



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

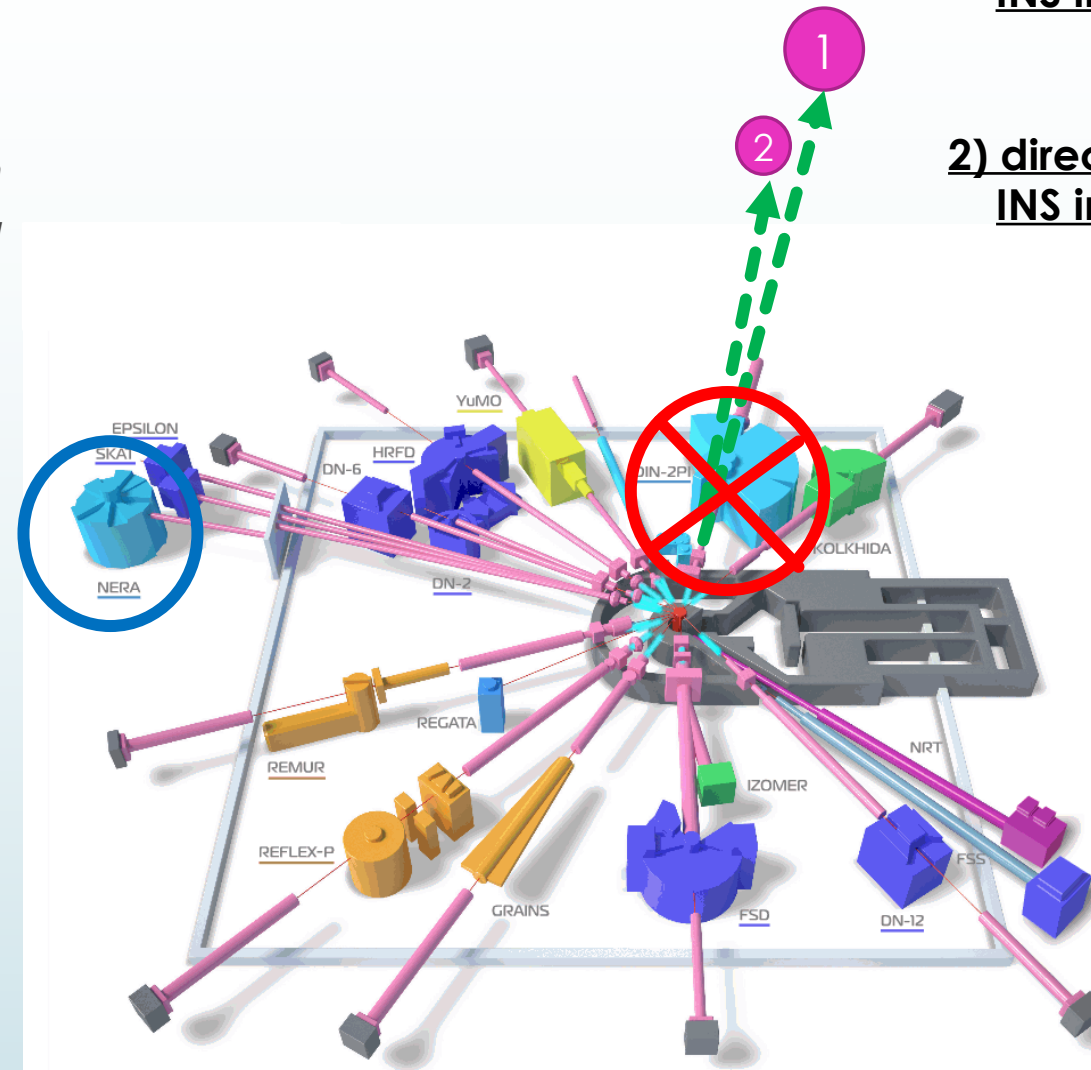
50th meeting of the PAC for Condensed Matter Physics

20 – 21.01.2020

51th meeting of the PAC for Condensed Matter Physics

23.03.2020

FLNP Science and Technology Council



**1) inverse geometry
INS instrument**

**2) direct geometry
INS instrument**

- ❖ Research directions realizing on NERA spectrometer
- ❖ New research directions

Slightly oversubscribed

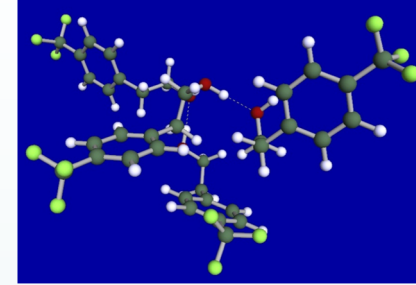
2016	2017	2018
20	13	18
PL/RU/RO	PL/RU/DE	PL/BU/RU/DE

Reasons: - low luminosity → large samples or long counting time
- limited energy transfer range
- high background

Scientific motivation

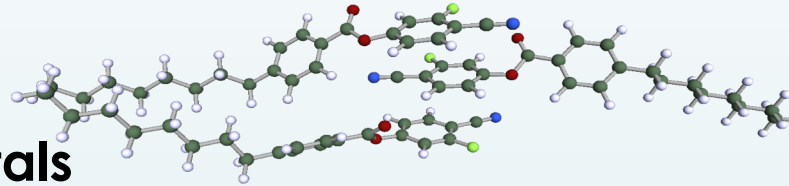
Research directions realizing on NERA spectrometer

Hydrogen bonds in molecular matter (vibrational analysis)



