Structural Analysis of Submicron and Nanomaterials Based on the SANS Method

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Small-Angle Neutron Scattering (SANS)

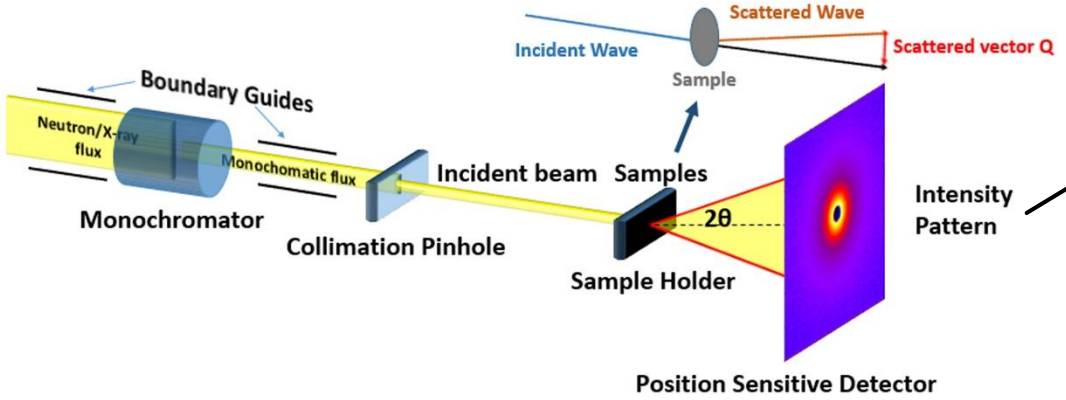


Fig. 1. The typical scheme of the SANS experiment.

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

$\sigma_s(r,q) \sim r^6$ – a microscopic elastic scattering cross-section;

$n(r)$ – a concentration distribution of particles with the characteristic size of r.

The size range available for study is from 1 nm to 1 μm.

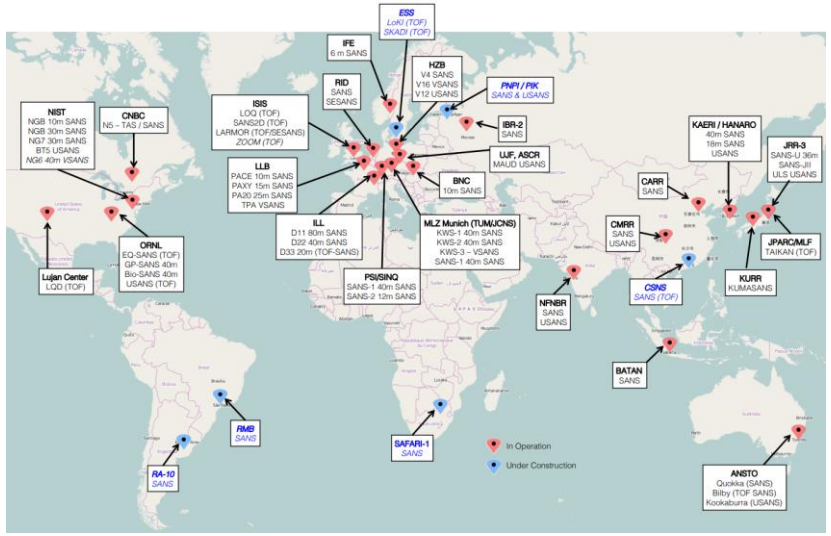


Fig. 2. The world map of SANS instruments.

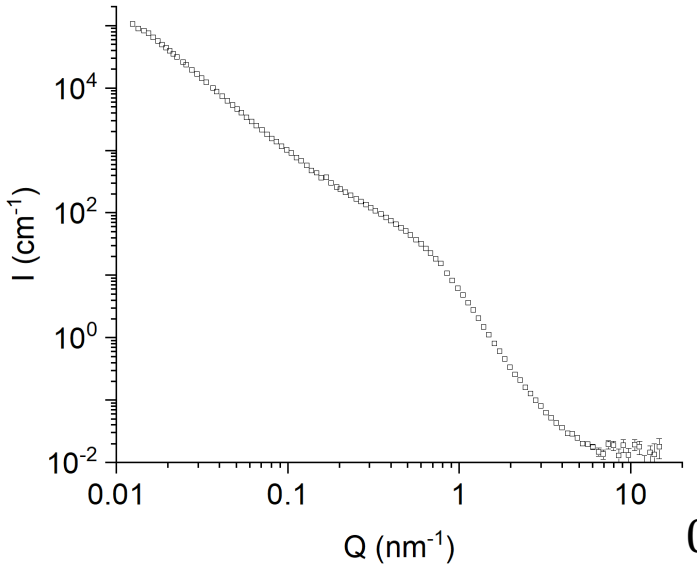


Fig. 3. Measured intensity I of scattered neutrons as a function of the transferred momentum Q for the powder of detonation nanodiamonds (DND).

$0.6\ nm \leq r \leq 200\ nm$

Small-Angle Neutron Scattering (SANS)

The diversity of SANS techniques:

- Very Small-Angle Neutron Scattering;
- Ultra Small-Angle Neutron Scattering;
- Grazing-Incidence Small-Angle Neutron Scattering
- Spin-Echo Small-Angle Neutron Scattering;
- Spin-Echo Modulation Small-Angle Neutron Scattering.

