

# Comprehensive Elemental Analysis of Nanodiamonds for Simulating the Properties of Cold and Very Cold Neutron Reflectors

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Neutron reflectors are widely used to store, extract, focus and deliver neutrons to experimental facilities. For the last almost 20 years, Detonation NanoDiamond (DND) powders have been actively studied as a material for efficient diffuse reflectors of Very Cold Neutrons (VCN) with the velocities of 40-150 m/s. Moreover, the DND powder reflects cold neutrons (up to 1000 m/s) quasi-specularly at small grazing angles of incidence of the neutron beam. The use of such reflectors will make it possible to increase the neutron fluxes and expand the scope of VCN applications. But the experimental research of the properties of advanced nanodiamond reflectors is a highly challenging task. It is connected with problems of having a large amount of DND powders and developing a complex system of neutron detectors. Therefore, the simulation seems to be the easiest way to study the characteristics of neutron reflectors made of DND.

In earlier works [1–3], we proposed the model of neutron transport in DND powders based on the data of small angle neutron scattering on DND and its agglomerates. We used this model to analyse the structure of DND powders and to simulate the reflection of VCN from the raw, deagglomerated, and size separated DND. However, the impurity composition of DND powders has never been counted due to the emphasis on structural analysis in these studies. Nevertheless, the impurities also affect the properties of nanodiamond reflectors to no lesser extent. Neutrons are captured by the nuclei of the trace elements in the DND powders. As a result, the performance of the nanodiamond reflector is degraded.

To calculate the total neutron capture cross-section, it is necessary to provide the most complete quantitative elemental analysis. In this work, we used x-ray photoelectron spectroscopy (XPS), prompt gamma-ray neutron activation analysis (PGNAA), and neutron activation analysis (NAA). Methods are sensitive to certain elements. They complement each other to identify all possible nuclei of elements that are responsible for neutron capture in DND powders. XPS provides information about the fractions of such elements in DND powders as carbon (C), oxygen (O), nitrogen (N), and fluorine (F). PGNAA and NAA are neutron methods that measure the induced activities for impurities. And it is the most natural way to study the absorbing properties of neutron reflectors. PGNAA allows obtaining the concentration of C, N, hydrogen (H), boron (B), chrome (Cr), chlorine (Cl), and others whereas NAA measures the concentrations of elements activated in high neutron fields (basically metals). Considering the full composition of impurities in DND powders allows simulating the properties of nanodiamond reflectors for different applications in neutron physics.

The methods of comprehensive elemental analysis of different DND powders, as well as the effect of impurities on the neutron reflection, will be discussed. We will also present the simulation results of neutron reflection from flat DND layers and the VCN storage inside spherical traps with walls made of DND powders.

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## References

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