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Proceedings of the 2nd International Advisory Committee on Biomolecular Dynamics Instrument DNA in MLF at J-PARC

November 12-13, 2008, J-PARC Center,
Japan Atomic Energy Agency
Tokai, Ibaraki, Japan

(Eds.) Masatoshi ARAI, Kazuya AIZAWA, Kenji NAKAJIMA, Kaoru SHIBATA and Nobuaki TAKAHASHI

Materials and Life Science Division
J-PARC Center

July 2009

Japan Atomic Energy Agency

日本原子力研究開発機構

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and Nobuaki TAKAHASHI

Materials and Life Science Division, J-PARC Center, Japan Atomic Energy Agency
Tokai-mura, Naka-gun, Ibaraki-ken

(Received May 14, 2009)

The 2nd International Advisory Committee on the "Biomolecular Dynamics Backscattering Spectrometer DNA" was held on November 12th - 13th, 2008 at J-PARC Center, Japan Atomic Energy Agency. This IAC has been organized for aiming to realize an innovative neutron backscattering instrument in the Materials and Life Science Experimental Facility (MLF) at the J-PARC and therefore four leading scientists in the field of neutron backscattering instruments has been selected as the member (Dr. Dan Neumann (Chair); Prof. Ferenc Mezei; Dr. Hannu Mutka; Dr. Philip Tregenna-Piggott), and the 1st IAC had been held on February 27th - 29th, 2008. This report includes the executive summary and materials of the presentations in the 2nd IAC.

Keywords: J-PARC, MLF, Inelastic Neutron Scattering, Backscattering, Indirect-geometry, Biomolecules

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※ Research Staff on Loan

J-PARC, MLF のダイナミクス解析装置 DNA に関する第 2 回国際アドバイザリ委員会会議録

2008 年 11 月 12 日～13 日：日本原子力研究開発機構 J-PARC センター
（茨城県那珂郡東海村）

日本原子力研究開発機構　J-PARC センター　物質・生命科学ディビジョン
（編）新井　正敏※・相澤　一也・中島　健次・柴田　薫・高橋　伸明

(2009 年 5 月 14 日受理)

2008 年 11 月 12 日~13 日に日本原子力研究開発機構 J-PARC センターにおいて、ダイナミクス解析装置 DNA の第 2 回国際アドバイザリ委員会が開催された。本委員会は、J-PARC/MLF に平成 20 年度より建設が開始されたダイナミクス解析装置 DNA の仕様検討に資することを目的に、背面反射型分光器に造詣の深い著名な 4 名の委員(Dan Neumann 博士(委員長);Ferenc Mezei 教授;Hannu Mutka 博士;Philip Tregenna-Piggott 博士)により組織されており、平成 20 年 2 月 27 日~29 日に第 1 回委員会が開催された。本報告書は、第 2 回委員会の答申、および委員会における講演資料を収録したものである。

J-PARC センター：　〒319-1195　茨城県那珂郡東海村白方白根 2-4
※ 出向職員

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Group photo

A group photo of the 2nd IAC held at HENDEL BLDG., JAEA on Nov 12-13, 2008.

Agenda

The 2nd IAC on the Backscattering Spectrometer DNA in MLF at J-PARC

Japan Atomic Energy Agency, Tokai Research & Development Center, Tokai, Naka, Ibaraki, JAPAN
February 27-29, 2008
Place: HENDEL BLDG, room310 (3F)

Wednesday, November 12, 2008

09:30 – 09:35	Welcome	Masatoshi Arai (JAEA)
09:35 – 10:00	Present Status of J-PARC Neutron Facility	Kenji Nakajima (JAEA)
10:00 –	Current status of the DNA	Kaoru Shibata (JAEA)
	Technical issues; session I	
12.00 – 13:30	Lunch Break	
13:30 – 17:30	Technical issues; session II	
17:30 – 18:30	MLF tour	
19:00	Banquet at Uoyasu: A Japanese style restaurant	

Thursday, November 13, 2008

09:15 – 12:00	Technical issues; session III	
12.00 – 13:30	Lunch Break	
13:30 –	Technical issues; session IV	
	Closed meeting of the advisory committee	IAC members
	Summary	Dan Neumann (NIST)
– 17:50	Preparing a report (paper work)	
17:50 – 18:00	Closing remark	Masatoshi Arai (JAEA)
19:00	Dinner at the Akogi-ga-ura club restaurant hall	

Technical issues

1.	Energy resolution and design of vacuum tank		Nobuaki Takahashi (JAEA)
	1.1	Energy resolution	
	1.2	Design of the vacuum tank	
2.	Repetition Rate Multiplication: RRM		Nobuaki Takahashi (JAEA)
	2.1	RRM	
	2.2	Requirements on the choppers	
	2.3	Further discussion on the neutron guide	
3.	Analyzer system		
	3.1	Reducing BG	Kaoru Shibata (JAEA)
	3.2	Q resolution	Kaoru Shibata (JAEA)
	3.3	Design of the analyzer bank	Nobuaki Takahashi (JAEA)
	3.4	Analyzer mounting device	Nobuaki Takahashi (JAEA)
	3.5	Analyzer alignment system	Nobuaki Takahashi (JAEA)
4.	Neutron transportation system		Nobuaki Takahashi (JAEA)
5.	Data analysis software		Yukinobu Kawakita (Kyushu U.)
6.	Other issues		

