Title: Minutes of 2nd CREMLINplus Diffraction (Structure) Subcommittee meeting

Wednesday 30 June 2021 at 14:00-16:00 CET via videoconference

Chair: A. Goukassov

Participants:

Subcommittee members:

A. Goukassov
W. Schweika
M. Meven
A. Balaguriov
V. Em
A. Senyshyn

PNPI speakers and attendees:

S. Grigoriev
A. Kurbakov
V. Ulyanov
V. Polyakov
I. Zobkalo
Yu Chernenkov

Brief Description:

In the introductory talk **I. Zobkalo** presented the current status of and time schedule of the instrumentation program of PIK reactor. Reactor should attain **megawatts** power in **December** 2021 and some of five "first-day" stations are operating at kWt reactor power. Other neuron instruments will be realized in the framework of the national program of the development of neutron and synchrotron research in Russia, **financially approved for the period 2020-2027**. The program consists of three stages of construction and includes consecutive delivery of diffractometers D1, DS1 and D3.

In the following talks project leaders presented the instruments under construction; High Resolution powder diffractometer **D1** (A. Kurbakov) and **DC-1** thermal single crystal 4-circle diffractometer (Yu. Chernenkov). Each presentation was followed by a 15-minute discussion. After these talks, a brief discussion of other diffractometer projects took place.

After a closed discussion between Subcommittee members, the following recommendations were formulated.

General remarks

We acknowledge the presentation of the status of PIK and the instrument construction plan, and appreciate that the construction of the D1 diffractometer is now in the advanced phase of design and

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procurement. Lead engineers are now nominated to all project, which should accelerate the decision making during the construction.

We acknowledge as well that accordance with our recommendation the single crystal diffractometer D1C is transferred to the hot channel and polarized neutron diffractometer DiPol to the thermal one. This is a good opportunity for studies on strongly absorbing materials, e.g. many RE multiferroics, high pressure and high Q studies.

D1: High Resolution powder diffractometer

We continue to believe that the high-resolution neutron powder diffractometer D1 remain the high priority instrument. Kurbakov's presentation has shown that most important units of D1 has been already designed and the procurement of some elements has started. The key units of D1 presented were the following: neutron guide between source and monochromator, focusing Ge-monochromator, set of Soller collimators, sample unit and one-dimensional detector.
We would like to stress that Ge monochromator with three possible take-off angles up to **155°/2theta should be** used as proposed. The choice of various Soller collimators (validated by McStas calculations) looks convincing.

Some doubts concern the shielding thickness of monochromator. In particular, at 155° take-off angle the background might be extremely high. We recommend performing more extensive optimisation of shielding by numerical simulations and using multilayer shielding structure. Load on the floor in the hall needs to be taken into account.
Retained option of the detector in a form of a set of individual He counters inclined by 45° is less ambitious than we expected. We understand, however, that this system has been adopted because of the budget and technical constraints. Though iIt would be nice to keep in mind a possibility of its "upgrade" to a version with position sensitive read out of tubes. The choice of such type of detector would considerably increase the capacities of D1.

We recommened also having automatic slits closer to the sample position rather than right after the monochtromator. Otherwise the general advancement of the project looks promising.

DC-1: Thermal four-circle single crystal diffractometer

The hot channel 8 is well suited for the implantation of the diffractometer. Monochromator take-of **42°** is optimum. A hot source with 1800°C as presented for PIK will boost the flux towards <= 0.5 Angstrom significantly. Thus, use of an Er filter is highly recommended for any monochromator with a wavelength whose lambda/3 (e.g. Ge311) or lambda/2 (Cu220) would be in this region to avoid contamination in the multiple percent range.

The limitation to a PG002 and Ge311 monochromator at 42 deg for a single crystal diffractometer at a hot source seems limiting the possibilities of using short wavelength (0.5 A). Even if Ge311 with 23deg will give a similar wavelength as a Cu220 monochromator the Ge reflectivity is significantly smaller

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below 1 Angstrom than for Cu. Moreover, using smaller Bragg angles for the monochromator will also raise more quickly the effective horizontal beam divergence for high Q. Compensation of this unwanted effect requires significant compensation by collimators which results in a corresponding loss of flux.

Thus it is recommended to design the monochromator setup in a way that also monochromators with high reflectivity (Cu) below 1 Angstrom can be used or added later.

A vertically focusing monochromator is definitively a good choice for improving flux. Nevertheless, a max. vertical divergence >= 3 deg. will most likely generate some problem,s like strongly distorted beam spots at the detector position and potential partial reflection overlaps (bad for modulated structures). A possibility of decreasing vertical divergence (for instance by slits) should be envisaged.

Primary horizontal collimation of white beam before monochromator is recommended, as this is the most effective way to tune the beam divergence and keep the gamma radiation generated while collimating inside the biological shielding. Radiation hardness of the (e.g. Gd coated) collimator foils is mandatory.

Biological shielding of DC-1 need to be presented in more detail.

Materials from the 2nd CREMLINplus Diffraction (Structure) Subcommittee meeting, including the agenda and the minutes of the meeting can be found on PNPI website [https://oiks.pnpi.spb.ru/cremlinplus-pnpi].

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