SAC _Cremlin_WP3 report 12.04.2021

1. Executive Summary:

- The SAC applauds the excellent scientific presentations that revealed the needs of Russian users in the fields of biology, chemistry, solid state physics, and materials science (engineering).
- It will be important for the success of PIK to demonstrate with a few selected high-class instruments that this installation is reliable and capable of hosting instruments with globally competitive performance in terms of flux, resolution, dynamic range and in particular background.
- The SAC is convinced that a funding period of less than 3 years for building an innovative neutron instrument is very demanding and challenging. From all experience at large neutron facilities, the SAC considers the construction of 20 instruments during a four years period as very ambitious. It may be advisable to focus first on a core set of essential instruments to start the user program.
- Initially, in the first round the selection of instruments should also be guided by the available expertise both in manpower as well in engineering capacities. For these first instruments, the challenge is international competitiveness on the highest level.
- The SAC emphasizes that some of the HZG instruments, such as NERO and TEX will be a valuable addition to the planned instrument program.
- The SAC notes that the necessary efforts to establish a scientific environment in terms of support facilities etc. and user support might be underestimated. However, the first priority of today for PIK is to build innovative instrumentation. The initial set of sample environments can be purchased from industry.
- The comparison of user demands and planned instruments shows that the PIK instrument program satisfies most users' needs.
- Modern solid-state physics needs polarized beams including polarization analysis. To reach this goal, He3 filters are mandatory. The SAC encourages any development in this direction.
- The bio-community that will increase in importance and numbers in the future, however, is not served well. Both a protein diffractometer as well as a high resolution NSE instrument are in strong demand and should be built.
- The engineering community is in demand of an imaging station that so far is not foreseen.
- Given that neutrons provide the ability to follow atomic and molecular motion in space and time, the SAC considers the 4 suggested inelastic instruments, three of them triple axis instruments, as not well balanced.
- A more balanced instrument suite should reduce the number of TAS instruments, prioritise the foreseen ToF instrument and consider high resolution NSE (as demanded by the biologists) and backscattering (NBS).
- Finally, in its next meeting, the SAC would like to focus on the instrumentation program and seriously evaluate the different suggested instruments.

2. Contribution of representatives of different science fields

The SAC praises lectures on the science cases and scientific communities as very informative and considers the quality of the presentations that were presented as high. They, in particular, allowed to get a good impression of the needs of the Russian user community. Reassuringly, this need is similar to what is known from the rest of the world. Historically, strongholds meet the requests stemming from impactful modern science.

3. General philosophy of instrument Program

The challenge that PIK is confronted with today is not supplying right from the start a suite of instruments that covers all needs of the community. PIK is a project that, as we have heard repeatedly during the meeting, remained in the starting blocks for more than 4 decades. This fact has to be taken clearly into consideration when giving recommendations on priorities. What PIK has to achieve over the next few years, is convincing all the parties involved (Russian funders, Russian community, international community) about its capacity to compete at a high level of excellence. This does not require that PIK offers immediately a complete instrument suite, nor complete services in sample environment or auxiliary services like deuteration. However, it will be important for the success of PIK to demonstrate with a few selected high-class instruments that this installation is reliable and capable of hosting instruments with globally competitive performance in terms of flux, resolution, dynamic range, and in particular background

Equipped with high class instruments, PIK at the PNPI has the potential of a large neutron facility with an international impact. It all depends on a timely development of the neutron source (including cold and hot sources) and a balanced instrument suite that meets the needs of the national and international user community.

The SAC is convinced that a funding period less than 3 years for building an innovative neutron instrument is very demanding and challenging. From all experience at large neutron facilities, the SAC considers the construction of 20 instruments during a four years period as very ambitious. Following our reasoning above first a set of internationally competitive instruments should be built that in a second step should be complemented by innovative instrumentation that needs more time to design and construct.

Finally, we note that instruments at a high flux continuous neutron source complement ESS instrumentation (such as TAS and NSE) and compete with instrumentation at ESS. And this competition is the driving force for excellence in instrumentation at spallation and continuous sources.