Committee member list

Name	Affiliation	part
Dr. Dan Alan Neumann	Group leader of Neutron Condensed Matter Science Group, NIST Center for Neutron Research, National Institute of Standards and Technology, MD, USA	Chair
Prof. Ferenc Mezei	Senior research professor of Institute for Solid State Physics and Optics, Budapest, Hungary Research scientist of Los Alamos National Laboratory, USA Invited researcher of J-PARC Center, Japan Atomic Energy Agency, Ibaraki, Japan	
Dr. Hannu Mika Ilmari Mutka	Deputy Group Leader of the Time-of-Flight High Resolution Group, Institut Laue-Langevin, Grenoble, France Co-responsible of the Time-of-Flight spectrometer IN5 at the ILL	
Dr. Philip Louis William Tregenna-Piggott	Senior research scientist of Neutron Spectroscopy Group, Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, Villigen, Switzerland Responsible of the backscattering spectrometer MARS at the SINQ	

List of attendees

Name	Affiliation
Kaoru Shibata	J-PARC, JAEA
Nobuaki Takahashi	J-PARC, JAEA
Kenji Nakajima	J-PARC, JAEA
Yukinobu Kawakita	Kyushu University
Taku J. Sato	Univ. of Tokyo
Hiroshi Nakagawa	QuBS, JAEA
Satoru Fujiwara	QuBS, JAEA
Itaru Tsukushi	Chiba Inst. Tech.
Masatoshi Arai	J-PARC, JAEA
Shinichi Takata	J-PARC, JAEA
Yasuhiro Inamura	J-PARC, JAEA

1. Executive Summary of the 2nd International Advisory Committee International Advisory Committee (Chair: Dan Neumann)

Overview

Inelastic neutron scattering is an indispensible technique for studying the dynamics of hydrogenous and magnetic materials. In particular, it is ideally suited to developing a detailed understanding of the dynamics of biomolecular systems. Due the simplicity of the neutron's interaction with matter, it is straightforward to directly compare neutron scattering data with molecular dynamics simulations. This provides an extremely stringent test of interatomic potentials, aiding the development of ever more predictive models.

The dynamics of biomolecules occur over a wide range of time scales. Thus it is essential that neutron facilities develop instrumentation that covers many orders of magnitude in time. In this regard particular attention should be paid to the ns time scale as this allows one to begin to address the bioactivity of enzymes and provides direct comparison of neutron results with today's state-of-the-art computer simulations.

The current design of the DNA spectrometer directly addresses these considerations and will undoubtedly provide Japan with a world leading capability in neutron spectroscopy. The excellent energy resolution of ≈ 1 μeV is achieved while maintaining a count rate comparable to the BASIS instrument at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory which has a resolution of only 3 μeV. Thus the Committee congratulates the DNA team for what is truly an impressive design.

DNA will consist of a pre-sample flight path using an advanced neutron guide design with a pulse-shaping chopper, additional choppers that allow repetition rate multiplication (RRM), and large-area Si(111) and Si(311) crystal analyzer systems. This design provides a very wide range of capabilities with the flexibility to trade resolution for intensity. It is noteworthy that the inclusion of the RRM technique would make DNA the first inverted geometry instrument in the world to employ this approach. The Committee also enthusiastically supports the ambitious goal of providing a "signal-to-noise" ratio of at least 10,000 to 1. If achieved, this could lead to qualitatively new science.

The Committee noted that the design as presented will undoubtedly be expensive to realize. However we were not able to see a way to significantly reduce costs without impacting the performance and flexibility of the design. We only note that we believe the highest resolution mode which employs the 1 cm slit on the pulse-shaping chopper and the Si(111) analyzer should be given the absolutely highest priority.

The rest of the report deals primarily with components of DNA.

1. Moderator

The high efficiency coupled cold moderators with water pre-moderator are trademark features of the J-PARC Materials and Life Sciences Facility (MLF). These moderators display exceptionally high peak brightness with 220 μs FWHM pulse length. Combined with a pulse shaping chopper, this capability will

make DNA the premier high resolution backscattering spectrometer at a spallation source. It will offer higher intensity at the same resolution than its strongest competitor at SNS. At the same time, the high peak brightness of the moderator allows one to trade intensity for resolution by employing pulse shaping choppers with only 1 cm slit width. This means that DNA will be the first backscattering instrument at a spallation source to achieve 1 μeV resolution. This projected success is made possible by skilfully using the brightness provided by the coupled cold moderator, a distinctive design strength of the MLF.

2. Guides

The DNA design team has made intelligent use of the capabilities offered by advanced supermirror technology. The current design is an optimized, focussing beam delivery system which provides a high neutron flux to an area of about 20x20 mm^2. This provides a concentrated flux on small samples of biomaterials while maintaining the excellent energy resolution. It is desirable to continue this work in order to minimize the cost by using the most powerful mirrors at the few critical locations in the focussing guide and by employing lower m-value sections wherever acceptable

3. Choppers

The chopper system is a crucial component of DNA, providing both the flexibility to trade resolution for intensity and the ability to scan an extended energy range. The pulse shaping choppers are the key to DNA's flexibility. Using a slit width of 1 cm, the source pulse has a FWHM of less than 10 μs providing an energy resolution ≈ 1 μeV. For those applications requiring higher count rates, pulse shaping choppers with 3 or 6 cm slit widths can be employed. One can even keep the full source pulse of 220 μs by stopping the choppers in the open position. The method of changing instrumental resolution will most probably involve physically changing the pulse shaping double chopper. The committee recommends studying ways to accomplish this task in a minimum of time thereby providing operational flexibility and swift response to user demand.

The innovative use of Repetition Rate Multiplication (RRM) in a backscattering spectrometer allows researchers to achieve pulse shaping without the usual restriction of the energy range of the measurement. The successful implementation of this feature will be a major milestone in the development of neutron instrumentation in general.