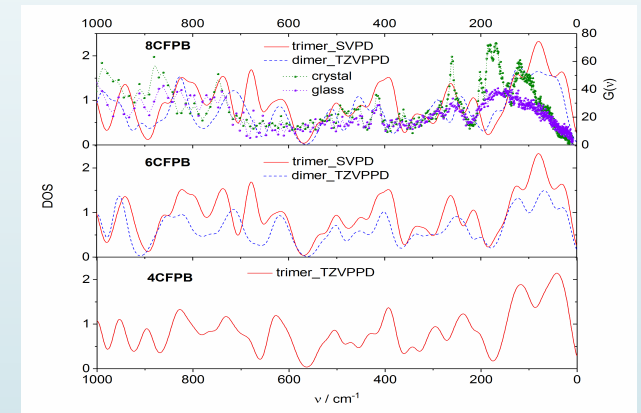
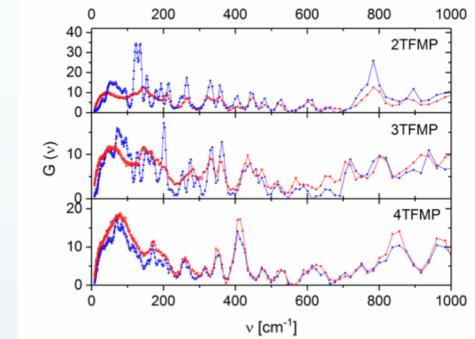
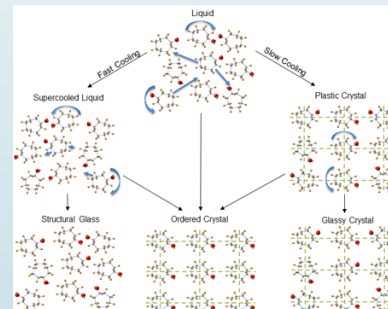
Dynamics studies of pharmaceuticals with studies under pressure

Dynamics studies of liquid crystals



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

Study of magnetic multilayers



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

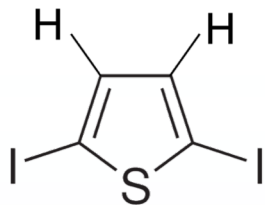
- “hard” nanomatrices (e.g. membranes)
- “soft” confinement (e.g. microfibres)

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

Catalysts

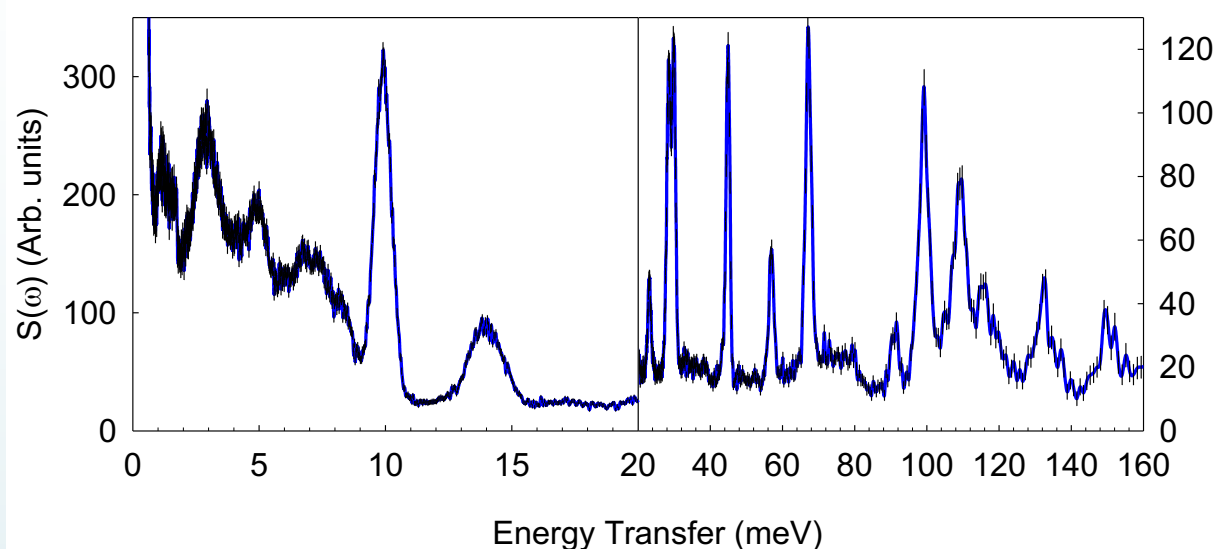
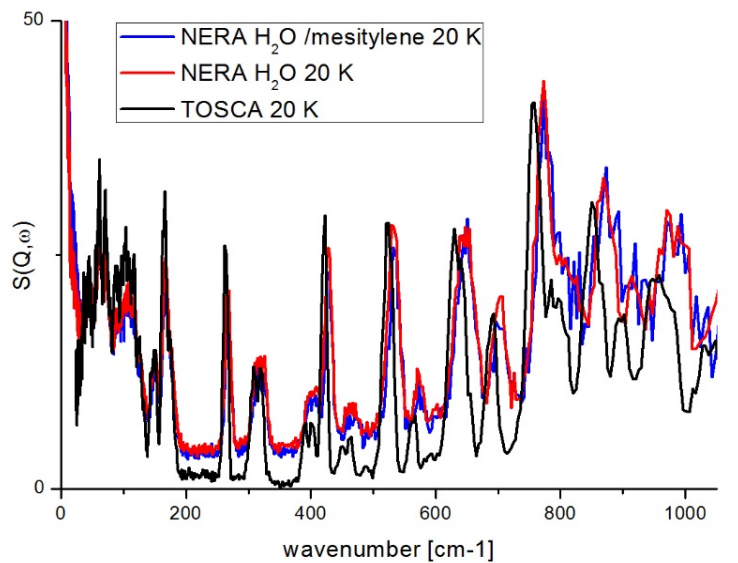
Photonic materials of industrial applications

