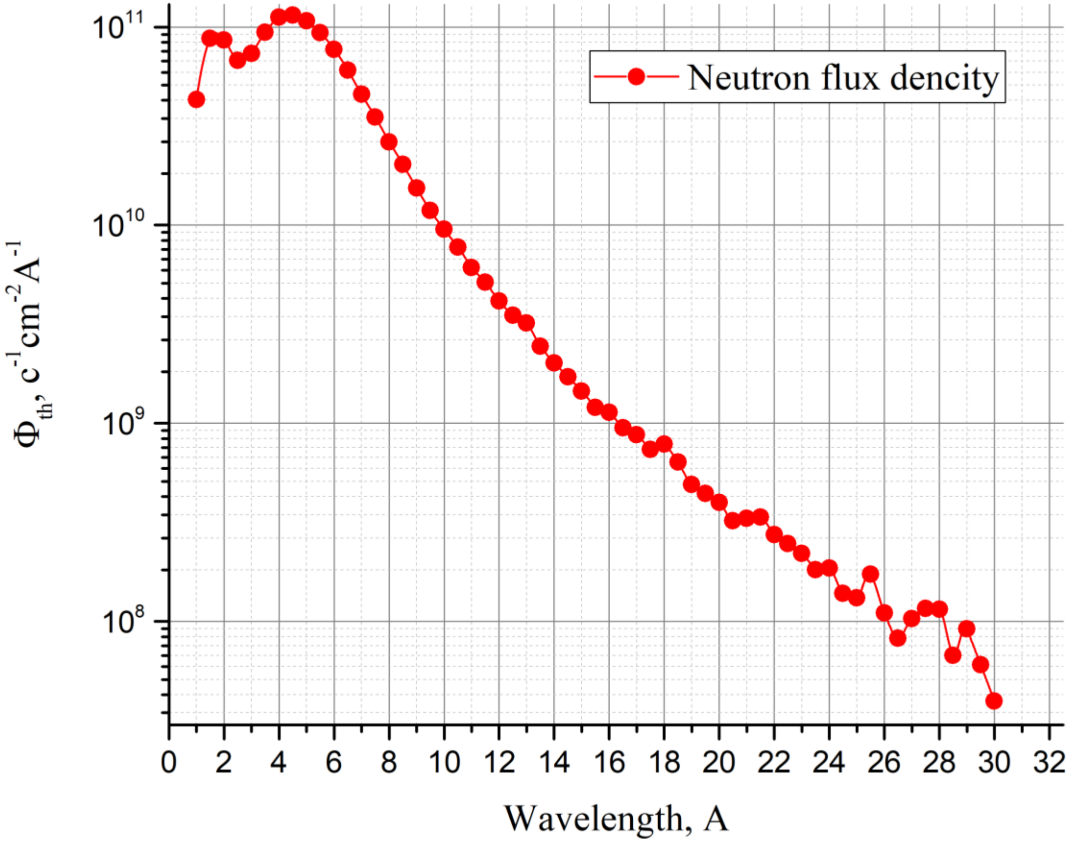
A Graphite Foil

Teflon Sample

Experiment general view

Intercalated Graphite Applications: Ultracold and Very Cold Neutron Sources*





A precise calculation performed using the MCNP program shows that in a hemispherical layer of liquid deuterium **20 cm** thick, the flux density of cold neutrons with a wavelength of 9 Å is $\boldsymbol{\Phi_c(9\text{Å}) = 1.54 \cdot 10^{10} cm^{-2} s^{-1} \text{Å}^{-1}}$.

*The presentation slide from "The first steps of development and construction of the high-intensity Ultracold neutrons source at the WWR-K reactor" by Dr. K. Turlybekuly at the AYSS-2023, Session of the Experimental Nuclear Physics on Wednesday, 01.11.2023.

Very Cold Nuetron Reflector

Criteria for the VCN reflector are minimum losses and maximum reflection.

Detonation nanodiamonds (DND) are the ideal candidate!