The proposed chopper system, including the three counter-rotating double-disc RRM frame separation choppers, is well optimized, offering state-of-the-art high performance disc chopper technology, without exceeding current technological limits. This provides excellent performance while minimizing technological risk. The detailed, geometrical chopper system design has been validated by Monte Carlo simulations, which reveal that the residual beam contamination will be below 1 ppm. The extensive and outstanding chopper system design work accomplished by the DNA team can be considered as largely completed.

What remains to be done is a detailed evaluation of the chopper timing and geometrical positioning

accuracy requirements to guarantee operation without creating background leakage. The evaluation of these aspects is an important part of the detailed design, but the Committee does not expect any difficulties in meeting the resulting spatial and temporal accuracy requirements.

One of the most challenging aspects of operating the RRM chopper system will be to avoid gaps in the coverage of the energy transfer domain. Continuous slewing of the phasing of the chopper system with respect to the source while maintaining very strict phasing between the different chopper discs seems to be too demanding. The Committee suggests that the DNA team examine providing a quasi-uniform continuous coverage of the broad energy transfer band by using a few discrete phasing configurations. Switching between these would only require a few minutes for the choppers to stabilize into new locked phases.

4. Sample Area and Scattering Chamber

The Committee is pleased to note that the proposed size of the sample flange has increased to a diameter of 40 cm, with a concomitant increase of the sample to analyzer distance to 2.3 m and that this has been achieved without compromising the resolution. This change allows DNA to accept J-PARC standard sample environments. Even though 40 cm is probably too small to mount a very high-field superconducting magnet, the increase from the previously considered 28 cm relaxes constraints concerning low field magnets (≤10 T) or high pressure devices. The use of specialized environments in an important aspect in neutron scattering experiments and therefore this increase allows DNA to be applied to even more scientific and technological problems. We remind the DNA team to allow for the alignment of single crystal samples.

Due to the design revision the evacuated scattering chamber has to be slightly bigger but this is still within the standard practice on time-of-flight instruments and with little impact on the fabrication or cost of the chamber.

5. Analyzer

The DNA team strives for the ambitious goal of achieving a signal to noise ratio of 10,000 to 1. To this end, they have worked to identify potential sources of background and devise ways to eliminate them. One source is the scattering from the epoxy resin and aluminum back plate upon which the silicon wafers are affixed. The DNA team proposes coating the back of each wafer with 20 μm of the neutron absorbing material boron carbide (B_4C), sandwiched between 5 μm aluminum films. This solution is innovative, but has never been used before in any backscattering instrument. Thus the method should be thoroughly tested before many square meters of analyzer are manufactured. We suggest affixing several crystals, with different absorbing materials, onto an aluminum plate of the correct curvature and subject the analyzer fragment to repeated vacuum cycles over a period of ~ 3 months. In our experience, any problems with the silicon peeling off should occur within this time frame. The DNA team could also explore the possibility of mounting the analyzer material directly on aluminum impregnated with boron. In the end, the Committee believes some arrangement of materials can be found that will allow the DNA

team to achieve their objective.

Given the radius of curvature of the analyzer banks, δd/d can be calculated as a function of the thickness of the crystals using standard elasticity theory. The DNA team has calculated that for the 2.3 m radius of curvature relevant to their instrument, a crystal thickness of 0.75 mm will provide the δd/d corresponding to the optimum intensity and resolution. In practice, the stress induced by bending the crystals is greater at the center than at the edges of the silicon wafers, with the consequence that the δd/d at the edges is lower than expected. Therefore a crystal thickness of 0.9 or 1.0 mm should give a little more intensity without comprising the resolution.

As a final point, the DNA team has concentrated their efforts on finding the optimum conditions for the Si(111) reflection. We trust that they will now demonstrate equal vigor for the Si(311) option that will enhance the Q-range of the instrument.

6. Detectors

The Committee fully endorses the proposed use of position-sensitive ^{3}He tubes for the detectors. Moreover, the detector arrangement is well-thought out. This combination will allow the DNA team to appropriately bin the data to minimize the energy resolution. This approach is being used at SNS and has been fully explored by the DNA team.

The Committee was also pleased by the provision of diffraction detectors which are very useful for monitoring the sample. Since the bandwidth for Si (111) is quite small, the simultaneous measurement of inelastic scattering and diffraction requires an angle dispersive measurement. Alternatively, if one was willing to stop the chopper, an adequate diffraction pattern could be measured by the usual time-of-flight approach.

7. Data acquisition

The event recording (or “list mode”) data acquisition approach generally adopted as the MLF standard offers an excellent solution for DNA. With a good number of chopper discs and complex sample environment equipment, it is important to collect a full record of all events as they occur, without losing any information by building histograms on the fly. The committee recommends developing a flexible tool for data visualization during data collection. This will be particularly challenging for the RRM mode of operation where several chopper phasing will be needed to obtain a complete spectrum.

Cost and Schedule

The Committee was not presented with the information necessary to comment in detail on the potential cost of the instrument. However as the instrument has both a large area crystal analyzer and five or six pairs of high-speed counter-rotating choppers, the design will undoubtedly be rather expensive to realize. However, we could see no way to reduce the cost of the instrument significantly without compromising performance. The schedule for completion in 2011 is quite optimistic, particularly in light of the fact that

construction funding is not in hand.

Acknowledgements

Once again the committee would like to extend their gratitude to the DNA team for their clear, carefully prepared presentations and for their hospitality during our stay. We have every confidence that they will be able to successfully realize their creative design of DNA and thus provide the Japanese scientific community one of the world's premier neutron scattering instruments for the study of dynamics on the ns timescale.

