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Methodology for simulating the properties of nanostructured reflectors for very cold neutrons

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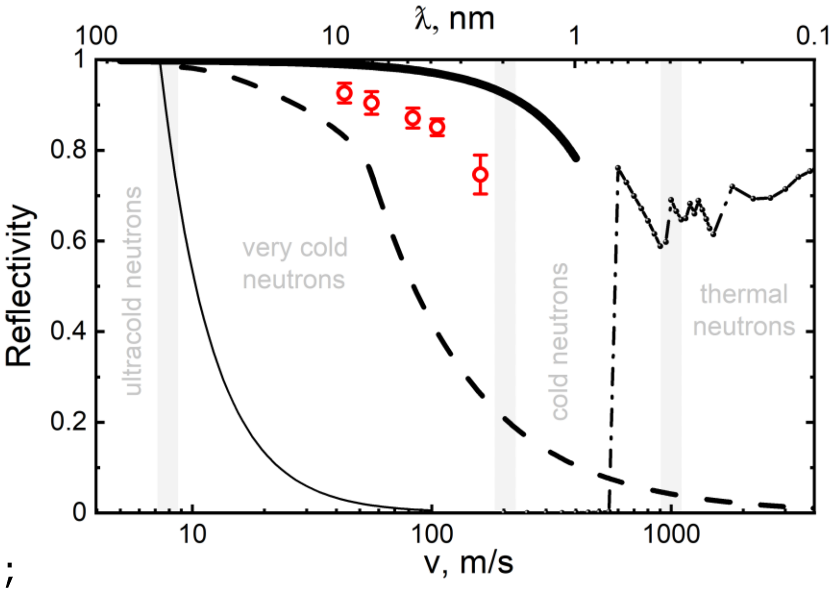
Low energy neutrons: what & why?

Very cold neutrons (VCN):
- the typical wavelengths are 2.5–60 nm;
- the velocities are 20–160 m/s;
- the energies are 0.25–130 μeV;
- the temperatures are 3×10^{-3}–1.55 K.

The VCN advantages are:
- long time of observation;
- larger phase shift;
- large coherent length;
- large capture cross-section ⇒ bigger contrast;
- structure analysis of large molecular complexes;
- large angles of reflections from mirrors; etc.

Neutron techniques **Fundamental physics**

<u>The main disadvantage is a low flux intensity!</u>



Workshops dedicated to the VCN applications and prospects:

21-24 August 2005, Argonne National Laboratory, USA. URL
13-14 February 2006, Paul Scherrer Institute, Switzerland.
27-28 April 2016, Oak Ridge National Laboratory, USA. URL
2-4 February 2022, European Spallation Source, Sweden. URL
9-10 May 2023, European Spallation Source, Sweden. URL
8-11 April 2024, Institute of Nuclear Physics, Kazakhstan. URL

Reflectors of very cold neutrons

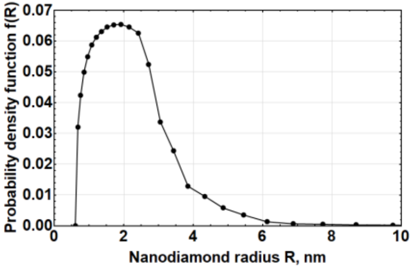
Criteria for the VCN reflector are minimum losses and maximum reflection.
Detonation nanodiamonds (DND) are the perfect candidate!

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

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

Positive Factors:
size distribution;
$b_{c.sc.}^{C} = 6.65\ fm$;
$\sigma_{c.sc.}^{C} = 5.55\ b$;
$\sigma_{abs}^{C} = 3.5\ mb$;
$\sigma_{in.sc.}^{C} \to 0\ (T \to 0)$;
$\rho^{Diamond} \approx 3.5\ g/cm^3$.