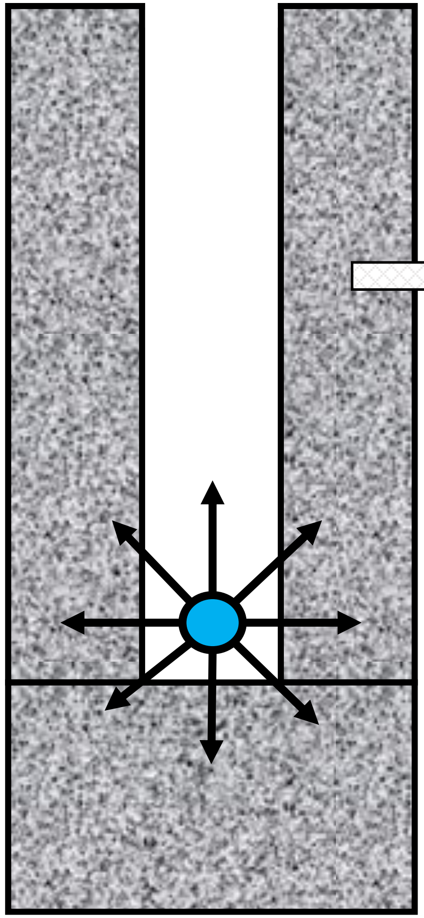
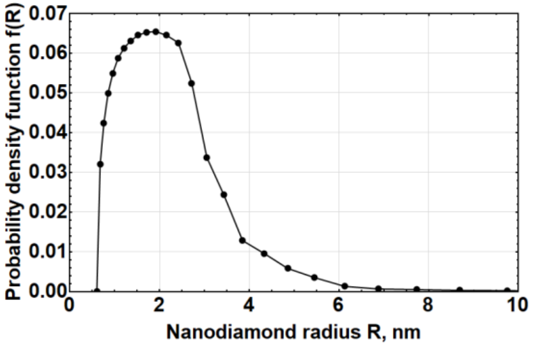


Fig. 2. The possible scheme of the VCN source.



$$\boxed{P_{REF}^{max}:\ R_{opt} \approx 0.27\lambda}$$

$$R_{opt}(\lambda) \approx 0.7 - 4.3\ nm,$$
$$\lambda \in [26, 160]\ \text{Å}$$
$$\text{or } v \in [25, 150]\ m/s$$

Positive Factors:

size distribution;

$b_{c.sc.}^{C} = 6.65\ fm;$

$\sigma_{c.sc.}^{C} = 5.55\ b;$

$\sigma_{abs}^{C} = 3.5\ mb;$

$\sigma_{in.sc.}^{C} \to 0\ (T \to 0);$

$\rho^{Diamond} \approx 3.5\ g/cm^3.$

$P_{REF} \sim 95\%$

Negative Factors:

~10 at. % of hydrogen,

$\sigma_{abs}^{H} = 0.33\ b;$

$\sigma_{in.sc.}^{H} = 108 \pm 2\ b;$

other impurities

< 0.15 at. %

neutron capture

neutron activation

Implemented solutions:

the fluorination of DND

$C/H = 7.4 \pm 0.2$ (before)

$C/H = 430 \pm 30$ (after)

the additional purification of DND

$\Sigma_{abs}^{after}/\Sigma_{abs}^{before} \approx 0.58$

$\Sigma_{abs}^{H} \approx 0.2\Sigma_{abs}^{after}$

But still significant activation!