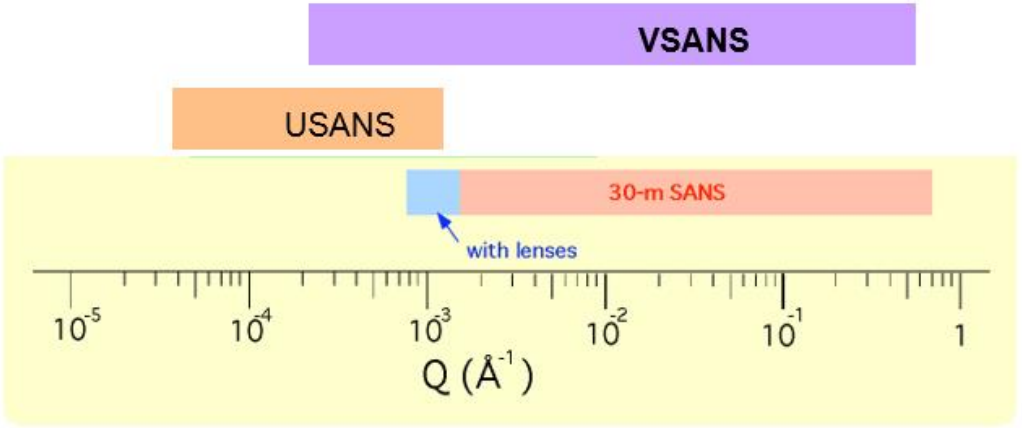


Fig. 4. The limits of Q range for different SANS.

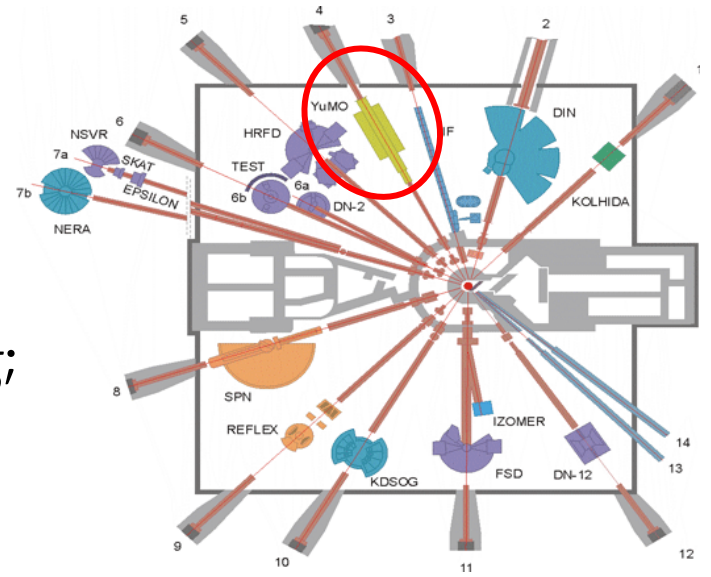


Fig. 5. The scheme of the IBR-2 experimental halls with the YuMO installation in Dubna, Russia.

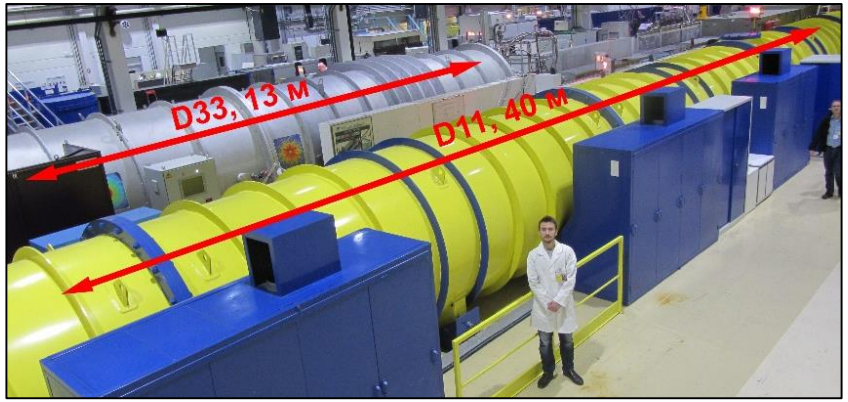


Fig. 6. The SANS installations of D11 and D33 at the ILL, France.

Exponential/Power-Law Approximation

$$I(q) = G \cdot exp\left(-\frac{q^2 R_g^2}{3}\right) + B \cdot exp\left(-\frac{q^2 R_{gS}^2}{3}\right)\left(\frac{1}{q^*}\right)^P + G_s \cdot exp\left(-\frac{q^2 R_{gS}^2}{3}\right) + B_s\left(\frac{1}{q_S^*}\right)^{P_S},$$

$$q^* = q\left[erf\left(6^{-1/2} k q R_g\right)\right]^{-3},\ q_S^* = q\left[erf\left(6^{-1/2} k_S q R_{gS}\right)\right]^{-3}.$$

R_g and R_{gS} are radii of gyration of the clusters and subparticles; P_S is the index that characterizes the surface of DND particles;
P is related to the fractal dimension of DND aggregates; k, k_S are empirical constants;
G, G_S, B, B_S are proportional to the density of scattering centers and to contrast; I_{bkg} is residual incoherent background.
The parameters without an index characterize the scattering by clusters; the parameters with index S apply to nanoparticles.