$\boldsymbol{P_{REF} \sim 95\%}$



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. %

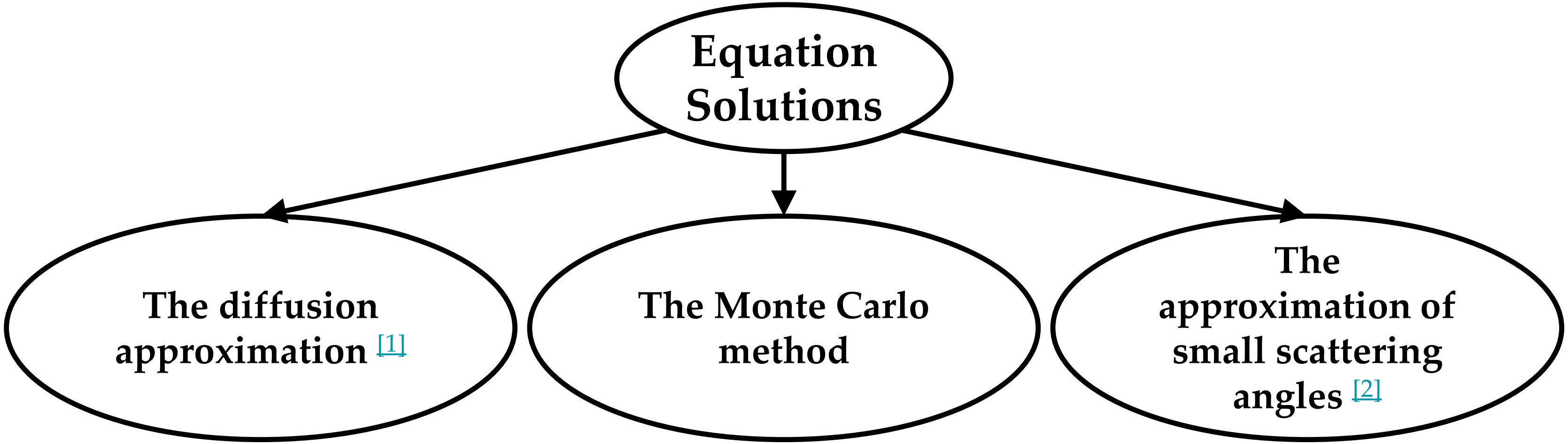
→ neutron capture
→ neutron activation

Neutron Transport Equation

Artem’ev V.A. // Vopr. At. Nauk. Tekh., Ser. Fiz. Yad. Reakt., Vol. 1–2, P. 7–12 (2003).

$$\frac{1}{v_{eff}}\cdot\frac{\partial\varphi}{\partial t} = -\mathbf{\Omega}\nabla\varphi - \Sigma_t\varphi + \int d\mathbf{\Omega}'\varphi(\mathbf{r},\mathbf{\Omega}',t)\Big[\Sigma_s W_s(\mathbf{\Omega}'\to\mathbf{\Omega}) + \Sigma_{coh}^{(m)} W_{coh}^{(m)}(\mathbf{\Omega}'\to\mathbf{\Omega}) + \Sigma_{coh}^{(p)} W_{coh}^{(p)}(\mathbf{\Omega}'\to\mathbf{\Omega})\Big] + q(\mathbf{r},\mathbf{\Omega},t)$$

Total cross-section
=
scattering + losses



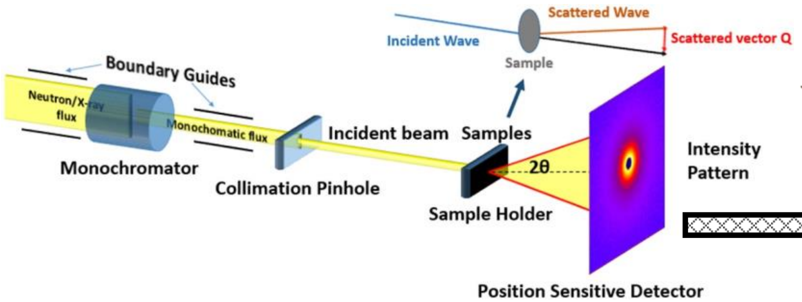
Equation Solutions

The diffusion approximation [1]