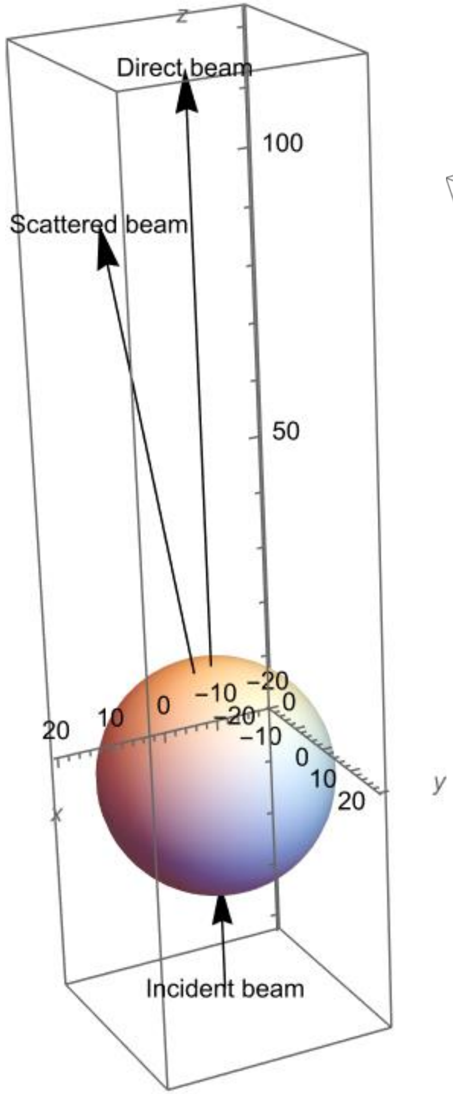
the deagglomeration of DND

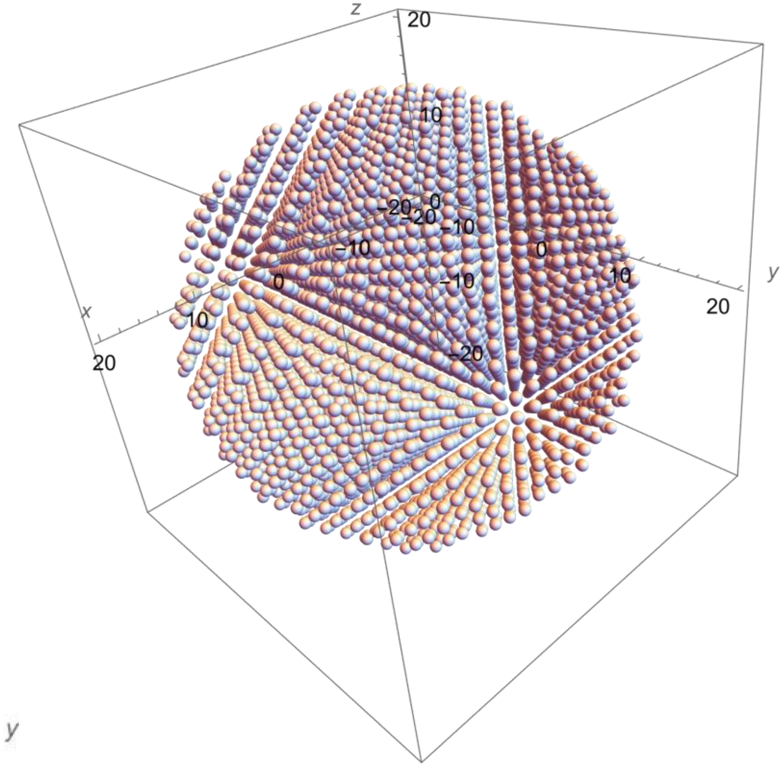
$P_{REF}^{after}/P_{REF}^{before} \approx 1.10$

$\rho_{bulk}^{after}/\rho_{bulk}^{before} \approx 3$

Diamond Nanoparticle Cross-Section Calculation

- Geometry of scattering: neutron beam with a wavelength λ and a unit vector $\boldsymbol{s}_i$ along axis Z falls on spherical nanoparticle, located at (0,0,0)
- Nanoparticle is a set of N atoms arranged in certain coordinates $\boldsymbol{r}_i$ defined by the unit cell of a diamond
- Cross-section of scattering at direction $\boldsymbol{s}_f$ results from the sum of waves, produced by each atom of a nanoparticle
- $\frac{d\sigma}{d\Omega} = \frac{1}{N} * \left| b * \sum_i e^{-\frac{2\pi i}{\lambda}(\boldsymbol{s}\cdot\boldsymbol{r}_i)} \right|^2$
    - b – carbon scattering length
    - $\boldsymbol{s} = \boldsymbol{s}_f - \boldsymbol{s}_i$ - scattering vector