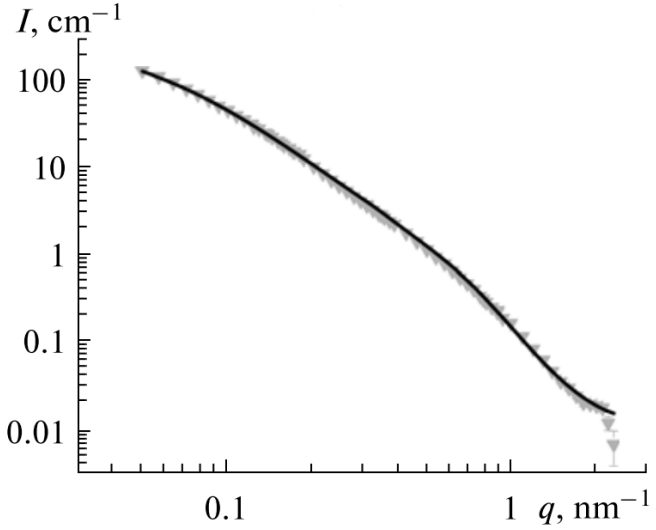


Fig. 7. An approximation example of a SANS curve for the DND solution of 1 wt % [2].

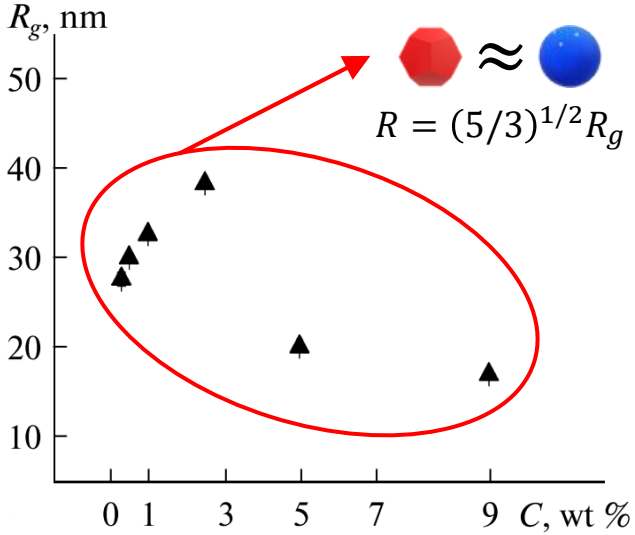


Fig. 8. The calculated radius of gyration R_g as a function of the DND concentration C [2].

More information in [1] by L.A. Feigin, D.I. Svergun.

R/R_g and other structure parameters are ONLY the averaged characteristics!

What if one wants to have the size distribution of scatterers?

It might be considered within a polydispersity index formalism [3], [4]. It is a model-depended approximation which one can't use in specific tasks, for example, in the scattering models of low-energy neutrons.

Developed Approach

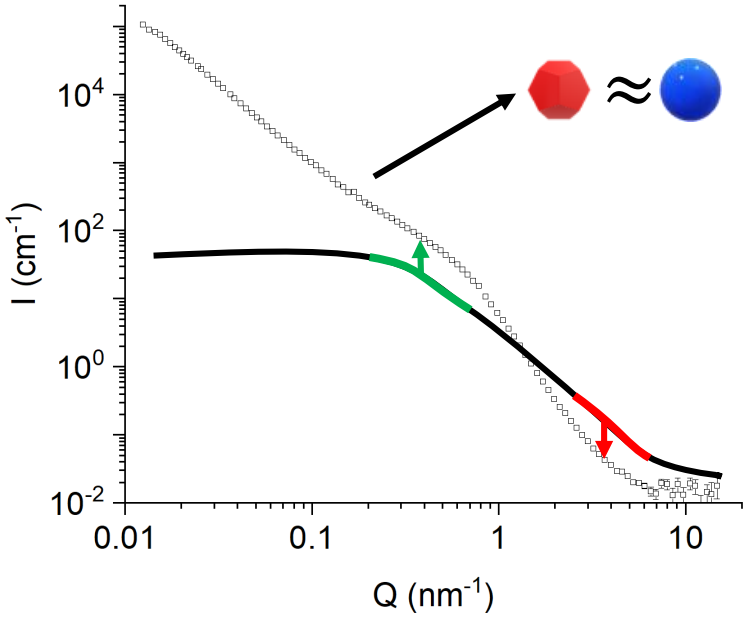
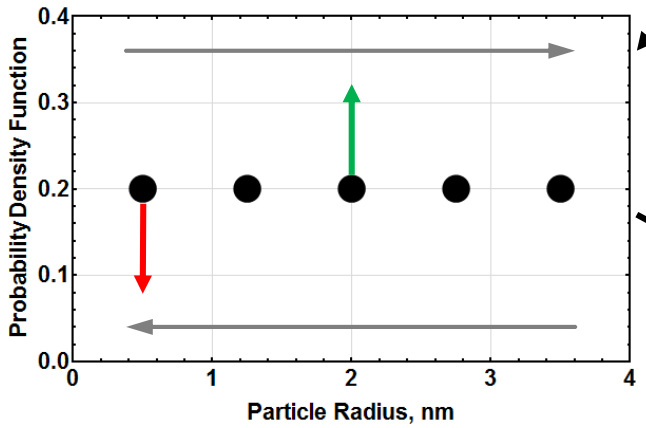


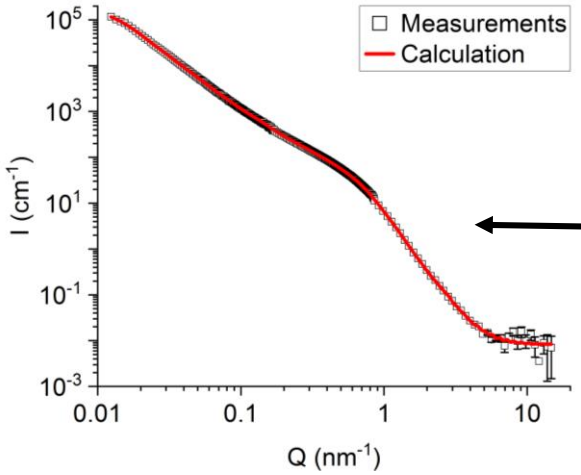
Fig. 9. Measured intensity for the DND sample.