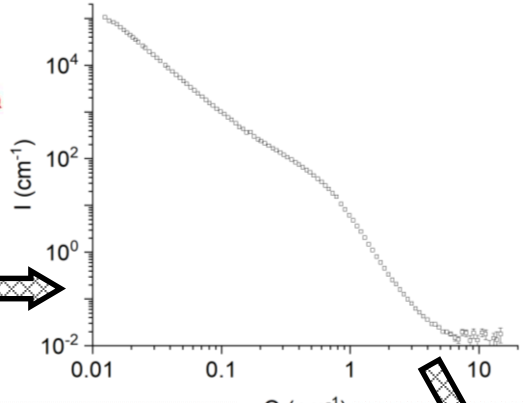
The Monte Carlo method

The approximation of small scattering angles [2]

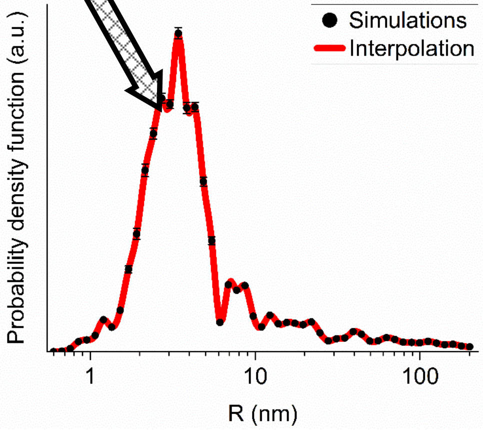
Models of nanopowder structure and neutron transport

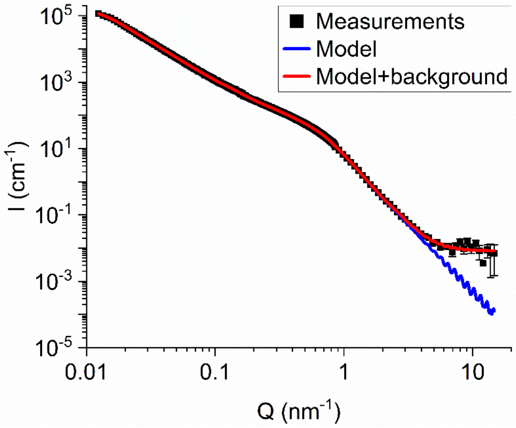


The typical scheme of the SANS experiment.

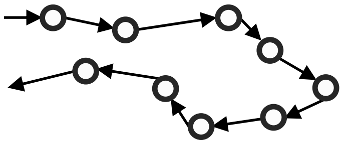


Measured intensity I of scattered neutrons as a function of the transferred momentum Q for the powder of detonation nanodiamonds.

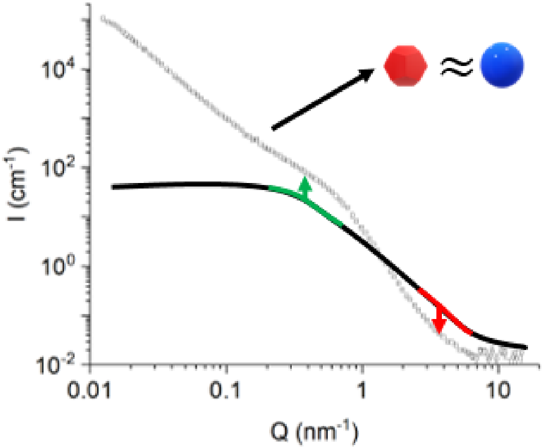




As a result, we have the capability to simulate a multi-scattering process via a single scattering cross-section.