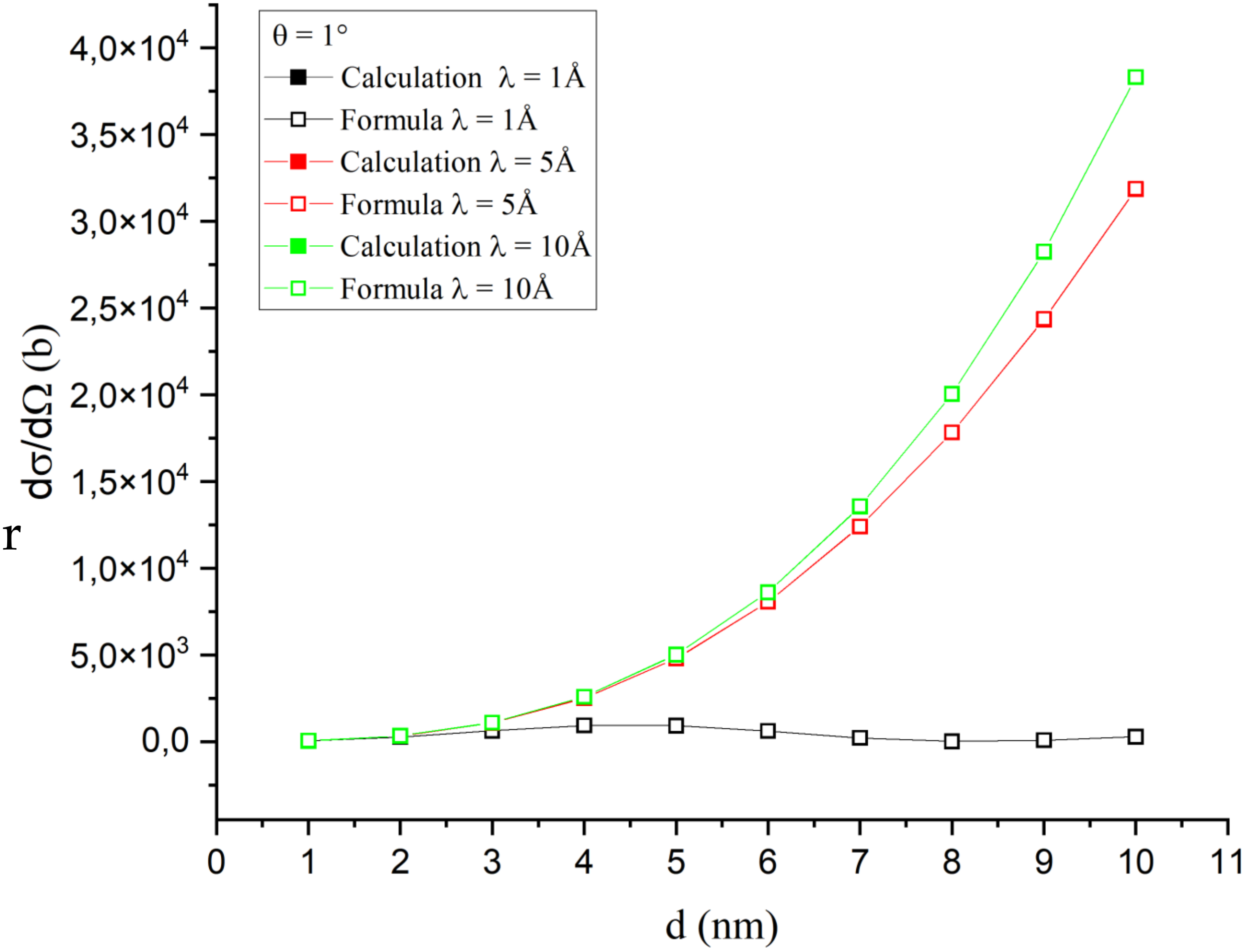
↑ Nanoparticle made of atoms
← Geometry of scattering