2,5 diiodothiophene (CH)₂(CI)₂S



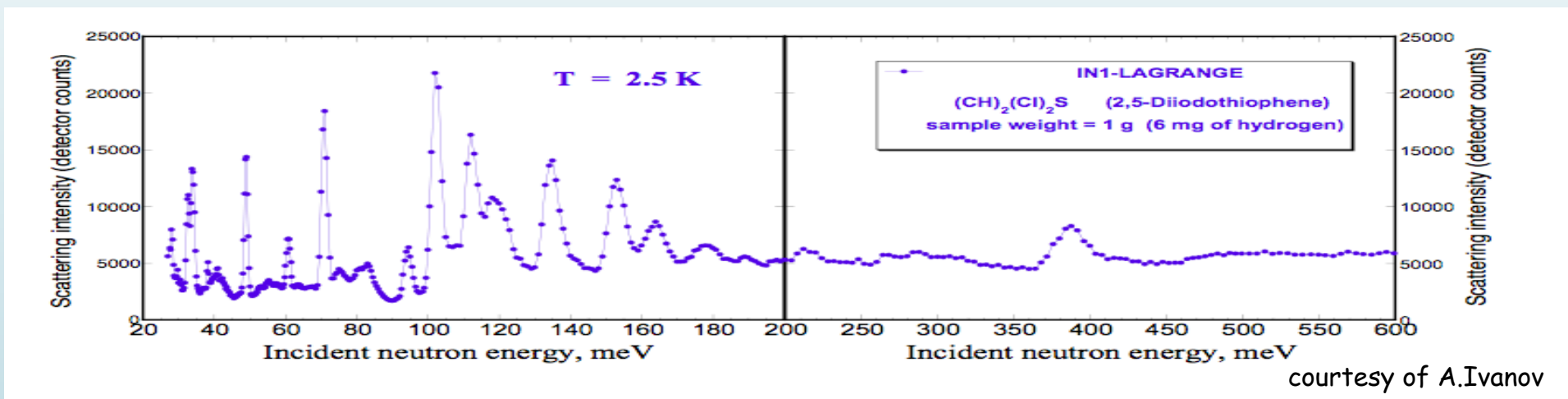
LAGRANGE, ILL, France

TOSCA, ISIS, England



5K 17h 18g

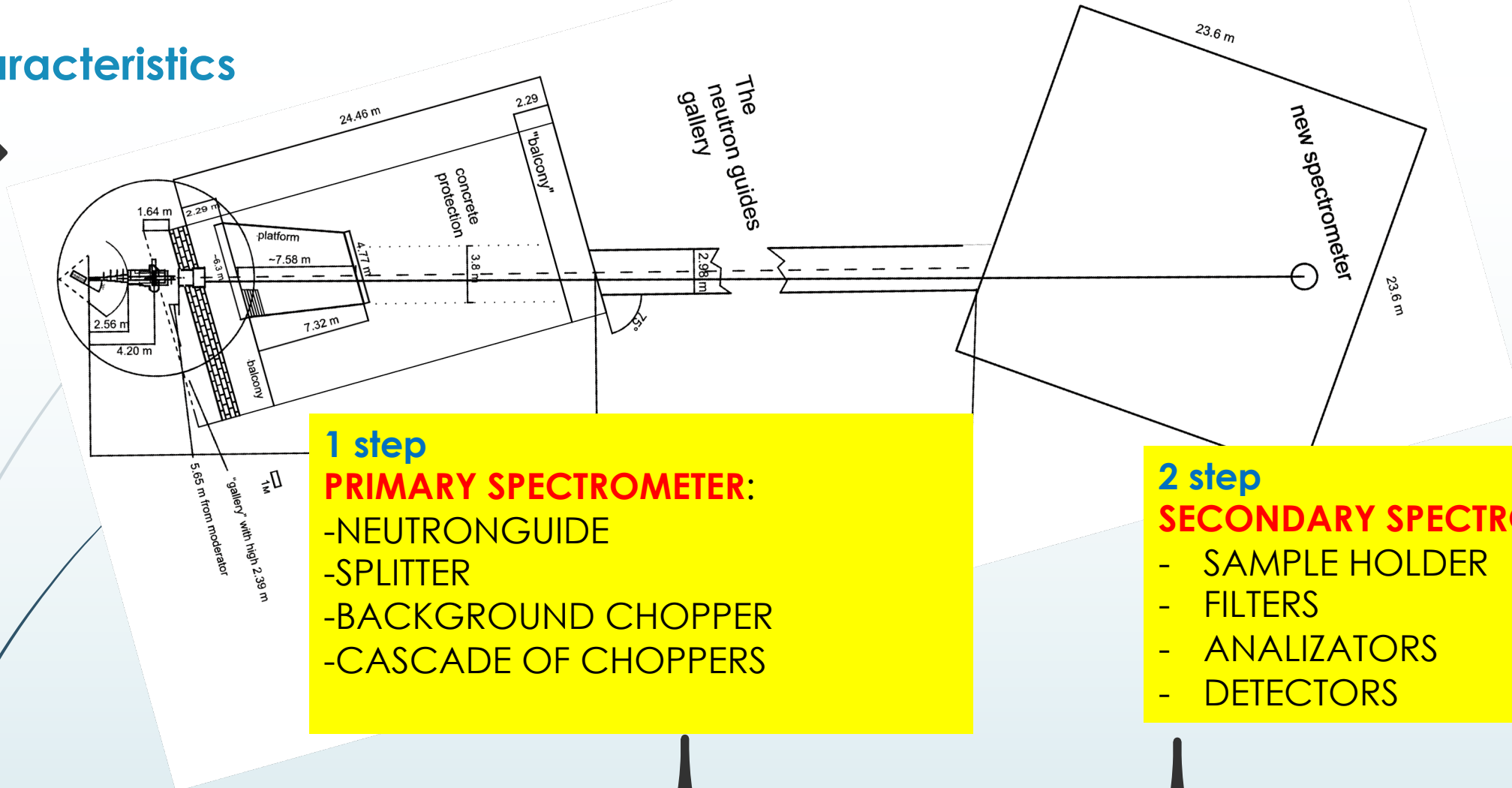
1 g / 4 hours (2+2 each panel) for raw scans