Model’s self-consistency and verification

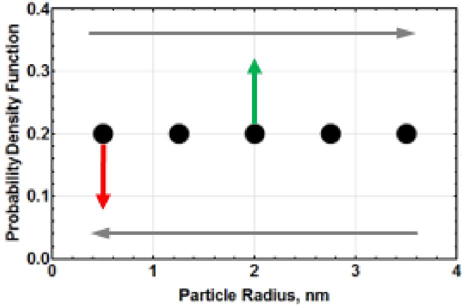


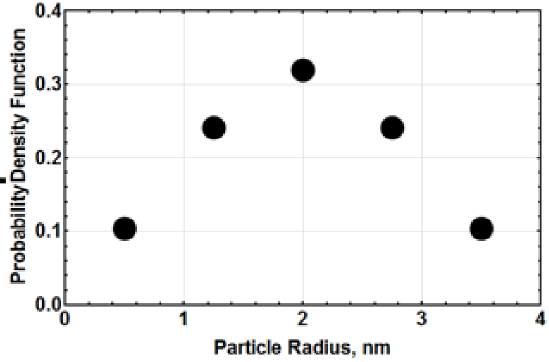
Measured intensity for the DND sample.

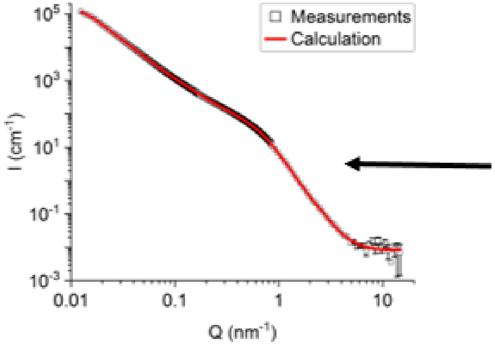
$$I(q) \equiv \frac{d\Sigma_s(q)}{d\Omega} = \int_{r_{min}}^{r_{max}} N \cdot f(r) \frac{d\sigma_s(r,q)}{d\Omega} dr$$

N – the averaged nanospheres concentration;

f(r) – a fraction distribution of particles with the radius of r.





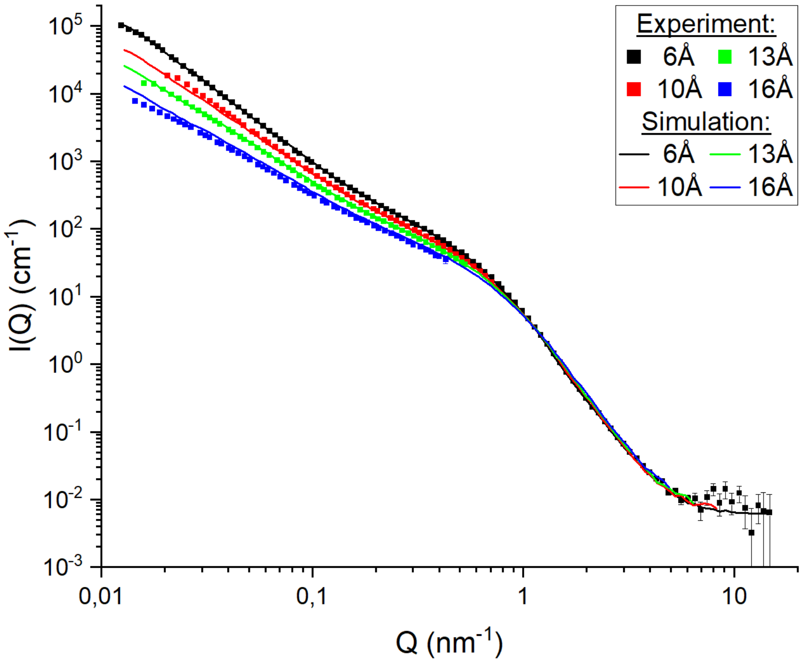


Self-consistency of the model was checked by variation of:

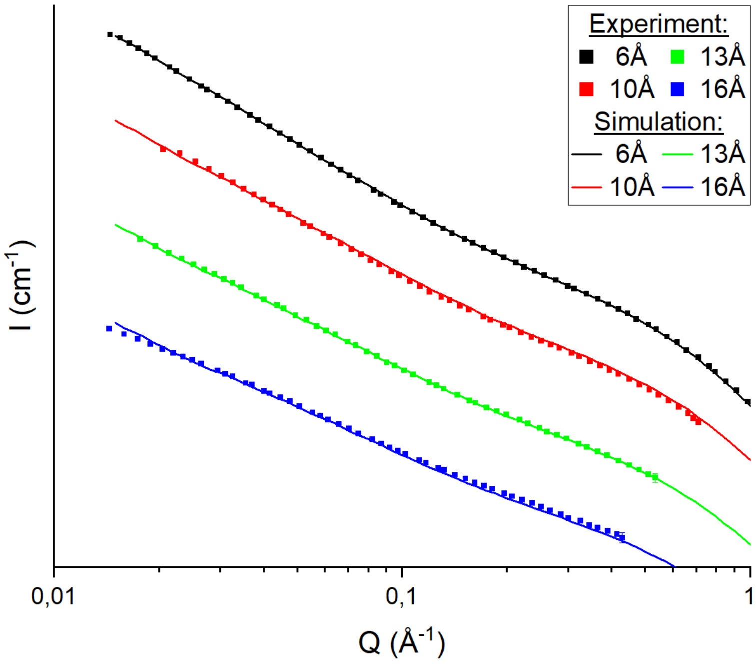
- variance σ of the initial distribution;
- number of discrete points;
- linear/log uniformity scales;
- etc.

Model's self-consistency and verification: Fluorinated nanodiamonds

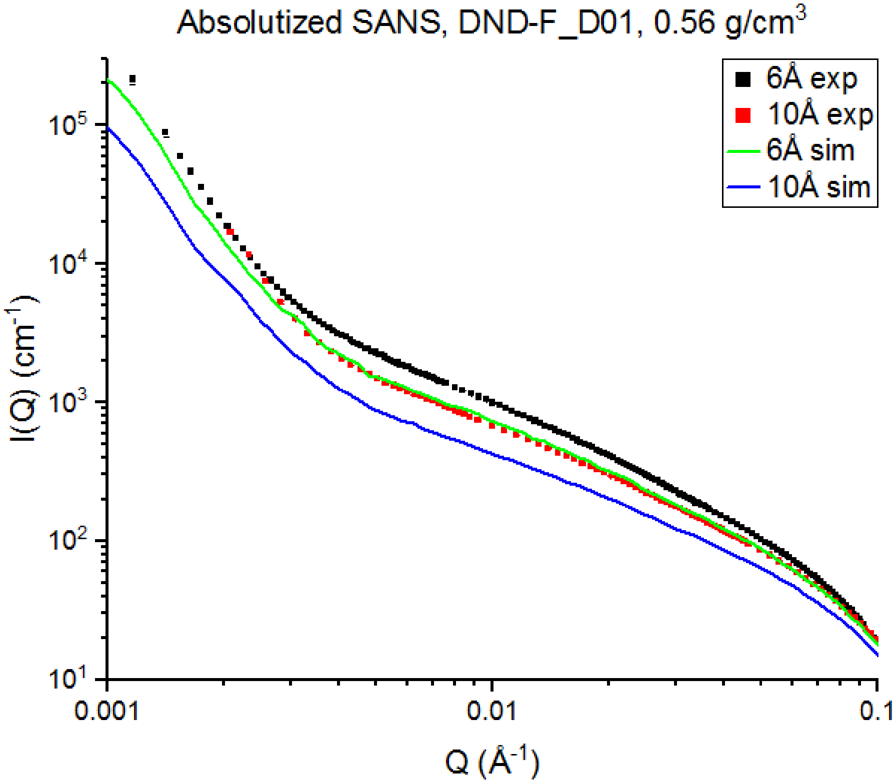
Absolutized SANS (F-DNDs, 0.39 g/cm^3)



F-DNDs SANS, 0.39 g/cm^3



Model's self-consistency and verification: Deagglomerated fluorinated nanodiamonds



- SANS was measured for a layer thickness of 1 mm.
- The bulk density of ~0.2 g/cm^3 is OK.
- The bulk density of >0.5 g/cm^3 is not OK.