2. Introductory part of the 2nd International Advisory Committee
2.1. Welcome
Masatoshi Arai (JAEA)

Recent Major Events

2008 2 — **Beam power of 5 kW/pulse (130 kW equiv.), 50 kW extracted at 3 GeV**

The safety regulation limits the power up to 4kW.

4

5 — **Injection, RF capture and extraction with 3 GeV beams at MR (5/22)**
Production of neutrons (5/30)

6

7

8

9 — **Beam power of 12 kW/pulse (300 kW equiv.), 210 kW extracted at 3 GeV**
Production of muons (9/26)

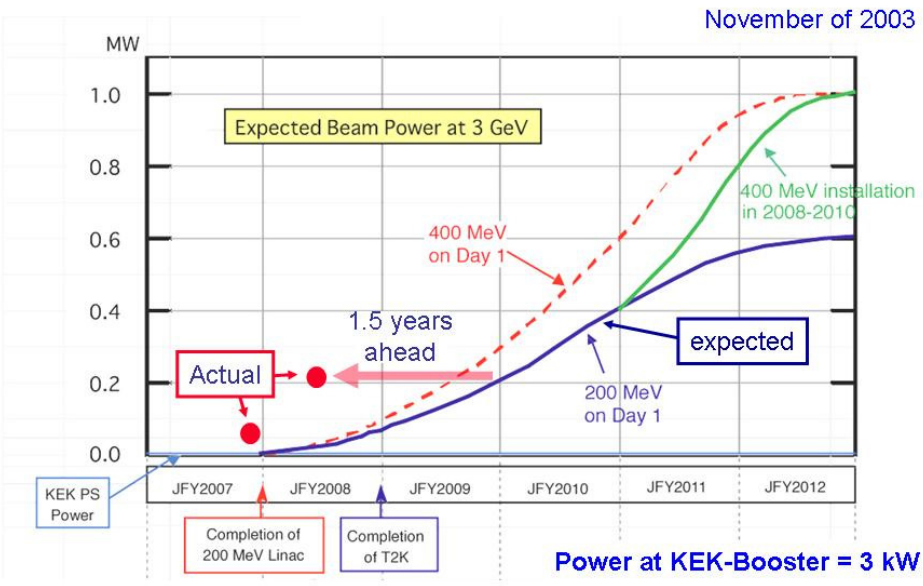
10 — Novel Prizes awarded for four Japanese scientists.
Prof. Nambu, Masukawa, Kobayashi

11

12 — **Acceleration of Beams at the 50 GeV MR**
Neutrons + Muons: Beam Usage for General Users

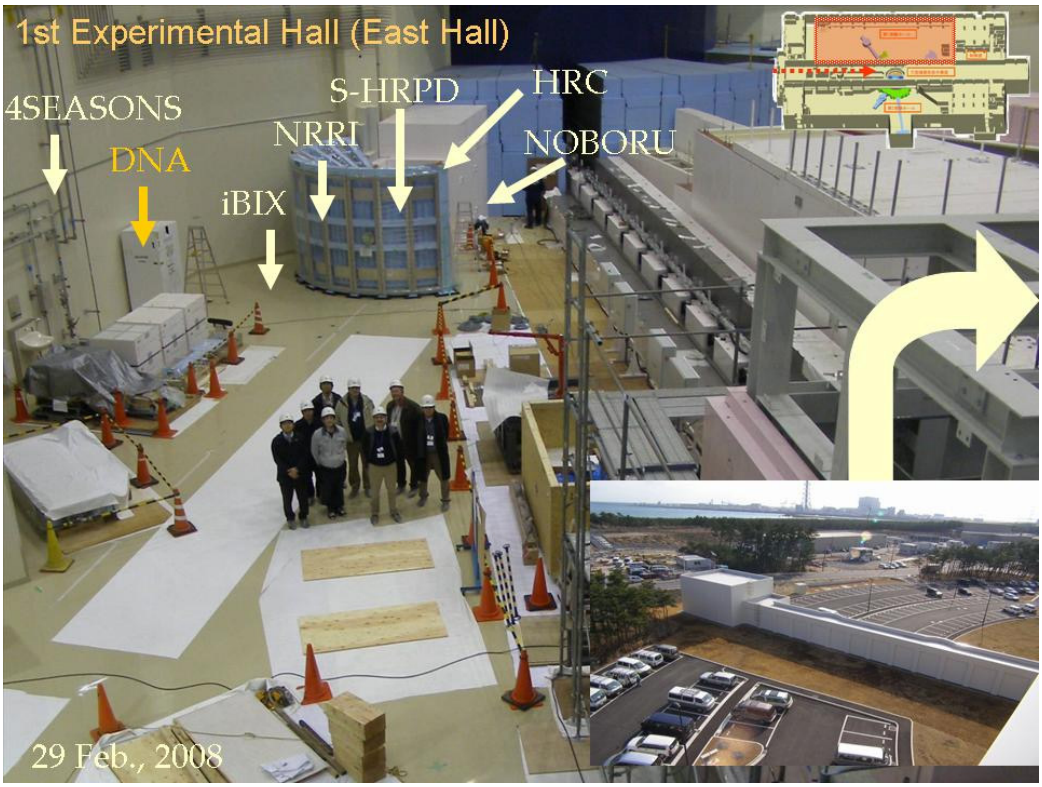
100kW.