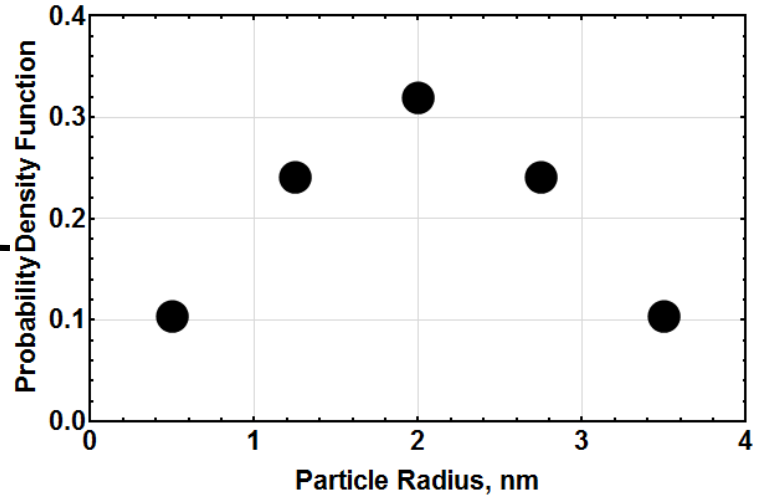
$$I(q) \equiv \frac{d\Sigma_s(q)}{d\Omega} = \int_{r_{min}}^{r_{max}} N \cdot f(r) \frac{d\sigma_s(r,q)}{d\Omega} dr$$



N – the averaged nanospheres concentration;

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

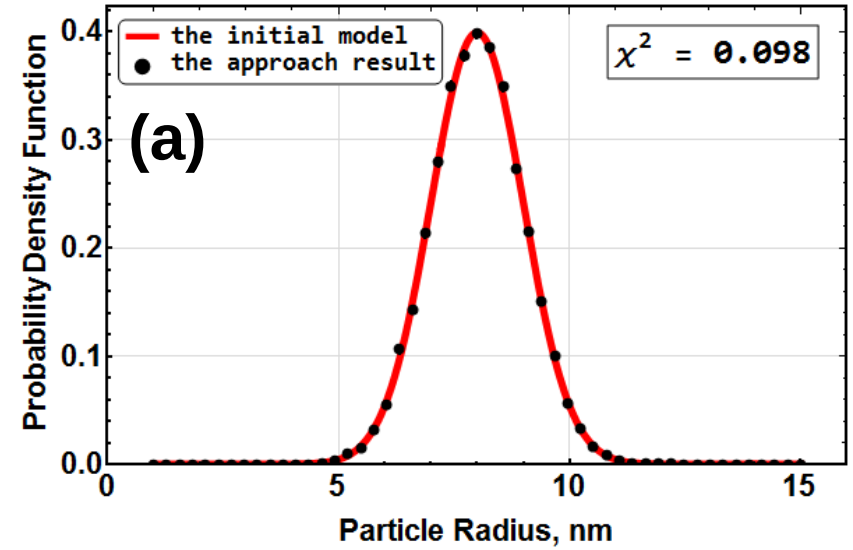


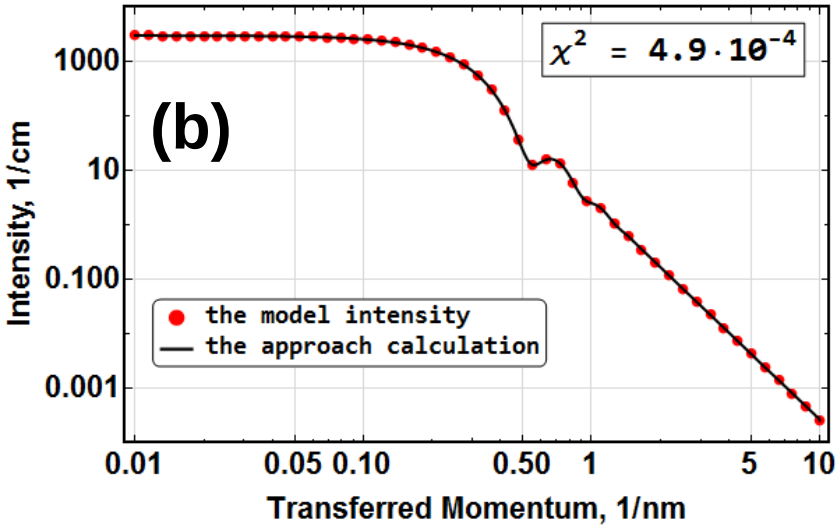


The approach is similar to the Maximum entropy method, implemented, for example, in the Iren package [5] for Igor Pro software.