One has to measure

a thinner layer of a nanodiamond powder

OR

a less denser nanodiamond powder

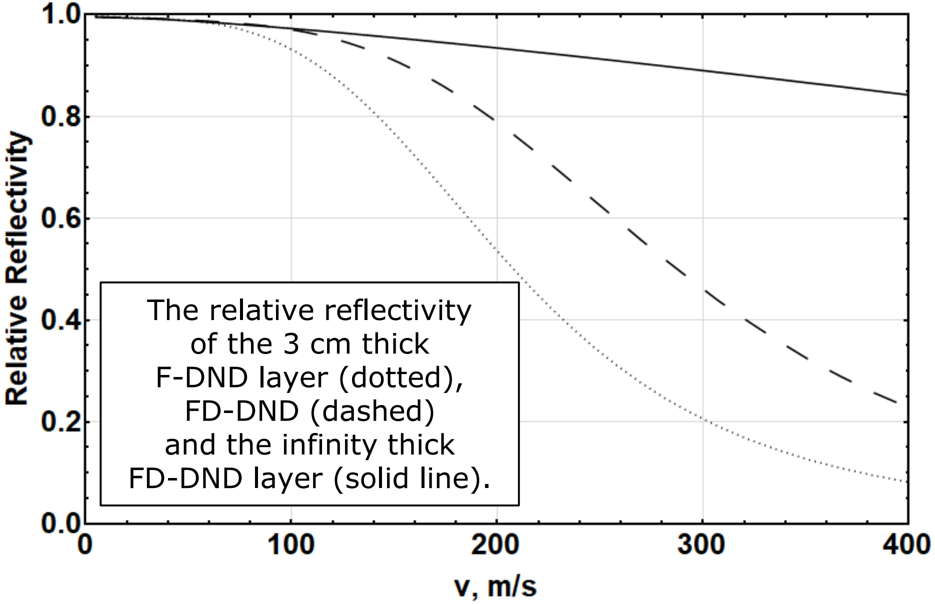
OR

to use a shorter wavelength of neutrons

for development the corresponding model.

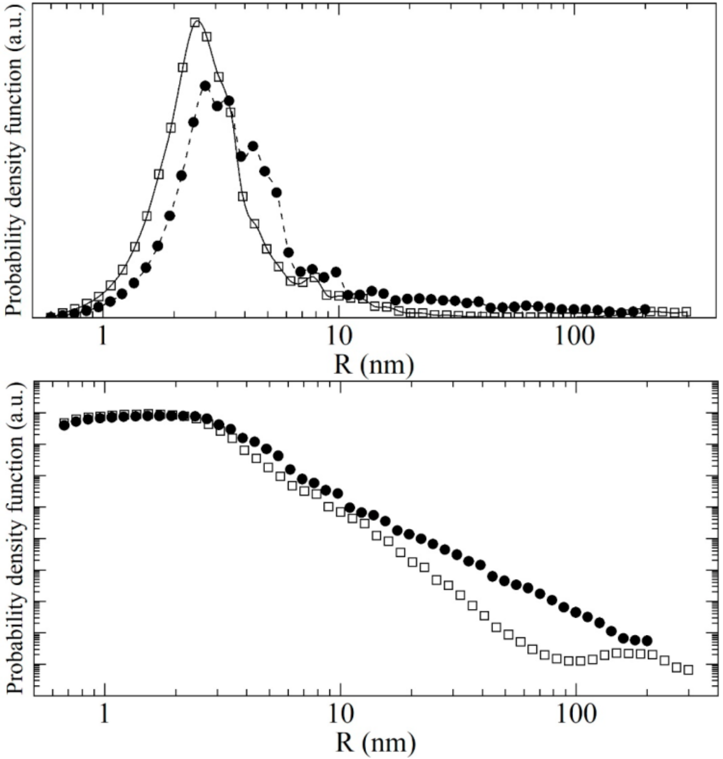
Deagglomeration: nanoparticle cluster breaking

$$P_{REF}^{after}/P_{REF}^{before} \approx 1.10$$
$$\rho_{bulk}^{after}/\rho_{bulk}^{before} \approx 3$$