4. In pile installation priorities

Cold neutrons are used in modern neutron beam research due to the high resolution and increased sensitivity available with them. So the main part of the neutron instruments at the PIK reactor uses cold neutrons. All these instruments serving condensed matter research are in the neutron guide hall. Altogether PIK will be able to support 40 experimental positions. Among them the two cold neutron sources that feed the wide neutron guide system, offer about 20 experiments. Effective use of the instruments situated at this neutron guide systems

will be possible only after commissioning the cold neutron sources. Therefore, the SAC emphasizes the need to launch cold neutron sources as soon as possible. It will give an impetus to the development of the scientific program at these instruments.

The progress in the installation of the second cold source appears to be is slow or even at risk. Up to now, the 2nd cold source is still in the conceptual design phase. The SAC sees a serious problem for the coming instrumentation and scientific program, if the second cold source is not constructed swiftly and installed soon.

5. Instrument Priorities

The 20 instruments currently planned, which are to be built in phases 1-3, are divided into 7 instruments for nuclear physics, 4 instruments for structural studies, 5 instruments for spectroscopic studies and 4 instruments for large-scale structures.

The SAC emphazises that initially the priority in instrument building should obey the following criteria:

(1) The first instrument suite must be chosen such that it exploits the source characteristics at the highest level.
(2) Whether these instruments are diffractometers, SANS machines or spectrometers is at this point secondary provided they are first class.
(3) To achieve first-class instrumentation requires first of all expertise. When choosing the first suite of experiments it is, therefore, essential to place particular attention on the availability of competent and motivated staff for building them.

Once PIK has shown to the world its capability of collecting high-quality experimental data, confidence in the installation is established. This confidence will free additional resources that will allow for the second step that consists in building up a fully-fledged user facility catering to the needs of the entire Russian community and reaching out internationally. At this point good coverage of all the relevant topics will be essential.

Present planning; Core instruments: Presently, in 3 phases extending over a period of less than 3 years each altogether 20 instruments are planned to be constructed and commissioned in the fourth quarter of 2024. From all our experience at large neutron facilities, the SAC considers this planning as veryambitious and extremely challenging. Instead, it may be advisable to focus on a core set of essential instruments to start the user program. If supported by the appropriate resources, one powder and one single crystal diffractometer, one SANS machine, one reflectometer, one TAS, one TOF and one high resolution NSE for the biologists may be considered as core instruments. This results in up to 7 instruments that can easily be expanded as time/budget/staff develop. In addition, those nuclear instruments may be installed that after upgrades are derived from existing instruments.

The recommendation of these core instruments is based on experiences made at other steady-state neutron facilities, and many of the proposed instruments are similar to those found in other locations. This leaves room for conceptual developments of new types of instruments that do not yet exist in biology and biophysical research, in materials science and in chemistry and that can contribute to societal challenges such as the climate change.

It was not clear to the SAC members what total budget would be available for instrument development. In any event, there are three main challenges to face: budget constraints, constraints on the number of skilled design and construction workers, and constraints on workshops inside or outside of PNPI, where many complex machines can be built in a short period of time. Therefore, as discussed above the choice of "demonstration instruments" in the first round should be also guided by the available expertise both in manpower as well in engineering capacities. For these instruments the challenge is international competitiveness on the highest level.

Nuclear and particle physics are a very important topic locally as well as for a wider Russian user community. This is mirrored in altogether 7 proposed instruments in this field. They were not presented at the SAC meeting. Nevertheless, given the long and successful Russian tradition in this field, such instruments are very important for the Russian community. But they will not further be commented on here.

HZG Instruments: To the SAC members it was not entirely clear, which of the HZG instruments will be part of the PIK instrument suite. However, apparently the former HZG instruments TEX (engineering diffractometer) and NERO (reflectometer) may become part of the instrument suite. Currently, TEX is equipped with a modern instrument control system and extended shielding. TEX using thermal neutrons is placed in the reactor hall, while NERO might serve as a high-resolution reflectometer in the neutron guide hall. Finally, TEX, as an engineering diffractometer, will be a vital part of a balanced instrument portfolio.