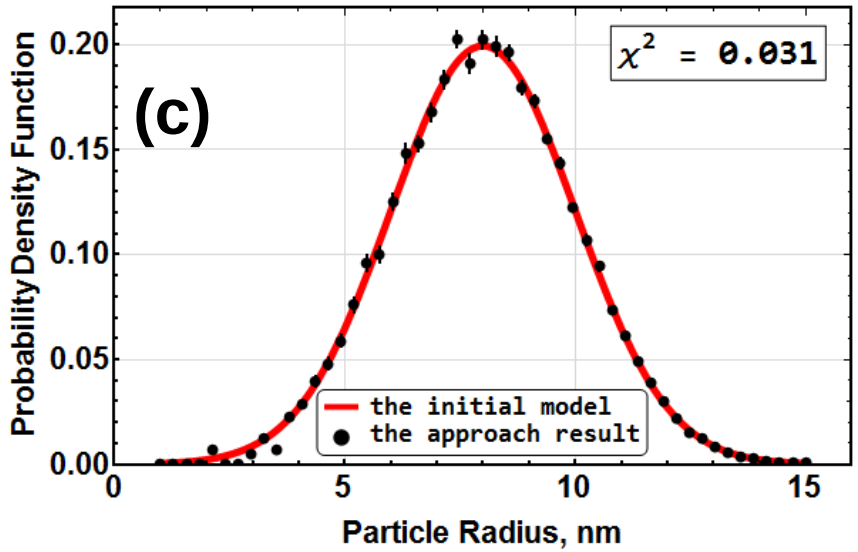
Approach Adequacy: the stability at different variance σ

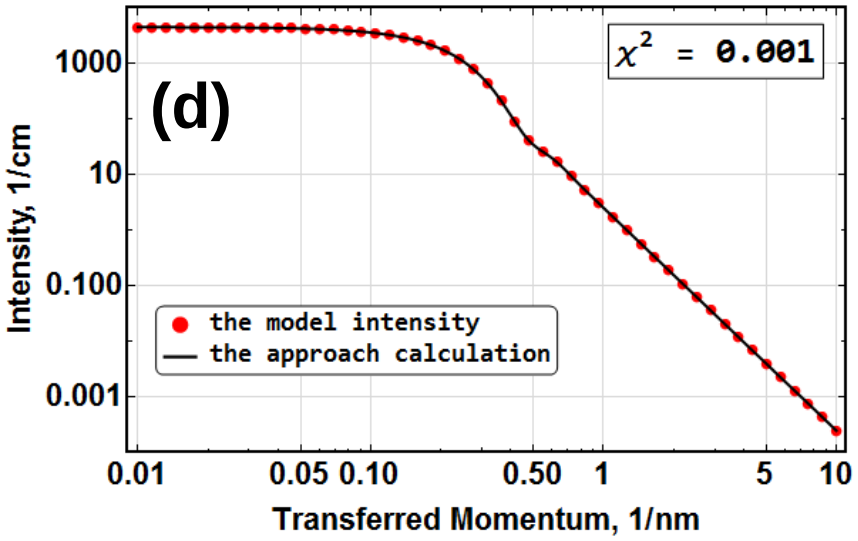
Preliminary results!