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

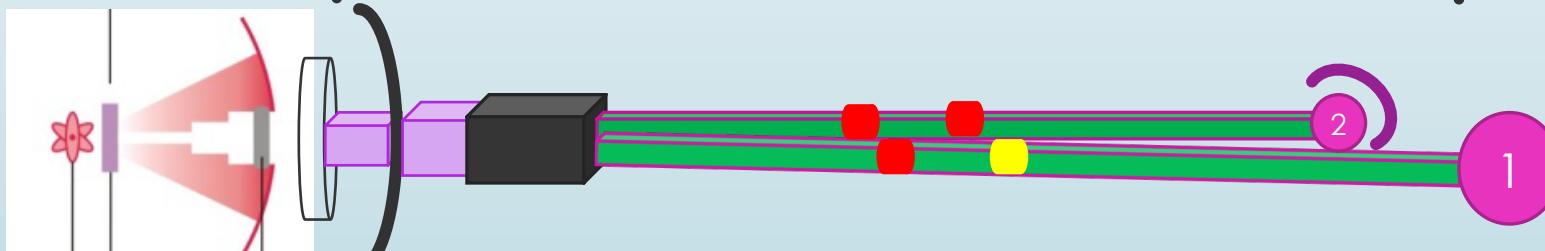
PRIMARY SPECTROMETER:

- NEUTRON GUIDE
- SPLITTER
- BACKGROUND CHOPPER
- CASCADE OF CHOPPERS

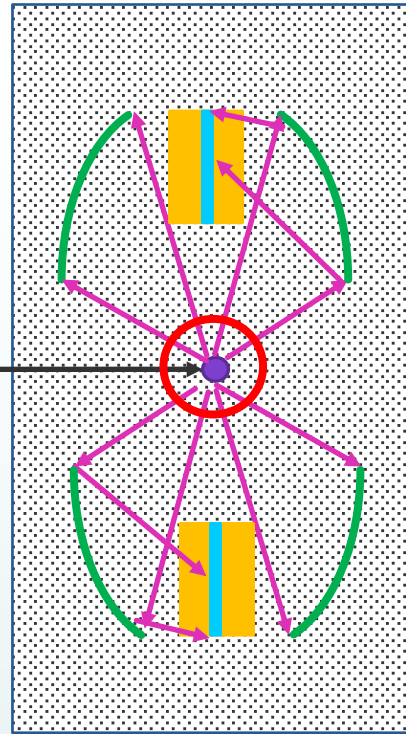
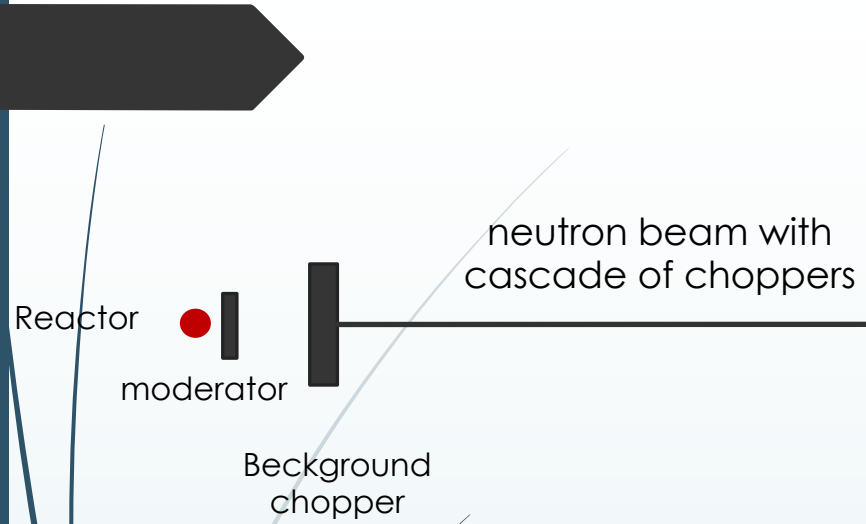
2 step