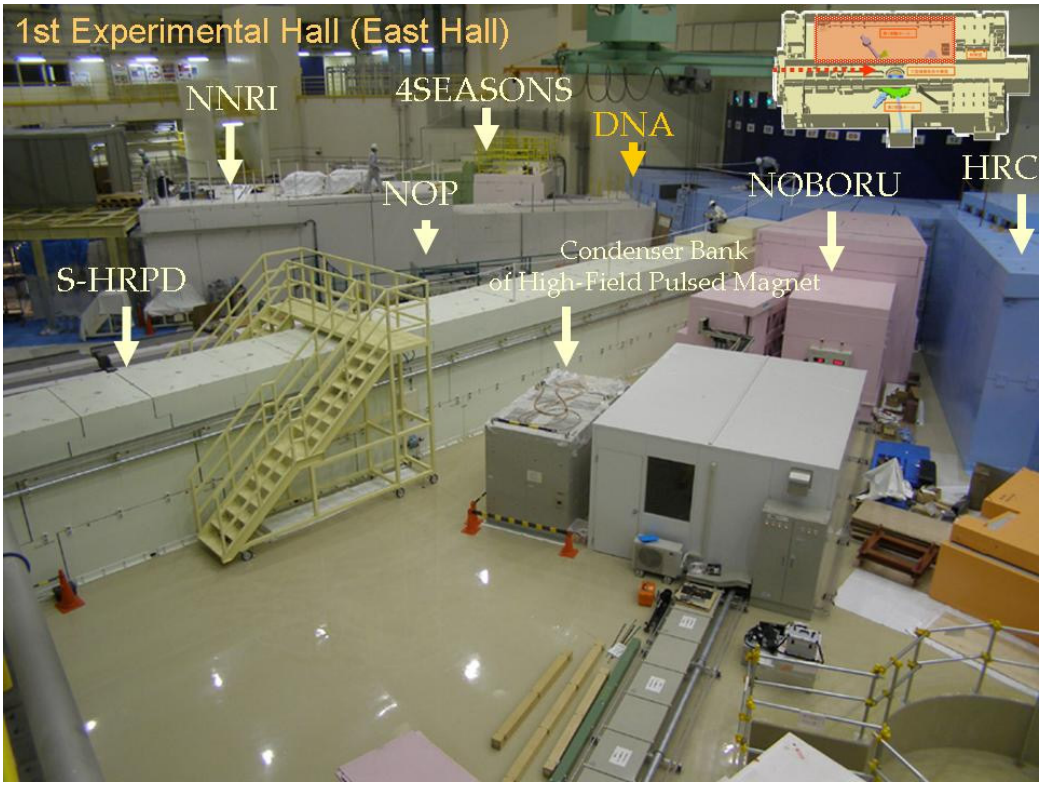
Expected Power vs. Actual Power
(ramping up status of the accelerators)



2.2. Present Status of J-PARC Neutron Facility

Kenji Nakajima (JAEA)




1st Experimental Hall (East Hall)
NNRI
4SEASONS
DNA
NOP
NOBORU
HRC
S-HRPD
Condenser Bank
of High-Field Pulsed Magnet


2nd Experimental Hall (West Hall)
AMATERAS
iMATERIA
NOVA
TAKUMI
November 2008

Recent Events at MLF, J-PARC

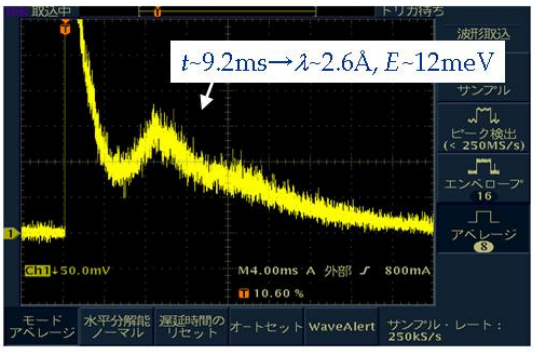
Major Events at MLF, J-PARC after the last DNA-IAC (Feb., '08)

- MLF was Designated a Controlled Area on 14 May, '08
- **The First Neutron Beam was Delivered to MLF on 30 May, '08**
- Run#16 & Run#17
  RUN#16: 30-31 May, 2008; 5mA, single shots
  RUN#17: 16-22 June, 2008; 5mA, 8.3Hz、25Hz (1.7~4kW)
  Commissioning of iBIX, NNRI, S-HRPD, NOBORU, iMATERIA started
- The First Call for Proposals for the MLF User Program; 8 July – 3 Sept., '08
- The First Muon Beam was Delivered to MLF on 26 Sept., '08
- Run#18 & Run#19
  RUN#18: 19-29 September, 2008; 5mA, 8.3Hz、25Hz (1.7~4kW)
  RUN#19: Cancelled
  Commissioning of 4SEASONS, TAKUMI, Muon Instrument started

The First Neutron Beam at MLF, J-PARC

The First Proton Beam was Delivered from RSC to MLF Target
@10:15, 30 May, 2008 (A pulse reached to the target at the first trial.)