σ = 1

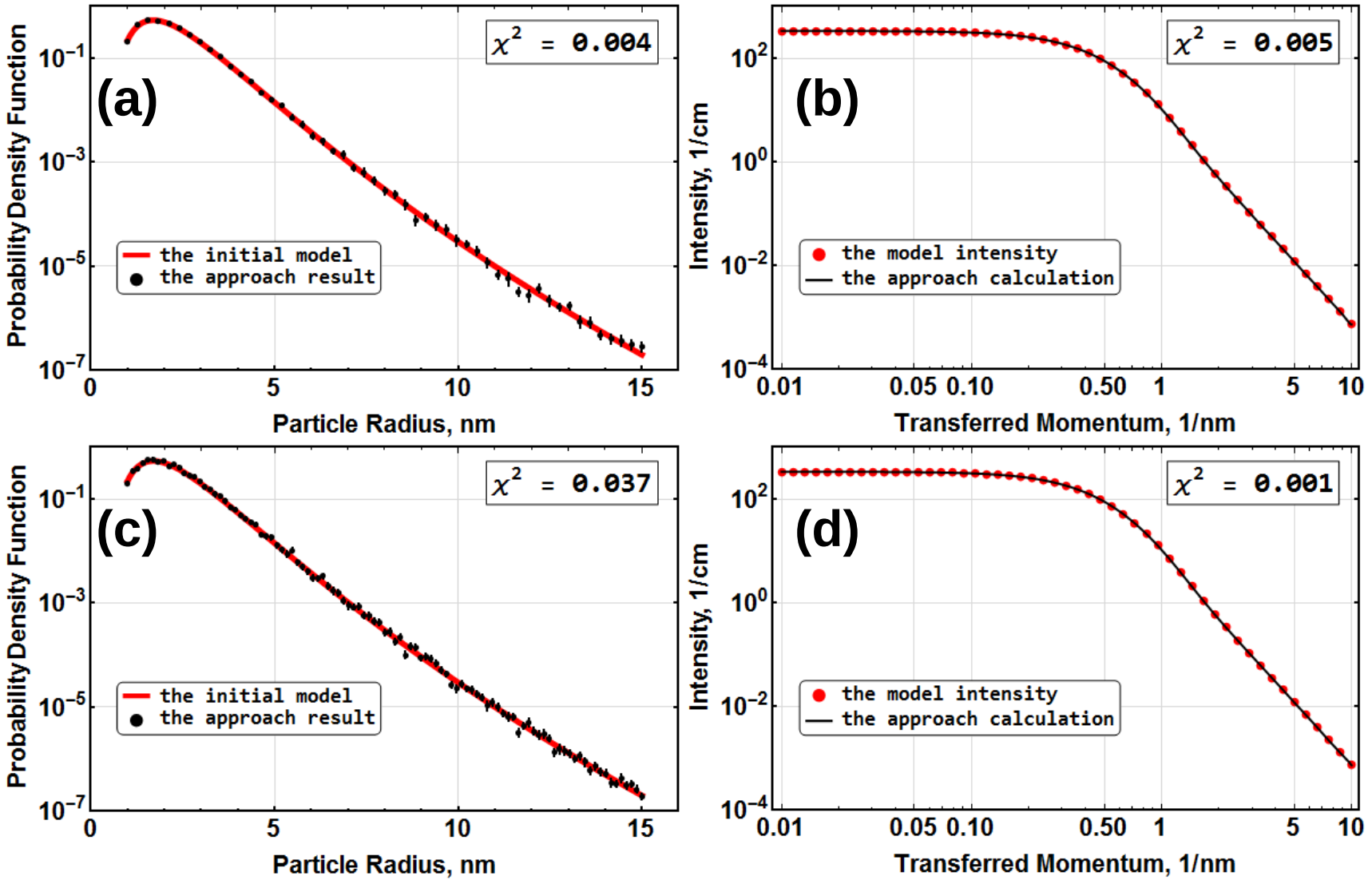




σ = 2

Approach Adequacy: different number N of points

Preliminary results!