Diamond Nanoparticle Cross-Section Calculation

- Calculation check using SANS formula

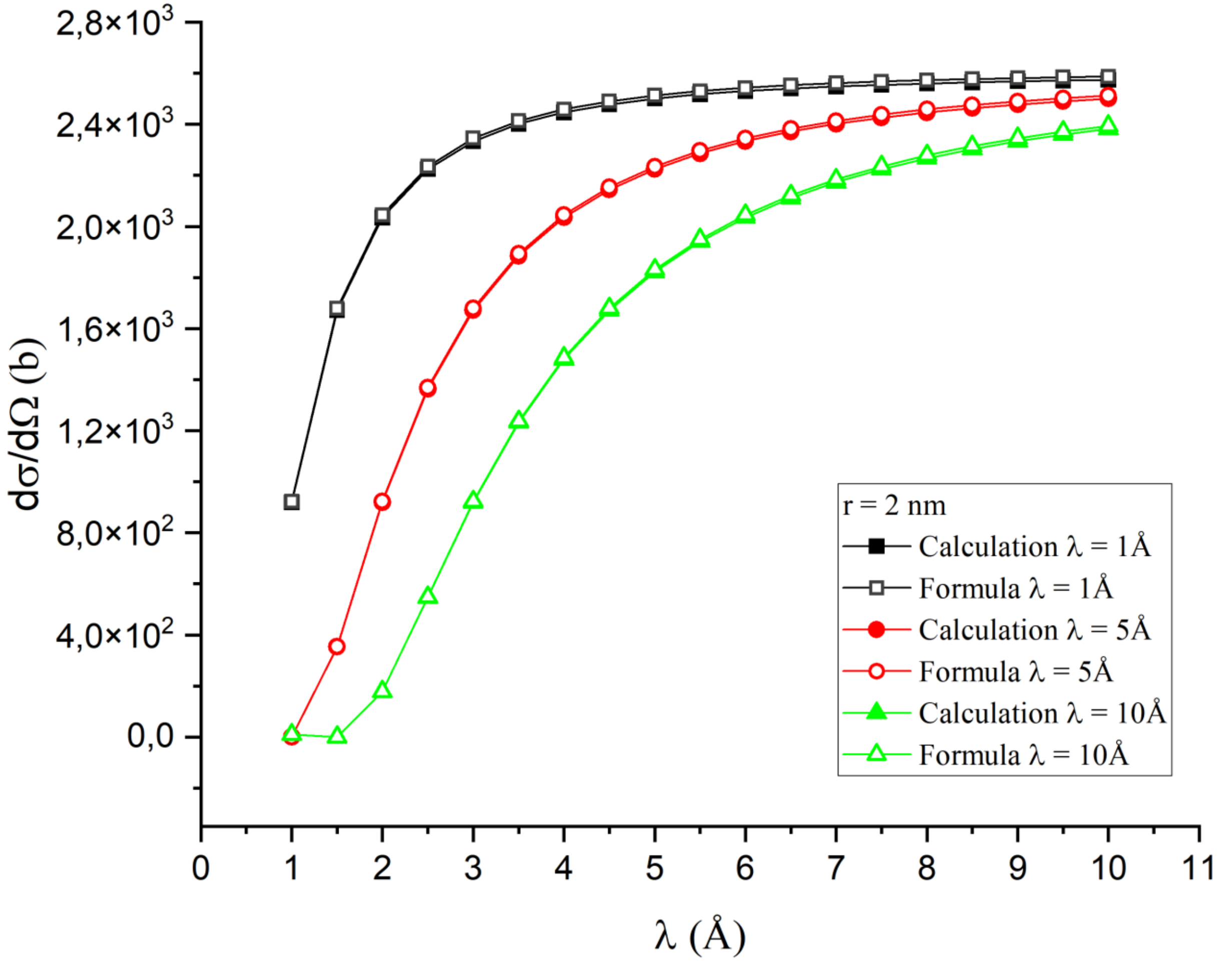
- $f(q) = \frac{2m}{\hbar^2} U r^3 \left(\frac{sin(qr)}{(qr)^3} - \frac{cos(qr)}{(qr)^2} \right)$
    - ○ $r = d/2$ – nanoparticle radius
    - ○ $q = \frac{4\pi}{\lambda} \sin\frac{\theta}{2}$ – momentum transfer
    - ○ λ – neutron wavelength
    - ○ θ – scattering angle

