Proposal for opening a new project

Development of an inelastic neutron scattering spectrometer in inverse geometry at the IBR 2 reactor

In the frame of Theme

Studies of functional materials and nanosystems using neutron scattering
Theme code: 04-4-xxxx-2021/2025

Dorota M. Chudoba
Introduction

28 – 29.03.2019
Workshop on the Construction of a new Inelastic Neutron Scattering Spectrometer

17 – 18.06.2019
50th meeting of the PAC for Condensed Matter Physics

20 – 21.01.2020
51th meeting of the PAC for Condensed Matter Physics

23.03.2020
FLNP Science and Technology Council
Scientific motivation

- Research directions realizing on NERA spectrometer
- New research directions

Slightly oversubscribed

<table>
<thead>
<tr>
<th></th>
<th>2016</th>
<th>2017</th>
<th>2018</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>20</td>
<td>13</td>
<td>18</td>
</tr>
<tr>
<td>PL/RU/RO</td>
<td>PL/RU/DE</td>
<td>PL/BU/RU/DE</td>
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</tbody>
</table>

Reasons: - low luminosity \(\rightarrow\) large samples or long counting time
- limited energy transfer range
- high background
Scientific motivation

Research directions realizing on NERA spectrometer

Hydrogen bonds in molecular matter (vibrational analysis)

Dynamics studies of pharmaceutics with studies under pressure

Dynamics studies of liquid crystals

Rotation-translation coupling – studies of Li – ion transportation in plastic crystals

Study of magnetic multilayers
Scientific motivation

New research directions – not possible to implement on NERA

Molecular crystals and glass-formers at low temperatures in connection with complementary studies and ab initio quantum chemical calculations.

Pharmaceuticals in bulk (native) state and as “micronized” or amorphized powders

Matter under spatial confinement
- “hard” nanomatrices (e.g. membranes)
- “soft” confinement (e.g. microfibres)

Materials for energy storage, e.g. plasticizer-SPE systems for Li batteries

Catalysts

Photonic materials of industrial applications
2,5 diiodothiophene
(CH)₂(Cl)₂S

TOSCA, ISIS, England

LAGRANGE, ILL, France

1 g / 4 hours (2+2 each panel) for raw scans

5K 17h 18g

courtesy of A.Ivanov
Main characteristics

• Based on the available space and needed time resolution and energy range the distance between the source and the sample was chosen equal 105 m.

• The optics was optimized for the 0.5 Å wavelength band (thus for large values of transferred Energy 0-330 meV (2661 cm⁻¹); now impossible to analyze above 100 meV).

• Two sample sizes was proposed: standard 3x3 cm² and small 1x1 cm².

• The distance between the end of optics and sample position is 0.35 m.

• Higher luminosity – 250 times higher than on NERA.
Main characteristics

1 step
**PRIMARY SPECTROMETER:**
- NEUTRON GUIDE
- SPLITTER
- BACKGROUND CHOPPER
- CASCADE OF CHOPPERS

2 step
**SECONDARY SPECTROMETER**
- SAMPLE HOLDER
- FILTERS
- ANALIZATORS
- DETECTORS
Main characteristics

- Reactor
- Moderator
- Background chopper
- Neutron beam with cascade of choppers

Side view
- Pyrolytic Graphite crystal
- Beryllium block-filter
- Detector

The moderator area for 2 channel: 33.5x40.5 cm² (WxH).
Main characteristics
Main characteristics
## Expected characteristics

<table>
<thead>
<tr>
<th></th>
<th>NERA</th>
<th>New INS Spectrometer</th>
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</thead>
</table>
| **Analyzer area**              | 15x3x25  
1125cm²            | 10000x2  
20000cm²                    |
| **Ratio input/output to neutronguides** | 16x5cm²/5x5cm²  
3.2       | 20x20cm² / 3x3cm²  
44.44    | a gain in flux density (without taking into account the higher quality of the neutronguide)  
44.44/3.2 = 14          |
| **Solid angle**                | ~ 0.2 sr                 | ~ 2 sr (1 pc of new spectrometer)  | Solid angle gain  
18                |
| **Ratio of luminosity of new spectrometer and NERA** |                          | 18x14 = 250 times higher i.e. measurements of a sample with the mass of 10-20 mg will be possible. |
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Authors:

<table>
<thead>
<tr>
<th>Author</th>
<th>Location</th>
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<tbody>
<tr>
<td>Chudoba D. M.</td>
<td>Dubna, JINR</td>
</tr>
<tr>
<td>Goremychkin E.</td>
<td>Dubna, JINR</td>
</tr>
<tr>
<td>Belushkin A.</td>
<td>Dubna, JINR</td>
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<tr>
<td>Bodnarchuk V.</td>
<td>Dubna, JINR</td>
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<tr>
<td>Kruglov A.</td>
<td>Dubna, JINR</td>
</tr>
<tr>
<td>Zając W.</td>
<td>Kraków, INP PAN</td>
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</tbody>
</table>

Project leader: Chudoba D. M.
Due to the regulations, it is possible to open the project for 3 years with the possibility of extension for another period (1-3 years).
### Proposed Project Schedule for inverse geometry INS instrument

<table>
<thead>
<tr>
<th>Task Description</th>
<th>2019</th>
<th>2020</th>
<th>2021</th>
<th>2022</th>
<th>2023</th>
<th>2024</th>
<th>2025</th>
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<tr>
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<td>The documents for opening a new project in the frame of FLNP theme within the topical plan of JINR submitted to PAC for CM</td>
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<td>Installation</td>
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<td>Testing/Commissioning</td>
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</table>
### Time schedule & Cost estimate

<table>
<thead>
<tr>
<th>Description of units and systems, resources, funding sources</th>
<th>Cost of units (k$). Resource requirements for 1st part of the project</th>
<th>Proposals of the Laboratory for distribution of funds and resources</th>
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</thead>
<tbody>
<tr>
<td></td>
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<td>2021</td>
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<tr>
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<td>Highly Orientated Pyrolytic Graphite</td>
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<td>$^3$He Detectors and electronics</td>
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<tr>
<td>Manufacture of vacuum, cryogenic systems and beryllium filters</td>
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<tr>
<td><strong>Total</strong></td>
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<td><strong>3700</strong></td>
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The second part of the project (2024-2025) is planned to cover rest costs for neutron quide system, manufacture of vacuum, cryogenic systems and beryllium filters (~2000k$).
<table>
<thead>
<tr>
<th>№</th>
<th>Description of cost items</th>
<th>Total cost</th>
<th>2021</th>
<th>2022</th>
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<tr>
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<td>1300</td>
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</table>
Partner companies and equipment suppliers

AMU, Poland
INP PAN, Poland
PNPI NRC «KI», Russia
ILL, France
FRAKOTERM, Poland
SwissNeutronics, Switzerland
Kompozit, Russia
Thanks for your attention!