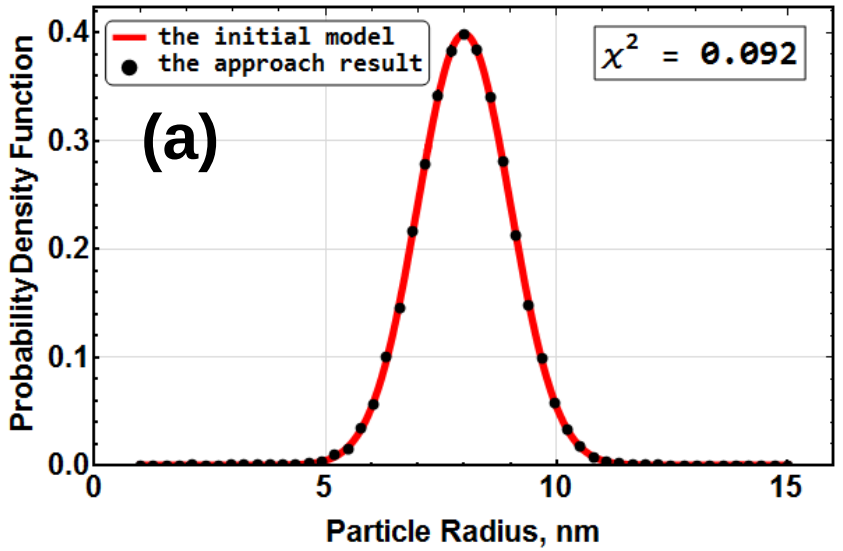
N=50

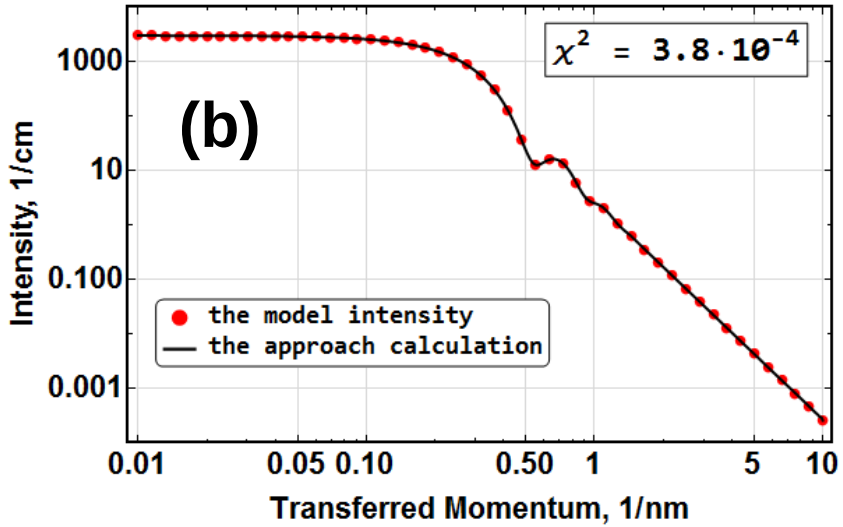
N=100

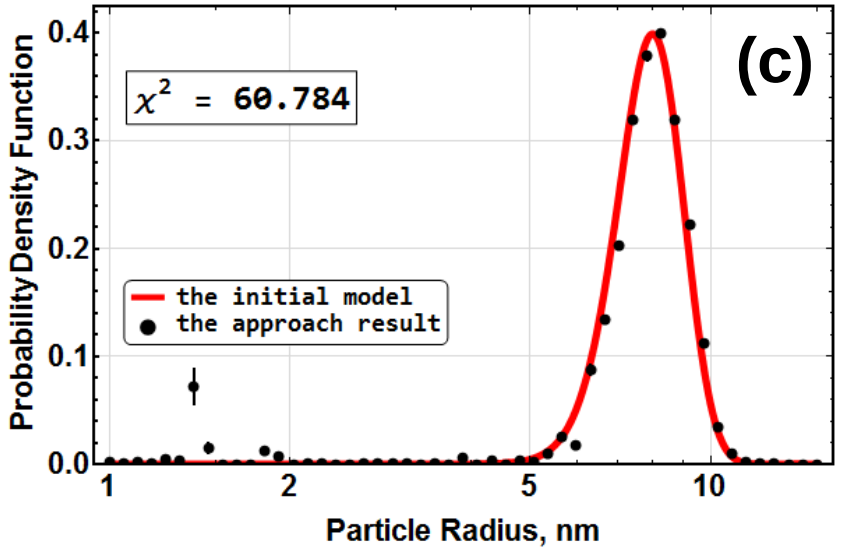
Approach Adequacy: the different uniformity scales

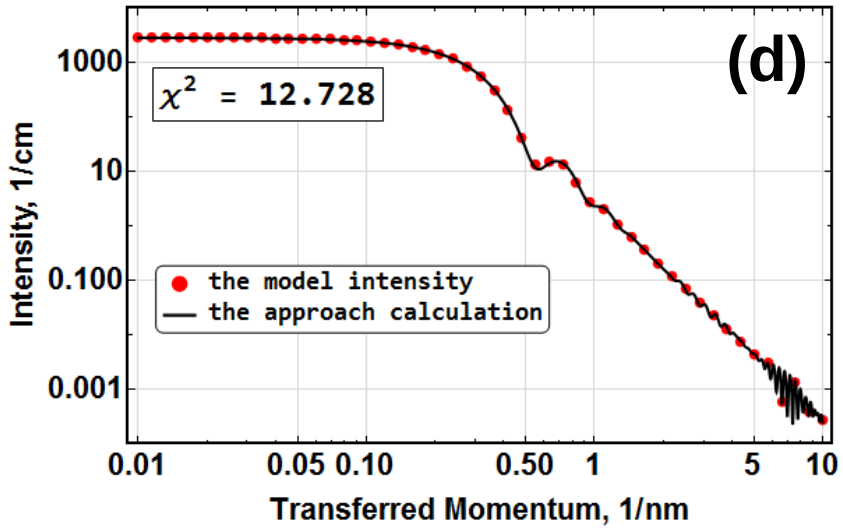
Linear

Log









The problem was solved in 2020!

