Methodology for Simulating the Properties of Nanostructured Reflectors for Very Cold Neutrons

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At the moment, many neutron research centers around the world are aiming to increase the range of useful neutrons while lowering their energy. Such neutrons are very promising for fundamental research and condensed matter studies. However, progress in this field is limited by the relatively small fraction of low-energy neutrons in the total flux and the low efficiency of their delivery to research facilities. Once the wavelength of neutrons reaches the interatomic distance, they begin to interact less efficiently with homogeneous media, pass through reflectors, and are not delivered to the facilities. The use of nanodispersed media, consisting of particles a few nanometers in size, solves this problem. Cold (CN) and very cold neutrons (VCN) are reflected from such materials due to intense coherent elastic scattering on an ensemble of nuclei, the individual nanoparticles [1].

Unique nanostructured reflectors of CN and VCN based on detonation nanodiamonds (DNDs), which have no effective analogs in the world, are being developed in the JINR FLNP. However, applications of such nanostructured reflectors and further optimization of their properties require the development of adequate models of both the nanopowders themselves and the propagation of slow neutrons in them [2]. The JINR FLNP has been engaged in the related studies for the last 20 years, and its results will be presented in the report.

For a quantitative analysis of neutron scattering on DNDs and their clusters, we developed the following model of discrete-size diamond nanospheres. We simulated both the DNDs and their clusters with diamond nanospheres. We assumed a discrete set of nanosphere sizes, in which the next generation nanosphere radius is larger than the previous one by a certain factor. In the calculations presented below, the radii are uniformly distributed on a logarithmic scale, with 20 values of the radius by an order of magnitude.

We adjusted populations of DNDs/clusters of each generation to fit the experimental data of small-angle neutron scattering. The fitting procedure is stable with respect to the parameter choice of the model (the initial populations of cluster generations, the step of increasing the mass of clusters of the next generation, the boundaries of the mass range if it sufficiently broad).

The obtained distribution of scatterers' sizes provides the differential cross-section of single elastic neutron scattering. We used this cross-section to simulate the multiple scattering of low-energy neutrons in a nanodispersed medium. Moreover, it does not matter in this case what method, exact or approximate, to use for the calculation of scattering cross-sections on a spherical particle. It is important that it be used for the simulation of neutron diffusion.

Models' benchmarking, various results of simulation of CN and VCN scattering on different nanodiamond powders will be presented.

References

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2. Frei, A., et al. "Fluorination of Diamond Nanoparticles in Slow Neutron Reflectors Does Not Destroy Their Crystalline Cores and Clustering While Decreasing Neutron Losses." *Materials* 13 (2020): 3337.