- $\frac{d\sigma}{d\Omega} = \frac{1}{N} |f(q)|^2$

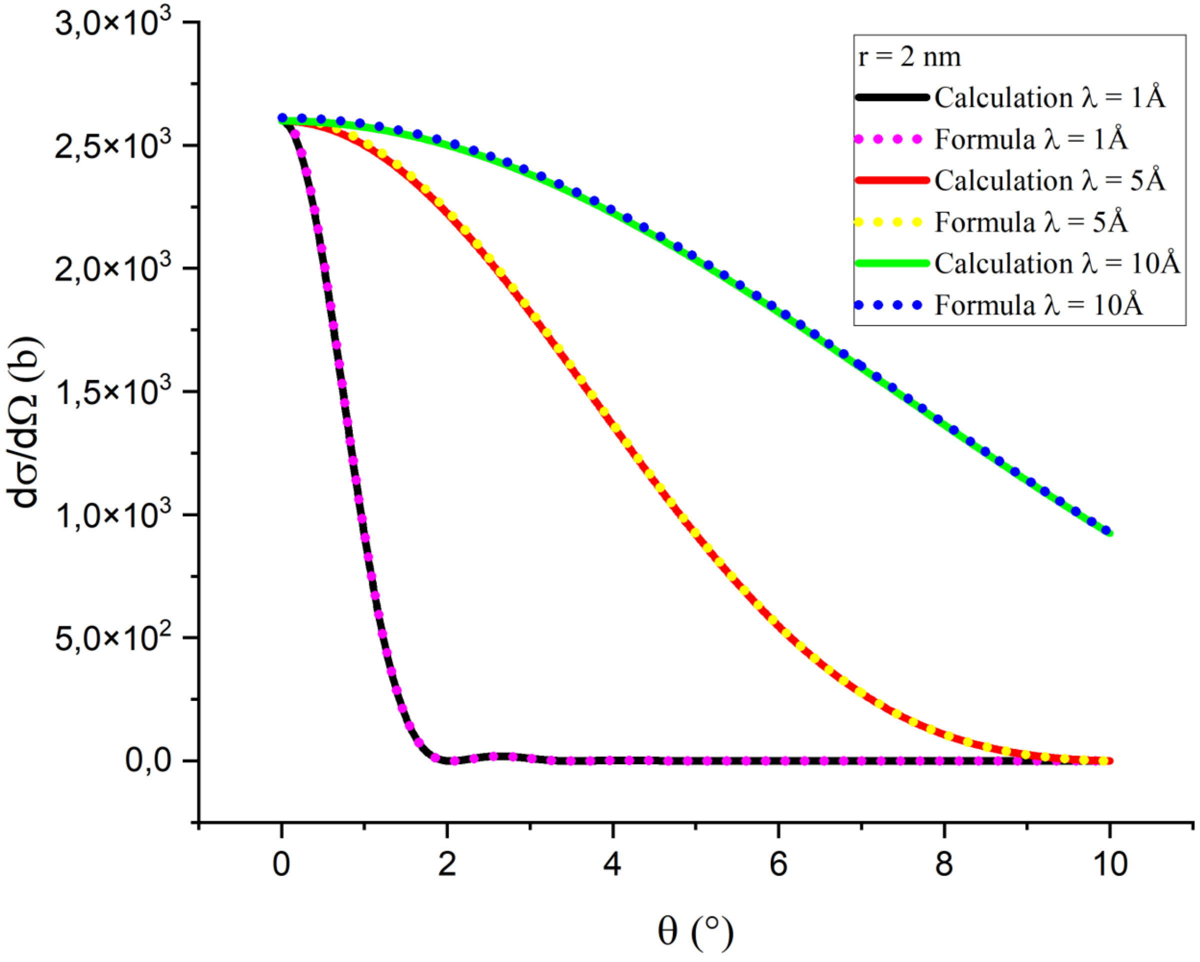


SANS check: size

Diamond Nanoparticle Cross-Section Calculation



