Title: 2nd Meeting of the Subcommittee on Fundamental Physics of WP3

Tuesday 08.07.2021 at 14:00-17:00 CET via videoconference

Chair: Valery Nesvizhevsky (ILL)

Participants:

Subcommittee members:

Sergey Grigoriev, PNPI // WP3 PIK

Ekaterina Korobkina, North Carolina SU // WP3 PIK

Egor Lychagin, JINR // WP3 PIK

Valery Nesvizhevsky, ILL // WP3 PIK

Vladimir Voronin, PNPI // WP3 PIK

PNPI speakers and attendees:

Sergey Grigoriev, PNPI // WP3 PIK

Vladimir Voronin, PNPI // WP3 PIK

Invited guests:

Artur Dideikin

Marc Dubois

Rolando Granada

Alexei Muzychka

Alexander Nezvanov

Alexander Vul'

Luca Zanini

Excused:

Hartmut Abele, TU Wien // WP3 PIK

Andreas Frei, TUM // WP3 PIK

Yuri Kopatch, JINR // WP3 PIK

Oliver Zimmer, ILL // WP3 PIK

Brief Description:

This FPS meeting was devoted to the review and coordination of the implementation of WP3, Task 3.3 of CREMPIL+ project, on Development of advanced Very Cold Neutron Source.

The meeting consisted of several presentations followed by their discussions.

The list of presentations is:

- **Sergey Grigoriev**, Introduction to the meeting, and the CREMLIN+ project,
- **Luca Zanini**, On simulation of VCN sources,
- **Rolando Granada**, Towards a new scattering kernel for solid deuterium,

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

- **Egor Lychagin**, On the preparation of a prototype VCN source,
- **Ekaterina Korobkina**, On the development of a solid-deuterium VCN convertor,
- **Alexander Vul'** and **Artur Dideikin**, On the deagglomeration and chemical cleaning of nanodiamonds,
- **Marc Dubois**, On the fluorination of nanodiamonds,
- **Vladimir Voronin**, On the potential feasibility of a VCN source at PIK.

At the end of the meeting, we had a general discussion on the progress of work on Task 3.3, WP3, CREMLIN+ project, as well as on a feasibility of a VCN source at the PIK reactor, and eventual involvement of PNPI.

Sergey Grigoriev started from the introduction on CREMLIN+ project, and in particular on Task 3.3 of WP3, Development of advanced Very Cold Neutron Source. During the following discussion, it was underlined that the good timing is chosen for the organization of this meeting. On one hand, some results have been already obtained by the participants of the project. On the other hand, discussion of these results and coordination of further activities are needed. Two publications have already resulted from this work:
- M. Herraiz, N. Batisse, M. Dubois, V.V. Nesvizhevsky, C. Cavallari, M. Brunelli, V. Pischedda, S. Radescu, A multitechnique study of fluorinated nanodiamonds for low energy neutron physics applications, J. Phys. Chem. C 124 (2020) 14229;
- A. Bosak, A. Dideikin, M. Dubois, O. Ivankov, E. Lychagin, A. Muzychka, G. Nekhaev, V. Nesvizhevsky, A. Nezvanov, R. Schweins, A. Strelkov, A. Vul', K. Zhernenkov, Fluorination of diamond nanoparticles in slow neutron reflectors does not destroy their crystalline cores and clustering while decreasing neutron losses, Materials 113 (2020) 3337;
- one more article has been submitted in the day of the meeting.

Luca Zanini presented the goals of theoretical studies associated with simulations of VCN sources: to determine yields of VCNs from candidate converter materials, and to determine the best converter material for the prototype experiment to be performed at the PF1B instrument at ILL. Candidate VCN converters include solid deuterium at the temperature of 5 K, liquid para-hydrogen at 14 K, liquid orto-hydrogen at 14 K, and solid methane at 22 K. Candidate reflector materials include magnesium hydrate at the temperature of 20 K (efficient for cold neutrons), and nanodiamonds at room temperature (efficient for VCNs). During the following discussion, participants underlined the importance of producing a reliable kernel for VCN production in solid deuterium. This topic was advanced in the following talk by Rolando Granada. The growing of solid-deuterium convertors with controllable properties was advanced in a following talk by Ekaterina Korobkina. A dedicated experiment at the end of the last reactor cycle at PF2/ILL on the transmission of VCNs through solid deuterium was discussed. Promising preliminary discussions with the beam responsible and the experimental groups, which own the setup, have been carried out. Main risks are COVID-related restrictions and high load on the beam responsible.

Rolando Granada presented the kernel for solid deuterium published in 2009: [R. Granada, Neutron scattering kernel for solid deuterium, EPL 86 (2009) 66007], and a new scattering kernel to describe the interaction of slow neutrons with solid deuterium. The main characteristics of this molecular solid are contained in the formalism including dynamical aspects related to: the lattice's density of states, the Young-Koppel quantum treatment of the rotational motion, the exact treatment of the one-phonon IA in the inelastic term, the internal molecular vibration. The elastic processes involving coherent and incoherent contributions are also fully described, as well as the spin-correlation effects caused by the coupling of the intrinsic and rotational angular momenta. To validate the new scattering kernel and its generated cross-sections, one needs experimental data. Measurements of VCN total cross sections for solid deuterium, in particular at 5 K, might be a relevant set of data for the validation. As follows from studies with UCNs, the most disturbing uncertainty is associated with the contribution of elastic scattering of neutrons on the inhomogeneity of solid deuterium. Therefore, one has to be able to produce solid deuterium converters with reproducible and controllable properties.