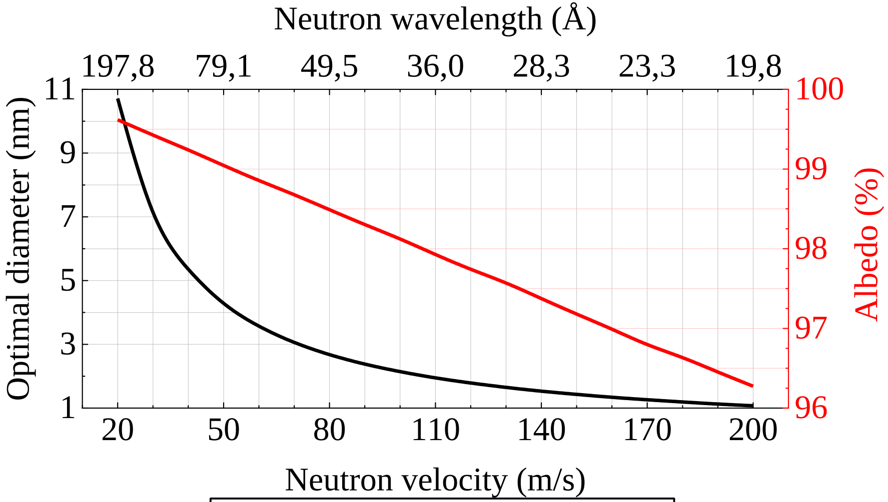


The relative reflectivity of the 3 cm thick F-DND layer (dotted), FD-DND (dashed) and the infinity thick FD-DND layer (solid line).

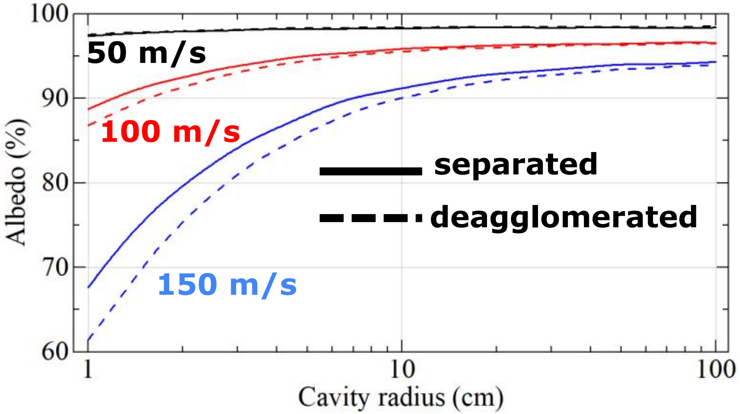
Size distributions of the fluorinated F-DND (dotted) and the deagglomerated FD-DND (solid).

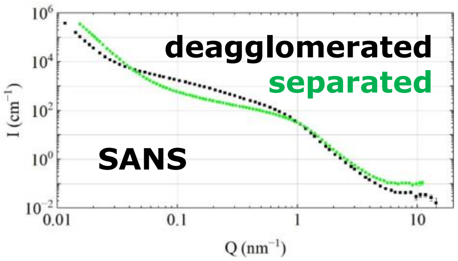


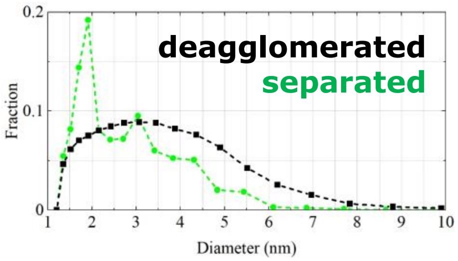
Size separation of nanoparticles

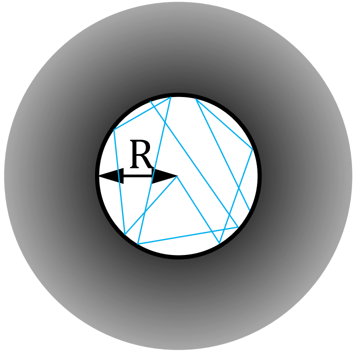


$$P_{REF}^{max}\colon\ R_{opt} \approx 0.27\lambda$$









Conclusions

- The MC numerical solution of the neutron transport equation was implemented.
- The approach for extrapolating the experimental results and extracting the structural parameters was developed.
- The model was validated and used to simulate the neutron albedo for different geometries.