SECONDARY SPECTROMETER

- SAMPLE HOLDER
- FILTERS
- ANALIZATORS
- DETECTORS



Main characteristics



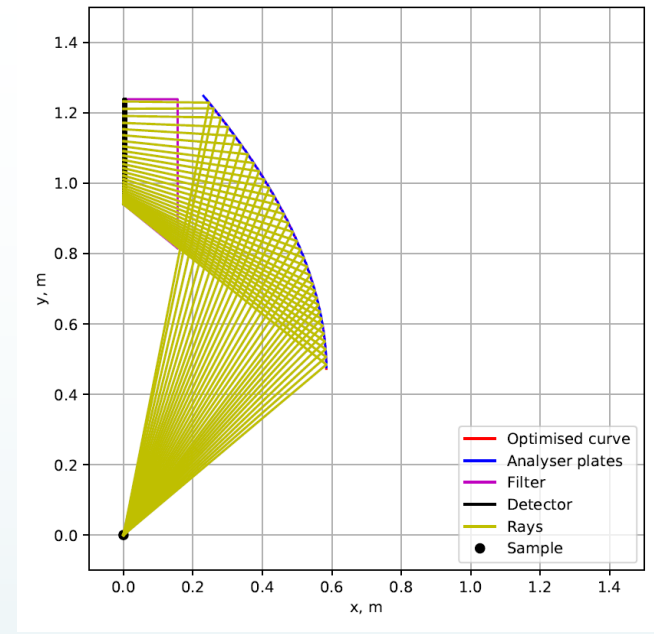
Detector

Beryllium block-filter

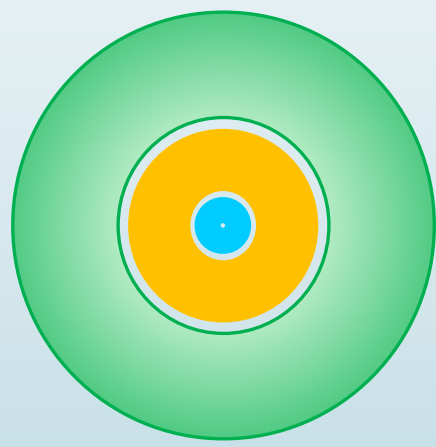