SANS check: wavelength

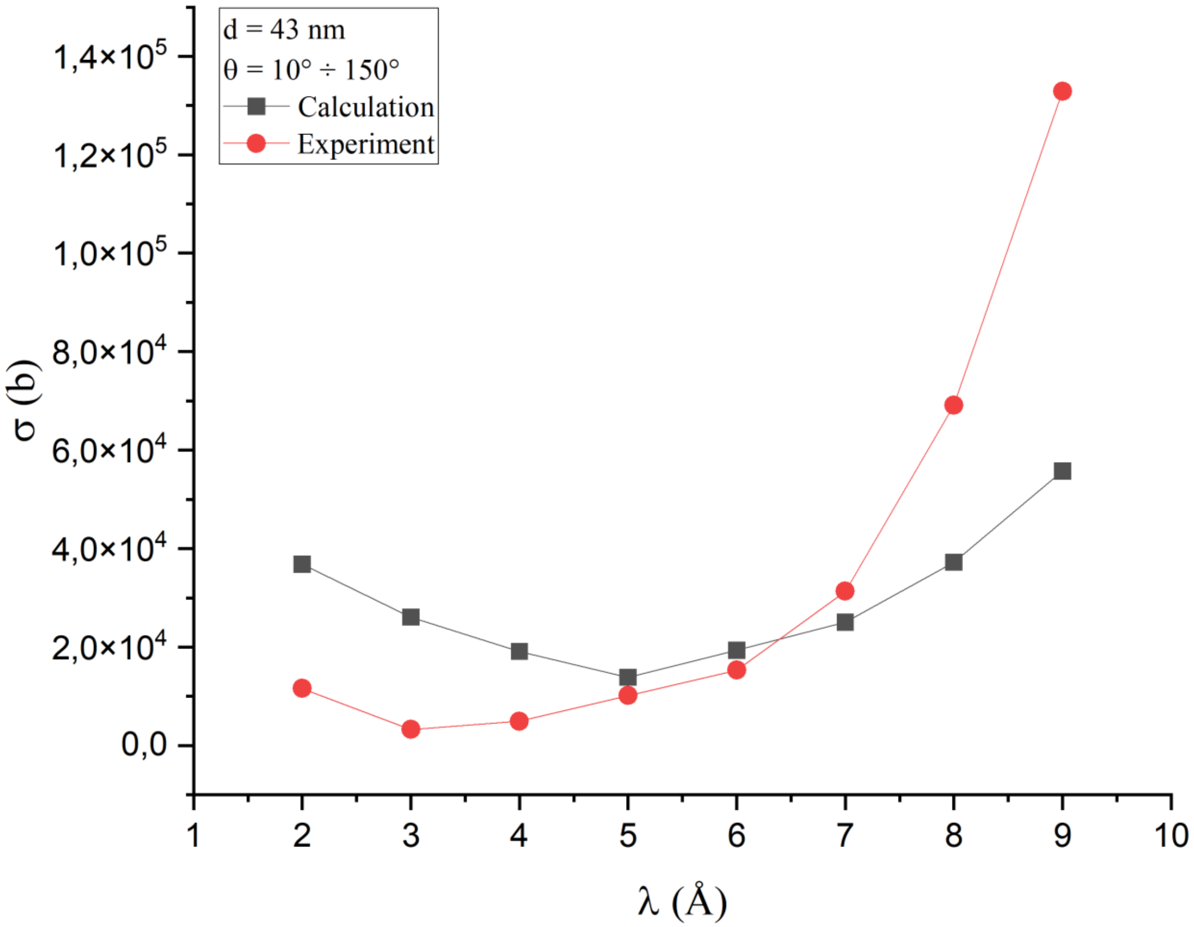


SANS check: angle

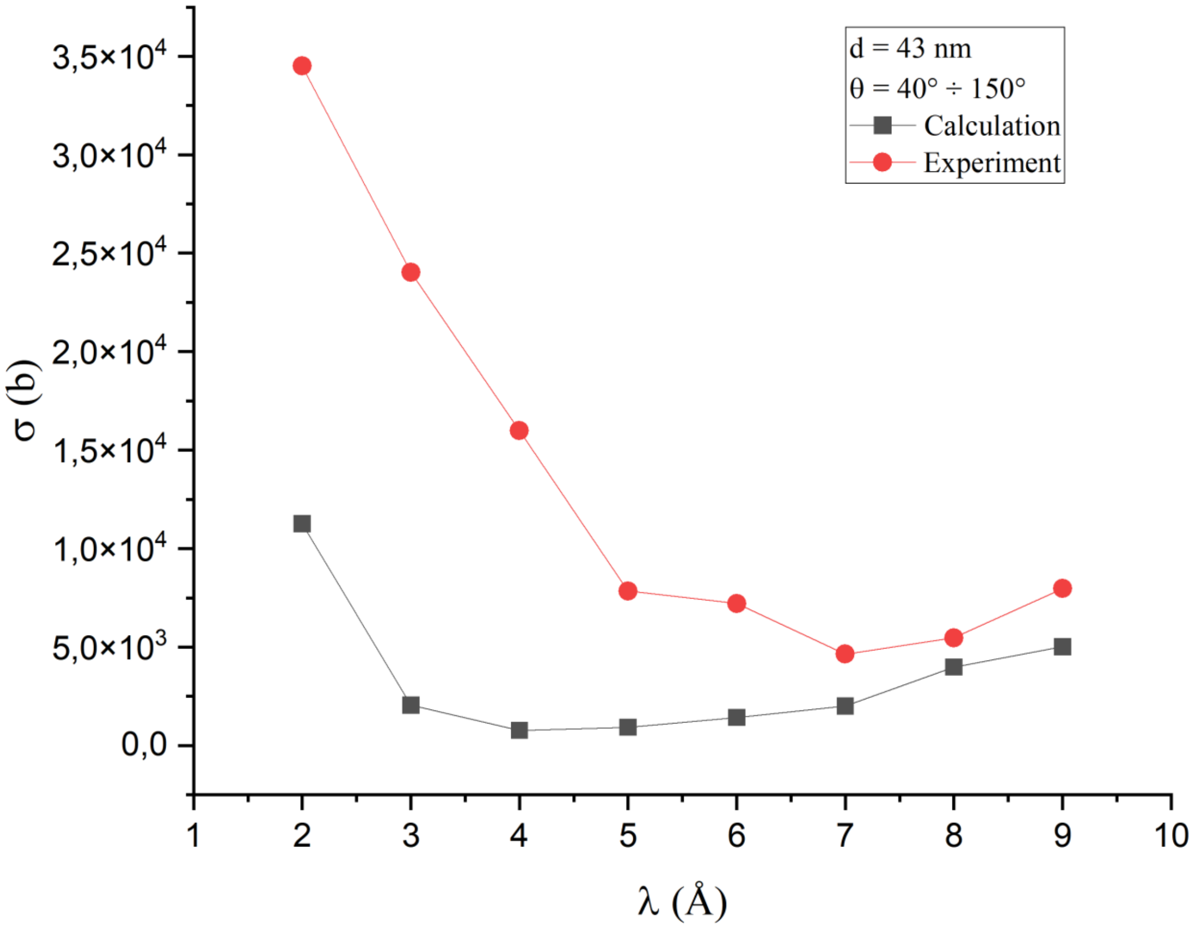
Comparison with the Experiment (preliminary)