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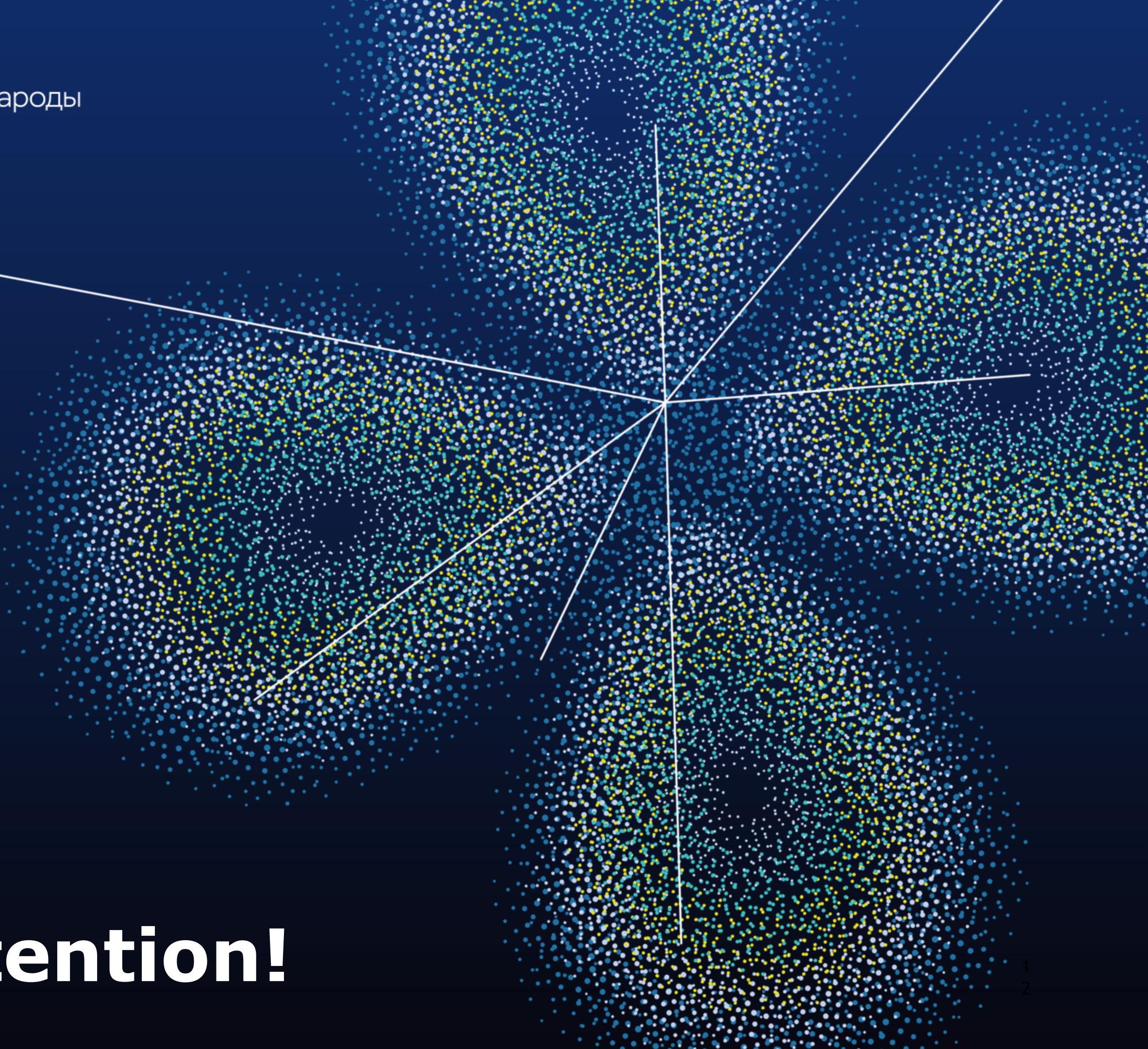

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