Pyrolytic Graphite crystal

Sample

Cryostat



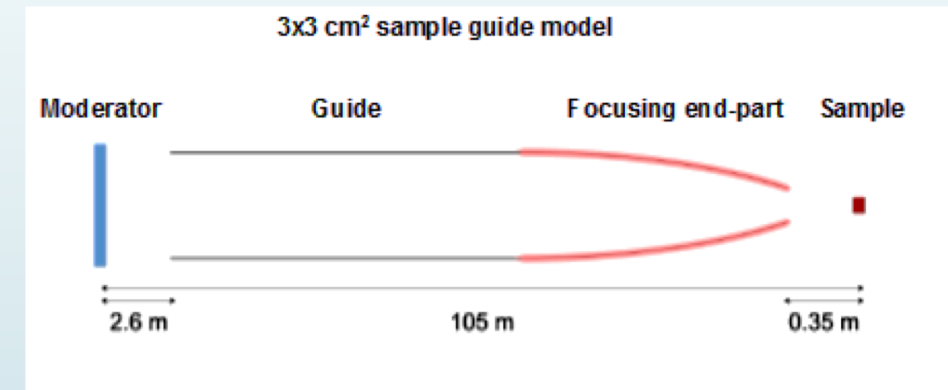
side view



Pyrolytic Graphite crystal

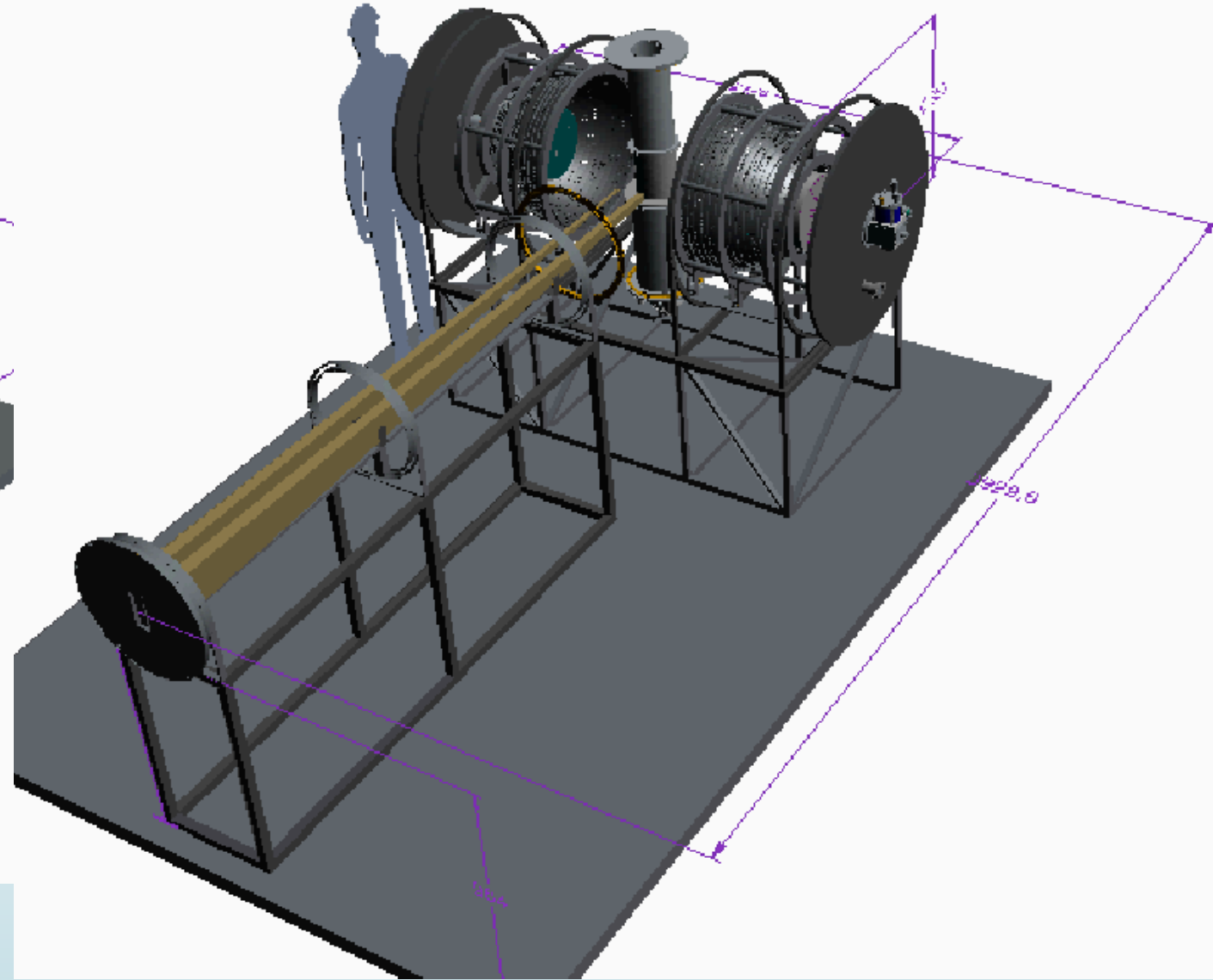
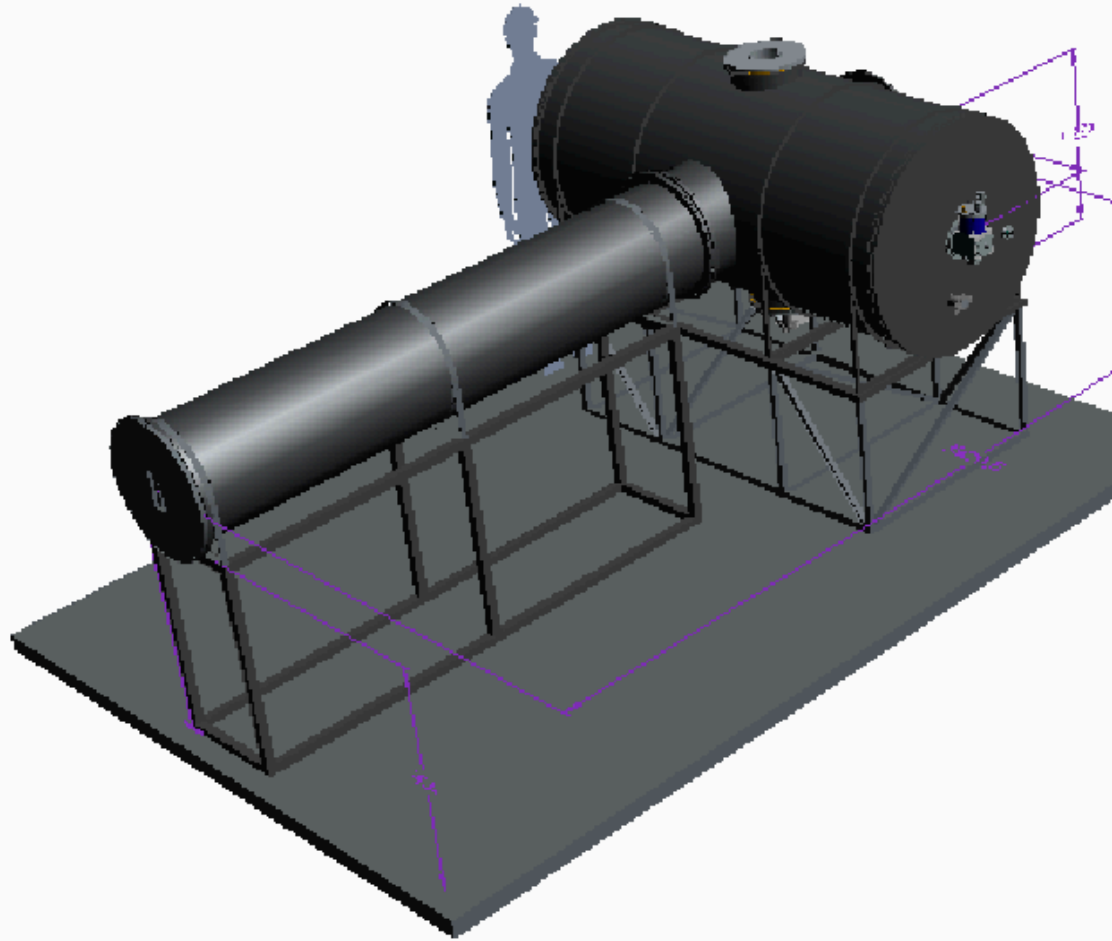
Beryllium block-filter