Egor Lychagin described the status of preparation of a prototype VCN source. The design should allow investigating both the VCN converter (VCN production as a function of VCN energy) and the VCN reflector (the gain in the VCN flux along the direction of the VCN extraction axis as a function of VCN energy). For the purpose of planning the experiment at PF1B, an approximately estimated VCN production rate is 1.6·106 n/s (v<100 m/s), and 2·105 n/s (v<50 m/s). The approximately estimated gain factors are 3-6 (v<100 m/s), and 4-15 (v<50 m/s) – the values to be refined by further calculations and experiments. For the preparation of this experiment at PF1B, beam shaping is provided by ILL, the cryostat for VCN converter and reflector as well as the orto-para convertor are being developed at JINR, nanodiamond powder is being produced and conditioned by Ioffe Institute (a following talk by Alexander Vul') and UCA (a following talk by Marc Dubois), the VCN chopper was developed by JINR and is located presently at ILL, the position-sensitive detector is provided by ILL. A scheme of the orto-para converter and the methodical developments on the internal parts of the cryostat were presented and discussed. The production of relevant parts has started. More model calculations of this experiment are planned.

Ekaterina Korobkina explained main ideas and showed the data relevant for the development of the solid-deuterium VCN converter. In particular, she commented on the need for para-orto conversion of deuterium, on the differences between condensation of solid deuterium from gaseous and liquid phases, on the process of growth of solid deuterium in various conditions, on the fact that the solid deuterium crystal has to be grown horizontally for the prototype VCN source experiment. The development of the solid-deuterium VCN source is based on the current development of the UCN source at North Caroline State University (NCSU). This connection is particularly useful because the parameters and properties of solid deuterium in these two sources are quite similar, and therefore the experience gain at NCSU can have direct application to the VCN source prototype. The process of growing of solid deuterium is quite complex and depend on temperature, in particular on gradients of temperature, on the temperature cycling, etc. On the other hand, quality and shape of the crystal can be predicted if we know the temperature distribution of the cryo-container walls.

Alexander Vul' and **Artur Dideikin** discussed the results and future prospects related to the preparation and conditioning of the nano-diamond powder for the VCN reflector. In particular, the reflection efficiency of nano-diamonds depends on the state of aggregation of nanoparticles in the powder. This effect is especially pronounced for the 3D geometry when the trap size is comparable to

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the wall penetration depth. Another way of improving the reflectivity of powder for VCNs consists of removing neutron-absorbing impurities. Therefore, nearly 1 kg of nano-diamond powder was chemically cleaned and deagglomerated at the Ioffe Institute for the production of the nanodiamond reflector for the solid-deuterium VCN prototype source. The next step of preparation of the powder is being done at Clermont-Ferrand (a following talk by Marc Dubois). Further developments, which can help to improve the quality of nanodiamond powder, can include further reduction of neutron-absorbing impurities, in particular nitrogen. The method could consist of other methods of production the initial powder.

Marc Dubois described the process of fluorination of (already deagglomerated and chemically cleaned at the Ioffe Institute) diamond nanoparticles used for the construction of a reflector for the solid-deuterium prototype VCN source. Fluorinations allow replacing the main impurity in nanodiamonds, which are responsible for neutron losses: hydrogen with its huge inelastic scattering cross section. Fluor replaces hydrogen nearly completely. Moreover, fluorinated nanodiamond powder does not reabsorb hydrogen from air in any form for very extended periods for time, of the order of a few years. Fluorination also removes sp2 carbon from the surface of the diamond cores of nanoparticles, which improves their scattering properties. The resulting powder was characterized using several complementary techniques including solid-state nuclear magnetic resonance, Raman light scattering and others. At the moment, a first fraction of the powder has been fluorinated and the rest is going to be done during the following several months. This presentation prompted an interesting scientific discussion going even beyond the direct topic of the VCN source development.

Vladimir Voronin presented the status of construction of the high-flux PIK reactor at the National Research Center “Kurchatov Institute”, Petersburg Nuclear Physics Institute, Gatchina. Participants of the meeting welcomed the progress achieved with putting in operation the PIK reactor and developing the national instrument program at this reactor. An emphasis was made in the presentation on the potential feasibility of a VCN source at PIK and the main corresponding constraints: limited space for the scientific equipment and the fact that national instrumental program at PIK is almost fixed. During the discussion after the presentation, participants decided that the most straightforward procedure to go forward with this discussion is to write a conceptual project of a VCN source in the form of an article. It would be distributed some time before one of the next FPS meetings among potential PNPI participants and would give the basis for more detailed discussions. A first draft of such an article will be presented in the form of ISINN proceedings.

Materials from the 2nd fundamental physics subcommittee meeting, including the agenda, available slides from the talks, and the minutes of the meeting can be found on PNPI website [https://oiks.pnpi.spb.ru/cremlinplus-pnpi].

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