The First Neutron Beam Observed at MLF, J-PARC
14:25, 30 May, 2008 @NOBORU(BL10)



4×10^{11} Protons/Pulse
C-TOF with ^{6}Li Scintillator
Moderator Temp.: 18K
$L_{mod.-detector}$=14m

- Observed neutron flux well agrees with calculation within the accuracy of 30%.
- 12 meV Peak ->100% of Para-H_2 at Moderator

Pulse Character: J-PARC vs. KENS

MLF, J-PARC (Mod.: Para-H_2) vs. KENS, KEK (Mod.: Methane)

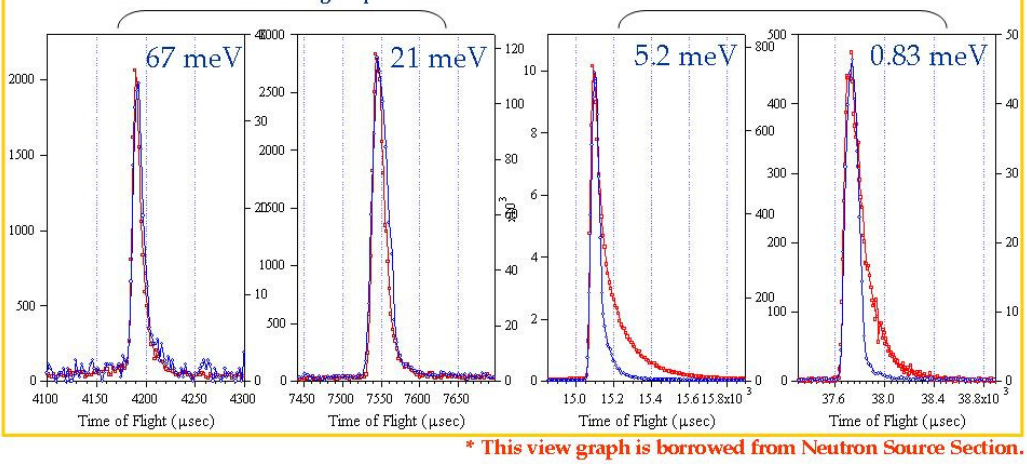
Methane has higher (×1.8) H-Density than H_2 does.
Methane can not last at high-flux condition.

Pulse Shape from Decoupled Moderator (BL10)

KENS
MLF

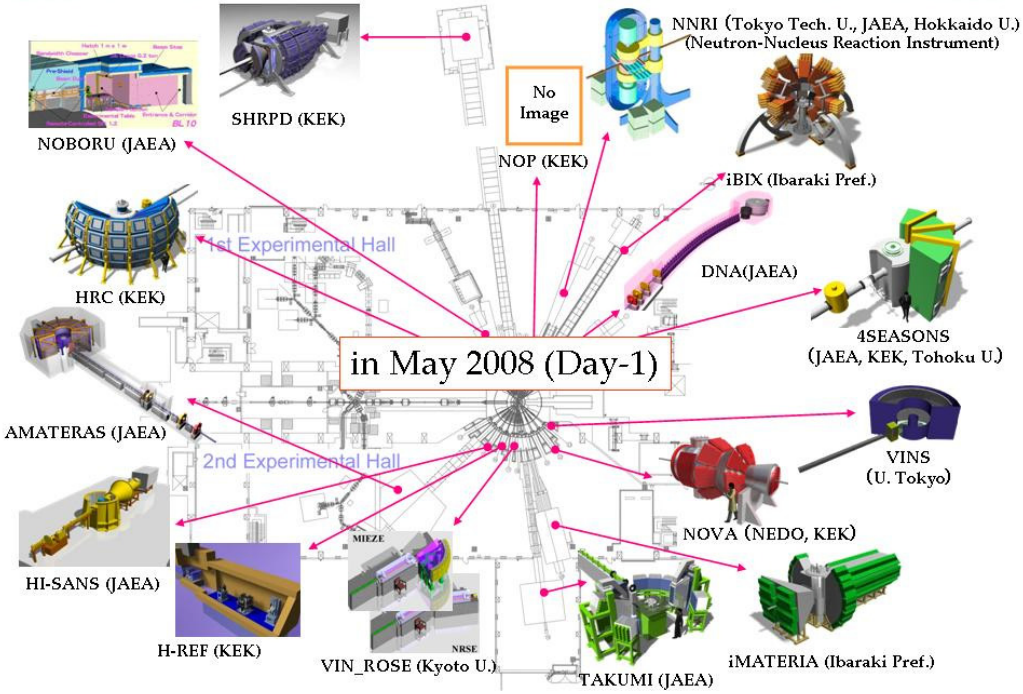
Comparable Peak Width is Comparable to KENS, although H_2 has Lower H-density.
→Result of Moderator Design Optimization

Peak Shape is Better than that from KENS Moderator.→Advantage of Para-H_2.



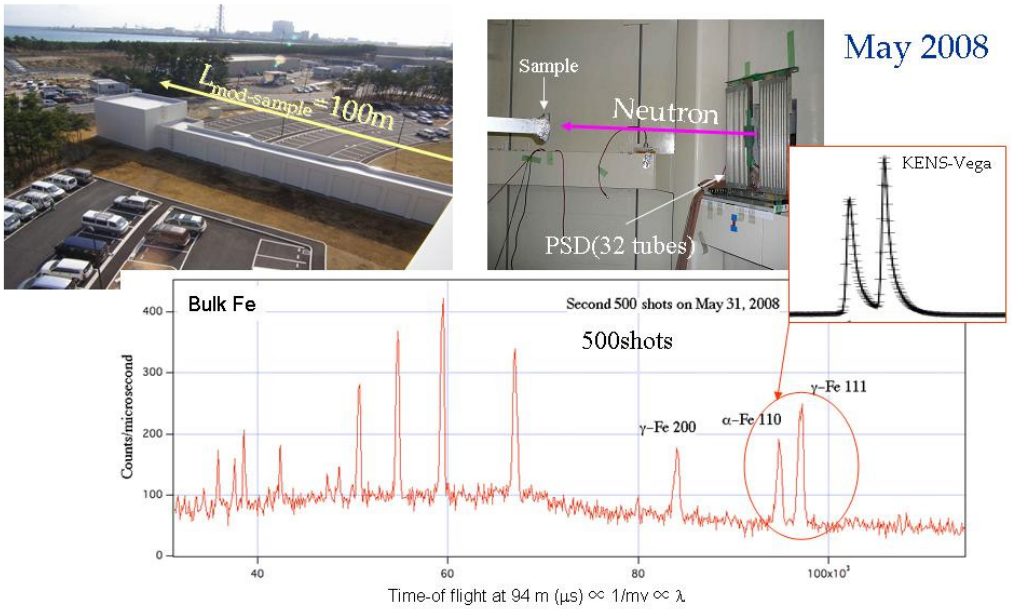
* This view graph is borrowed from Neutron Source Section.