Detector

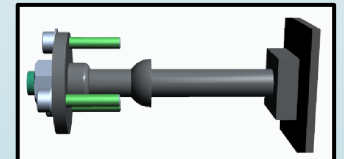
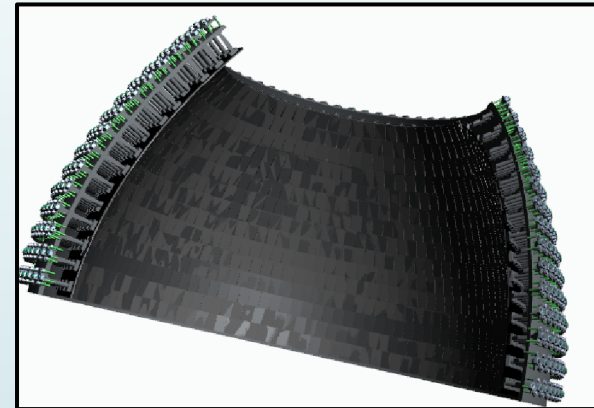
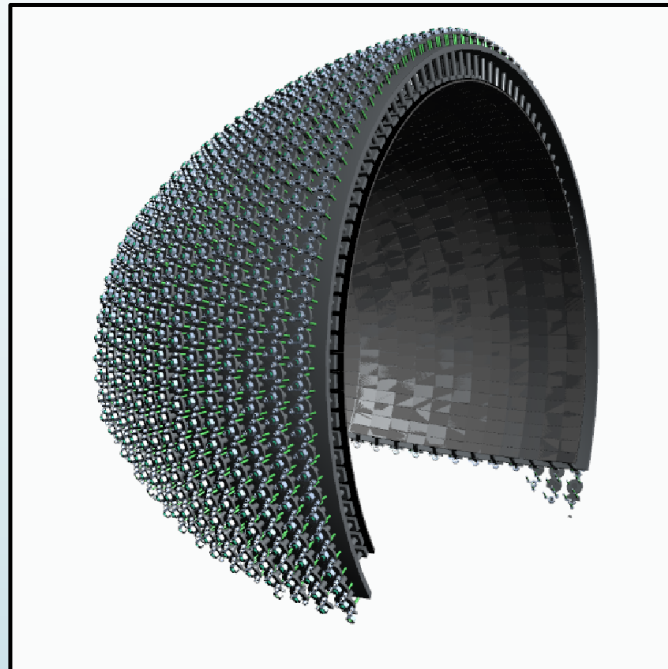
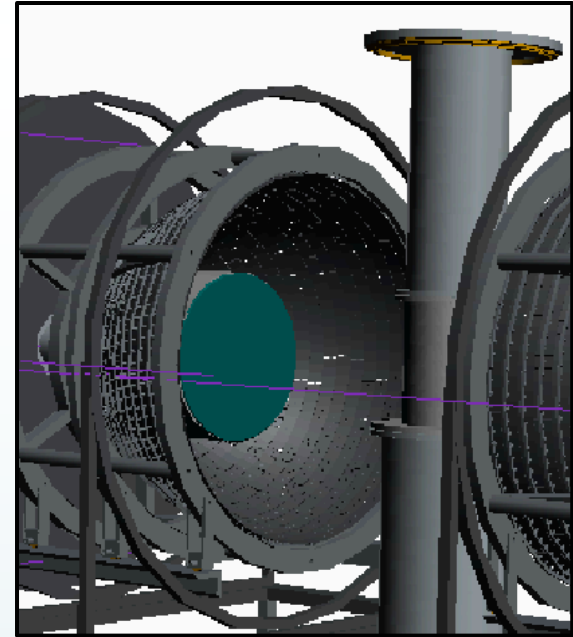
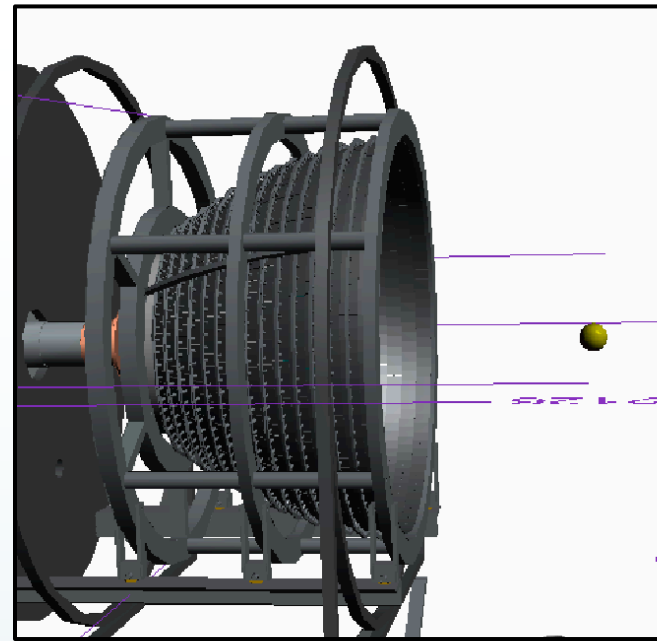
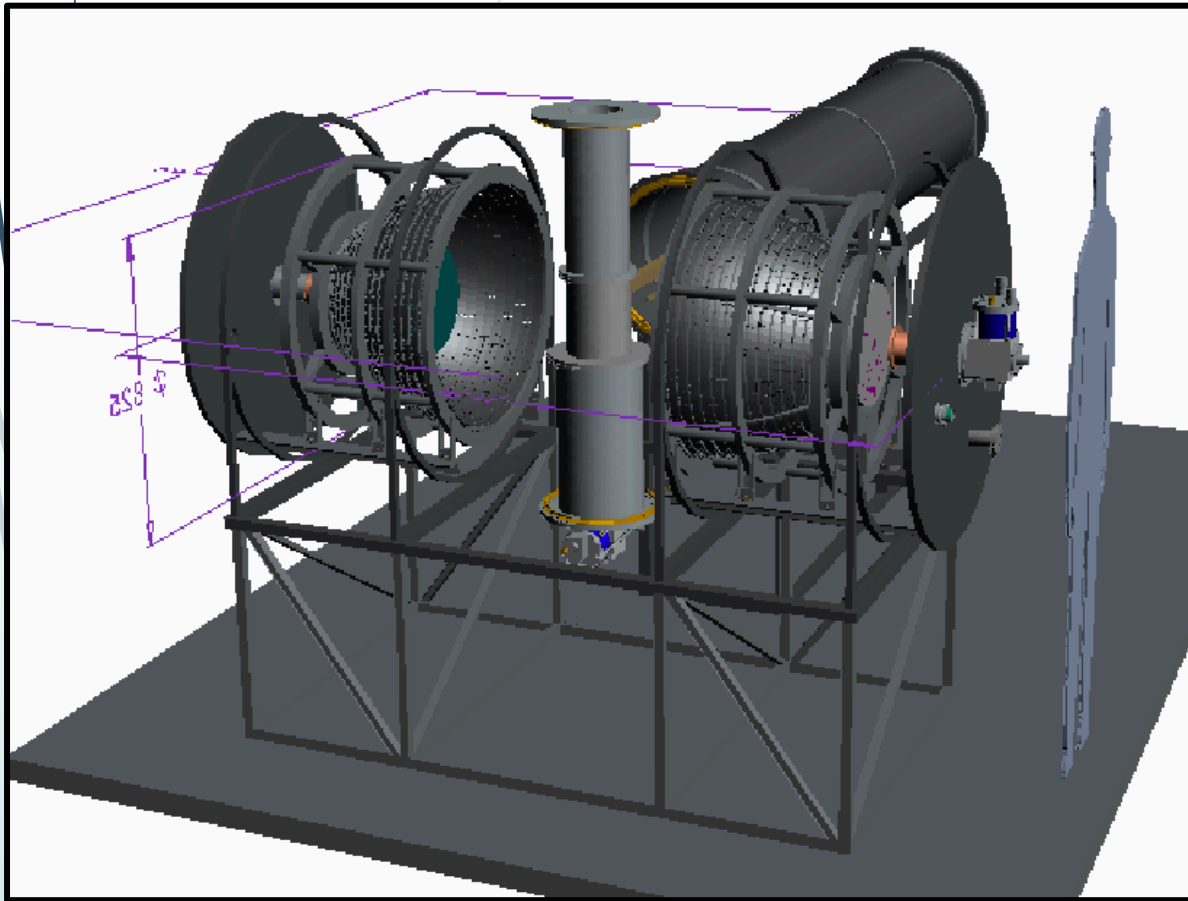


The moderator area for 2 channel:
33.5x40.5 cm² (WxH).