Orphee contribution: As proposed by PNPI, there is some ground for collaboration between LLB and PNPI regarding instrument/parts transfers. Early talks on what can be done (beyond the tasks set out in the PNPI 20 instrument project) will be initiated soon.

6. Priorities Infrastructure

For the medium-term future, SAC members stress the need for adequate instrumentation infrastructure, including furnaces, cryostats, pressure cells, and a deuteration laboratory. Also, it would be helpful, if users had access to on-site sample characterization facilities such as magnetometer, light scattering, transport experiments, etc. Similarly, access to a chemistry laboratory, a mechanical workshop and an electronic workshop would be advantageous. The SAC notes that the necessary effort to establish a scientific environment in terms of support facilities etc. and user support might be underestimated.
Nevertheless, the first priority of today for PIK is to build innovative instrumentation. A first set of sample environments can be purchased from industry.

7. Relation between PIK instrument Program and Users Demands

A comparison of the declared needs of the different scientific communities with the instrumentation program at PIK as it stands by now is shown in table 1.

Table1: Comparison of the foreseen instruments at PIK, including some of the former instruments from FRG at HZG

Instrument program PIK	Instrument Community	Science discipline
TEX	Stress Diffractometer	Materials
None	Imaging	Materials
None	Protein Diff.	Bio
?SEM?	High Res. NSE	Bio
SESANS	USANS	Bio
SONATA	Horizontal Reflectometer	Bio
MEMBRANA;	TR-SANS	Bio
DC1	Single Crystal Diff	Diffraction Comm.
D1	High Res. Powder	Diffraction Comm.
D3	High Int. Powder	Diffraction Comm.
D3	TR-Powder	Diffraction Comm.
MEMBRANA	SANS	Chemistry
SONATA	Reflectometer	Chemistry
One of IN1; IN2 or IN3	Polarized TAS	Solid State
D3	Polarized Powder	Solid State
DC1	Polarized Single Crystal	Solid state
TENZOR	Polarized SANS	Solid State
GARMONIA	Polarized Reflectometer	Solid State
IN-4	Cold Time of Flight Instrument	Very versatile: Would serve Bio, Chemistry and Solid State

The comparison of user demands and planned instruments shows that the PIK instrument program satisfies the needs of a large part of the anticipated user community. As pointed out by the Russian solid-state community, modern solid-state physics needs polarized beams, including polarization analysis. To reach this goal, in particular for polarization analysis, He3 filters are mandatory. The SAC encourages any development in this direction.

Table 1 shows that the bio-community, which is expected to increase in importance and numbers, is not served well. A protein diffractometer is missing and the present layout of SEM is not in the direction of a high resolution NSE instrument. Both are in strong demand and the future planning should satisfy the requirements of the biologists. Furthermore, the engineering community will need an imaging station which has not yet been included in the planning.

Beyond this comparison, the SAC members like to emphasize that the uniqueness of neutron scattering lies mainly in its ability to follow atomic and molecular motions in space and time. In this context we note that only 4 instruments in the instrumentation program are "IN"-instruments, i.e. spectroscopic: 3 x Triple axis (TAS) and 1x Time of flight (TOF) instruments; in addition the portfolio includes SEM, a medium resolution NSE. Thus, presently TAS is overrepresented with 75 % of the 4 inelastic instruments. There is only one TOF instrument (1 out of 4) that is planned for phase III. A more balanced instrument suite should reduce the number of TAS instruments and consider high resolution NSE (as demanded by the biologists) and backscattering (NBS).

Finally, in order to achieve a balanced portfolio and in view of the endeavor to establish an international user facility, not only the needs of the Russian neutron community should be

taken into account. If PIK has the ambition to become an international user facility, the question of access by foreigners cannot be avoided.

8. **Future SAC Meeting on Instrument choices:**

The SAC can certainly help building a balanced instrument suite; but for doing so, we need a dedicated meeting where the instrument concepts are seriously evaluated as we do for our own upgrade programs. Thus the SAC suggests to focus in the next SAC meeting on the instrumentation program.