Possible Applications – Modification of Nanosystems

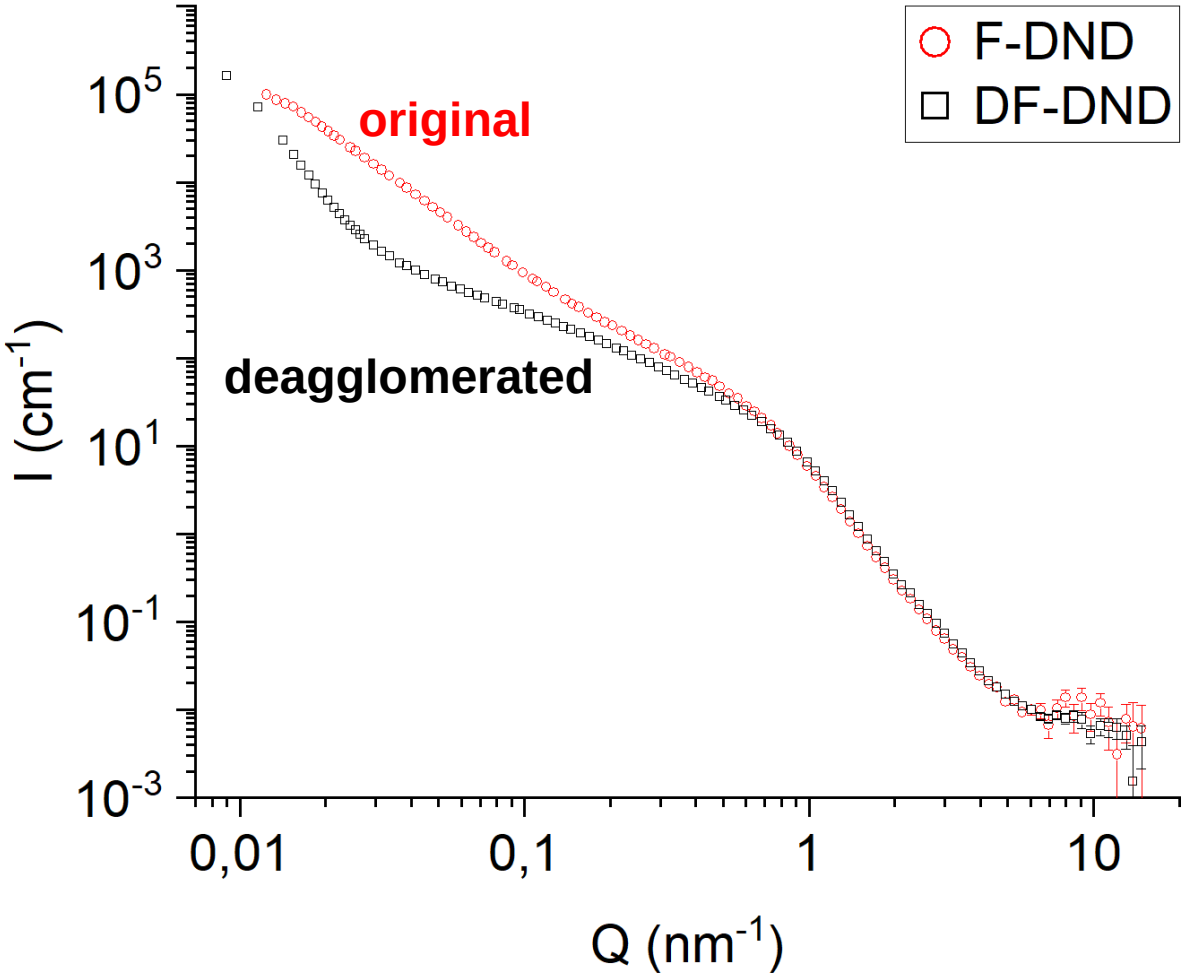


Fig. 10. Measured intensity I of scattered neutrons as a function of the transferred momentum Q for the powder of DND.

Preliminary results!

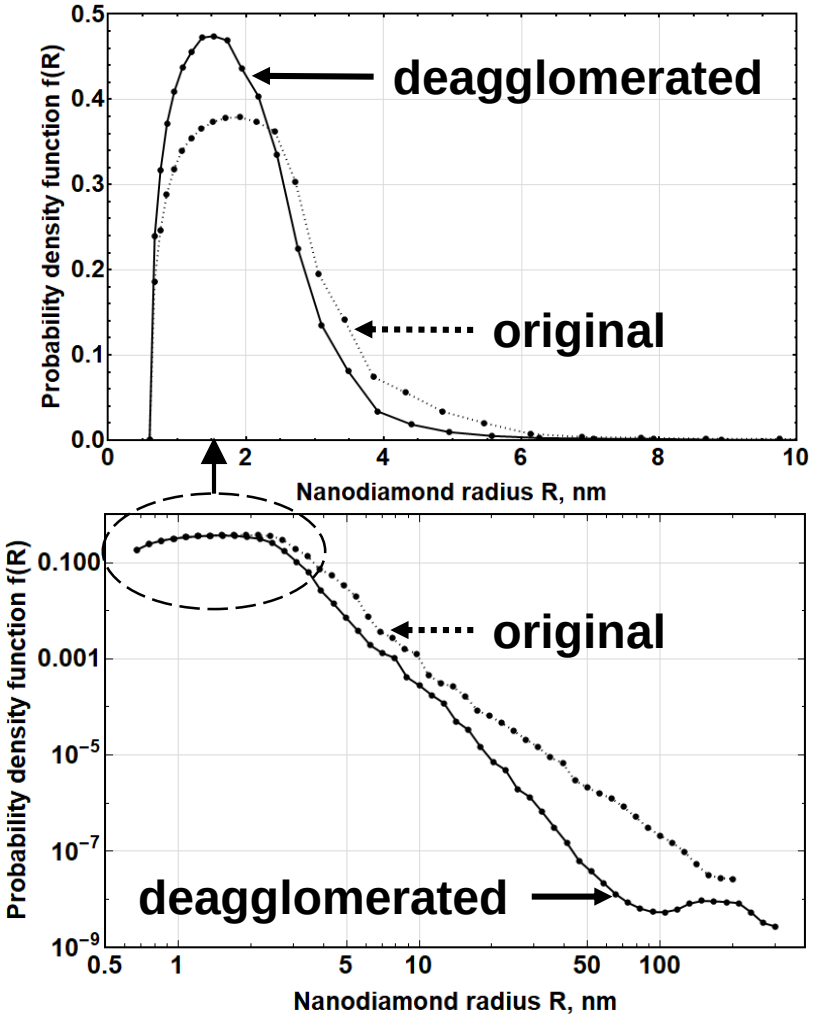


Fig. 11. Size distributions of the original and deagglomerated DNDs.

Scientometrics & Plans for the Close Future


РОССИЙСКАЯ ФЕДЕРАЦИЯ

СВИДЕТЕЛЬСТВО

о государственной регистрации программы для ЭВМ

№ 2020662675

Structural Nanopowders Analyzer Based on Small-Angle Scattering Data (SNASAS)

Правообладатель: Объединенный Институт Ядерных Исследований (RU)

Автор: Незванов Александр Юрьевич (RU)

Заявка № 2020661661
Дата поступления 05 октября 2020 г.
Дата государственной регистрации в Реестре программ для ЭВМ 16 октября 2020 г.

Руководитель Федеральной службы по интеллектуальной собственности

Г.П. Ивлиев

The certificate of state registration of the software "Structural Nanopowders Analyzer Based on Small-Angle Scattering Data (SNASAS)", RU2020662675.

SNASAS results were used in 2 articles.

We are constantly working on testing, modifying and improving the approach.

We will continue to investigate the approach stability:

- the mean value of the distribution;
- accounting for statistical errors in experimental data;
- description of SANS data from particles with a multimodal size distribution.

The detailed approach description would be published in 2021–2022.

Conclusions

1. The approach has been developed for extracting the model-independent size distribution of scatterers.
2. It is tested for self-consistency and stability.
3. It is successfully applied on real SANS data.
4. The application is found in problems of low-energy neutron transport. Are there others?

Thank you all for your kind attention!

Please share the presentation with your colleagues working with nanoparticles or its clustering!

Feel free to contact me if you are interested in your data processing.

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