Neutron Instrument at MLF, J-PARC



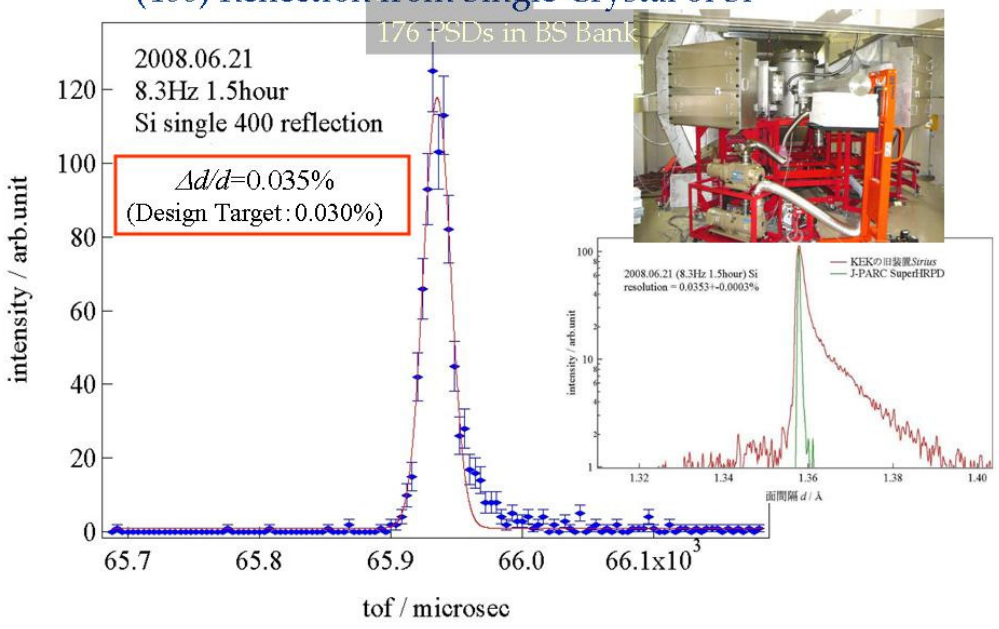
Super-HRPD(BL08)

S-HRPD: High Resolution Powder Diffractometer (J-PARC/KEK)