- Experiment:
  - PF1b, ILL (Grenoble, France)
  - ToF
  - $\lambda = 2 \div 9$ Å, $\Delta\lambda = 0{,}2$ Å
  - $\theta = 10° \div 150°$
  - Cylindric sample holder: $d = 1{,}2\ cm$, $h = 2{,}8\ cm$
  - $\rho_{sample} \approx 0{,}4\ \frac{g}{cm^3}$
- Calculation:
  - $\sigma = \int_\Omega \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} \int_{\theta_1}^{\theta_2} \frac{d\sigma}{d\Omega} \sin\theta\, d\theta d\phi$
  - No particle rotation (i.e. wrong diffraction treatment)!

Comparison with the Experiment (preliminary)



σ(λ): angle range 10° ÷ 150°



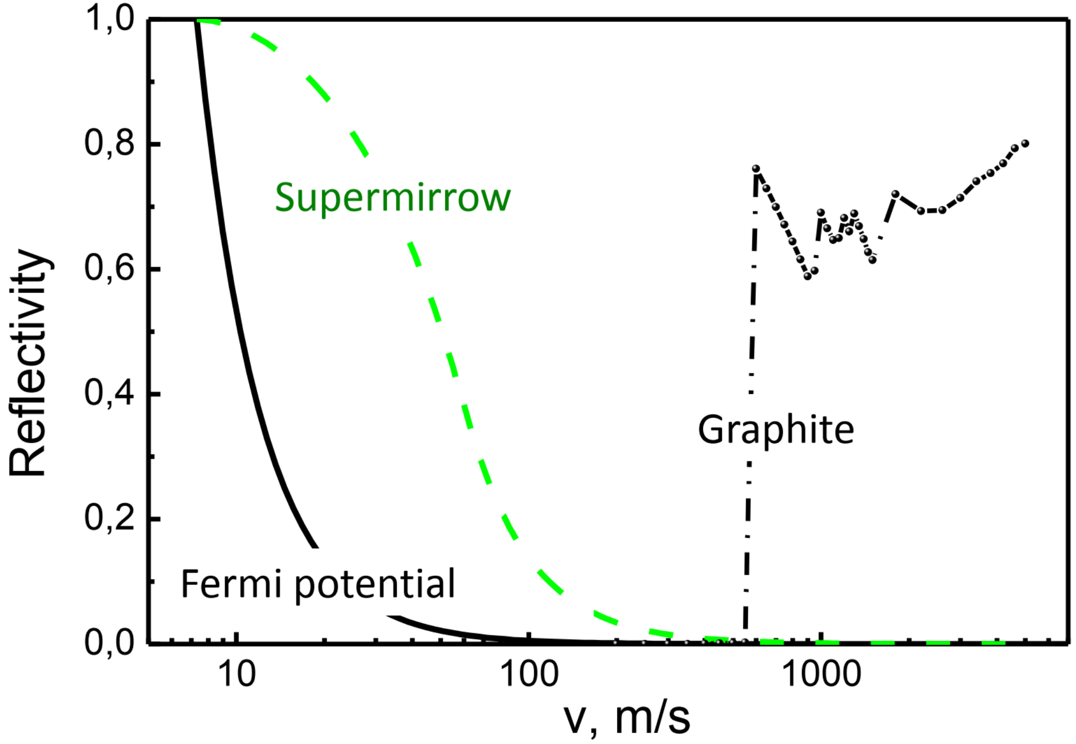
σ(λ): angle range 40° ÷ 150°

Conclusions and Future Plans

Ultracold Neutrons
<5-20 m/s

Very Cold Neutrons
~20-200 m/s

Cold Neutrons
~200-1000 m/s



The reflection probability for isotropic neutrons with different velocities.

Intercalated Graphite’s diffraction limit is around 9 Å.
Bragg’s cut-off for diamond is 4.1 Å.

<u>We continue to analyze the preliminary results.</u>

- However, the Intercalated Graphite seems to be an effective reflector for cold neutrons up to 9Å.
- Moreover, the nanodiamond diffraction data allow us to extend the existing models to cold and thermal neutron spectrum ranges.
- The results might be used for the development of advances reflectors, focusing systems, filters, environments of low-energy neutron sources!

Thank you all for your kind attention!

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