Main characteristics



Main characteristics



Expected characteristics

	NERA	New INS Spectrometer	
Analyzer area	15x3X25 1125cm²	10000x2 20000cm²	
Ratio input/output to neutronguides	16x5cm ² /5x5cm ² 3.2	20x20cm ² / 3x3cm ² 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:

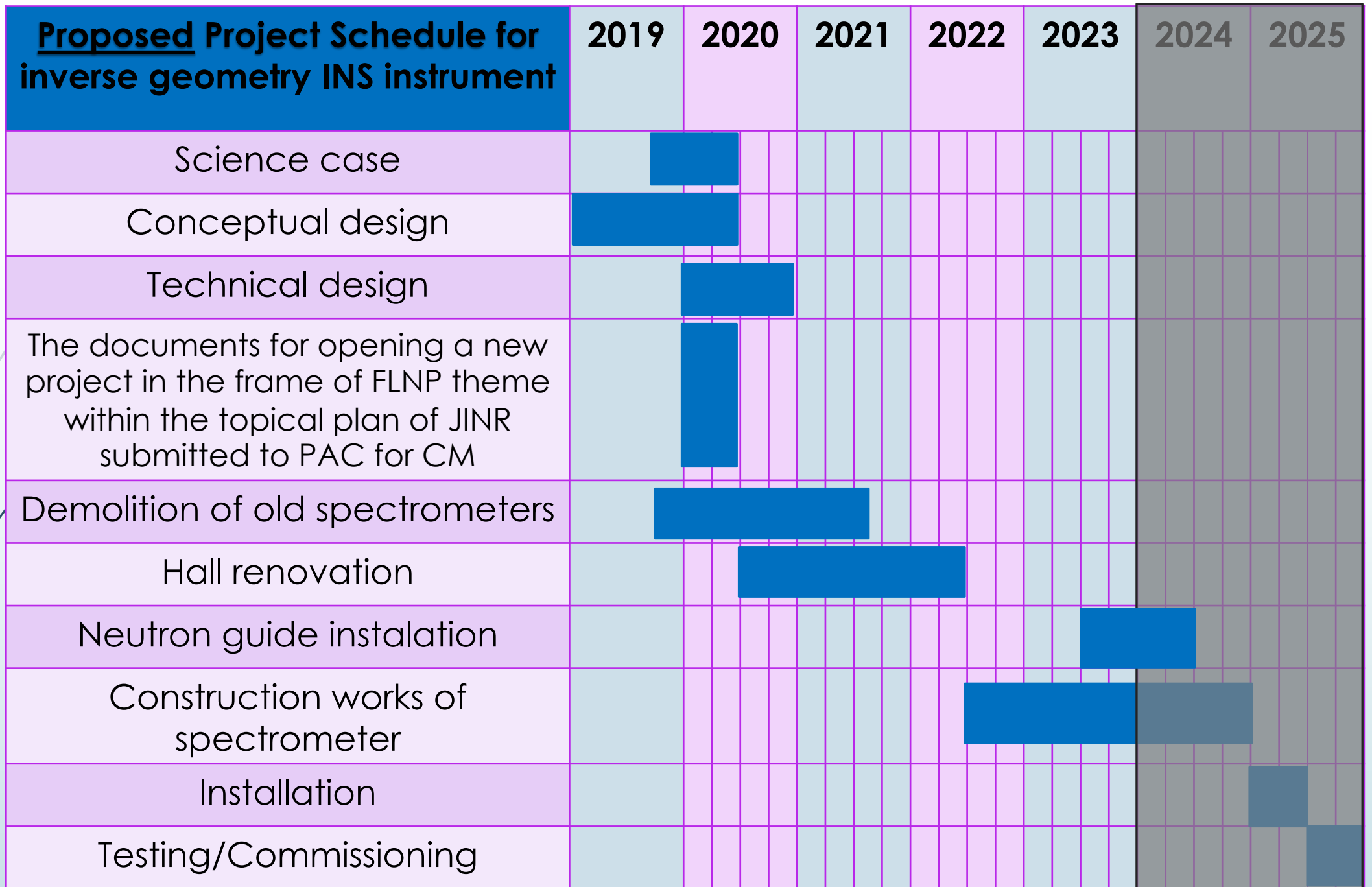
Chudoba D. M.	- Dubna, JINR
Goremychkin E.	- Dubna, JINR
Belushkin A.	- Dubna, JINR
Bodnarchuk V.	- Dubna, JINR
Kruglov A.	- Dubna, JINR
Zajac W.	- Kraków, INP PAN

Project leader: Chudoba D. M.

A dark grey arrow points to the right from the top left corner. Below it, several thin, curved lines in shades of blue and grey sweep across the left side of the slide.

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).**

Time schedule



Time schedule & Cost estimate

Description of units and systems, resources, funding sources	Cost of units (k\$). Resource requirements for 1st part of the project	Proposals of the Laboratory for distribution of funds and resources		
		2021	2022	2023
Neutron guide	2500	600	900	1000
Construction design and technical specification	250	250	-	-
Highly Orientated Pyrolytic Graphite	550	150	250	150
³ He Detectors and electronics	50	-	-	50
Manufacture of vacuum, cryogenic systems and beryllium filters	350	250	50	50
Total	3700	1250	1200	1250

The second part of the project (2024-2025) is planned to cover rest costs for neutron guide system, manufacture of vacuum, cryogenic systems and beryllium filters (~2000k\$).

Time schedule & Cost estimate

№	Description of cost items	Total cost	2021	2022	2023	
Direct expenses						
1	Design	k\$	250	-	-	250
2	Materials	k\$	150	250	200	600
3	Equipment	k\$	850	950	1050	2850
4	Payment for research performed under contracts	k\$	40	40	40	120
5	Travel expenses	k\$	10	10	10	30
Total		k\$	1300	1250	1300	<u>3850</u>

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 !