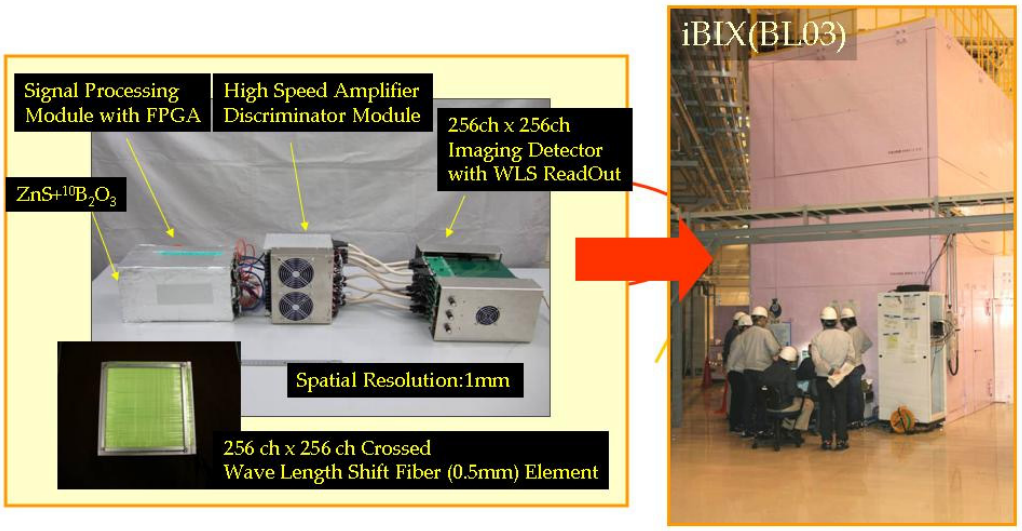
BL08:Super-HRPD

June 21, 2008
(400) Reflection from Single Crystal of Si



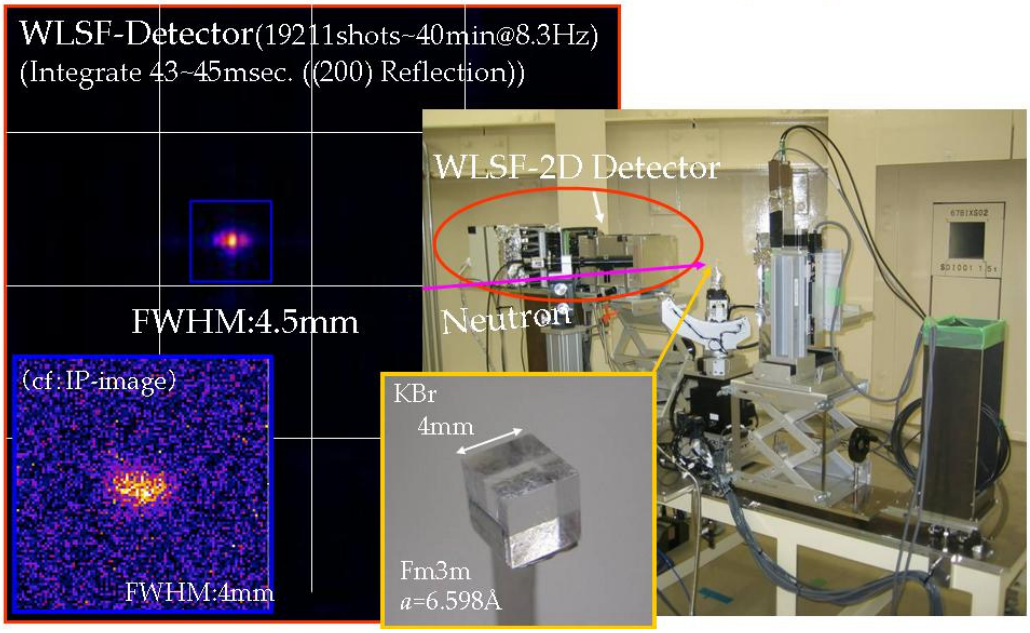
Wave Length Shit Fiber Detector @ iBIX(BL03)

2D Scintillation Detector with WLS R/O developed by J-PARC

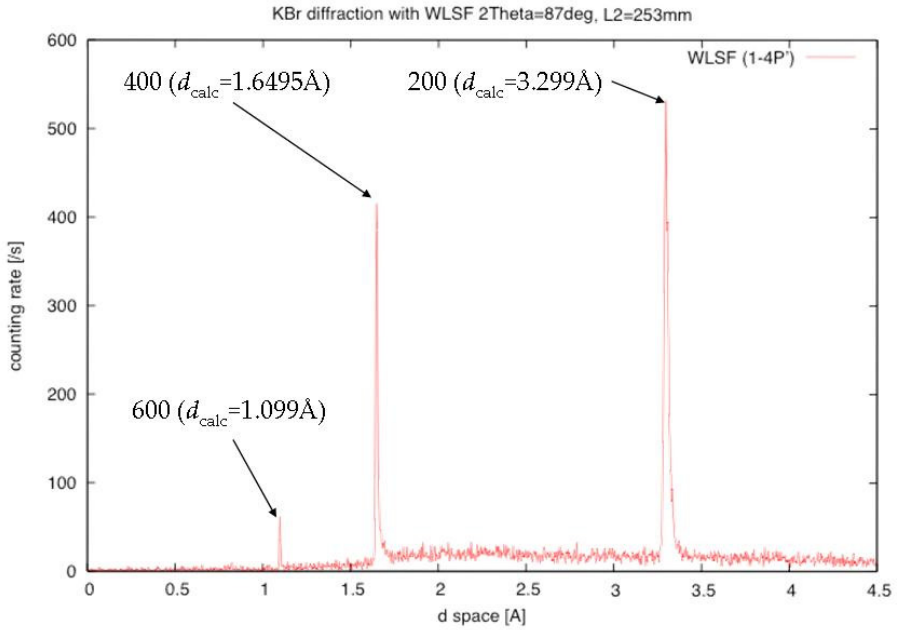


Wave Length Shit Fiber Detector @ iBIX(BL03)

2D Scintillation Detector with WLS R/O developed by J-PARC



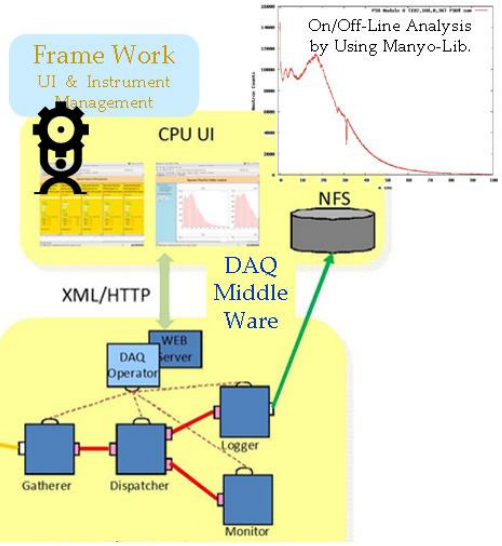
Wave Length Shit Fiber Detector @ iBIX(BL03)



DAQ System@iMATERIA(BL20)

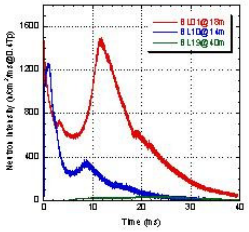
Newly Developed DAQ System is Applied to iMATERIA

- Network Distributed DAQ using SiTCP / Event Data Collection
- We have Confirmed the Function of the Full DAQ System
  - ✓Electronics
  - ✓Middle Ware
  - ✓Analysis Software
  - ✓Flame Work



4SEASONS Commissioning

- Commissioning@4SEASONS has been Started from September '08
- Major Equipments are under Delivering
  - ✓Scattering Chamber & Shieldings are OK
  - ✓Beam Transport: Front End Section Only
    Other Parts will Arrive in December '08
  - ✓Detectors: 112 Arrived in the Last Week
    88 will Arrive in the Next Week
  - ✓Fermi Chopper: will Arrive in December '08
  - ✓Vacuum System: will be Ready in 1-2 Months
- Flux at 18m Measured by C-TOF
- DAQ System without Actual Detectors Seems OK & Some Powder Patterns can be Measured



The First Call (JFY'08) for Proposals to MLF, J-PARC

Proposals for the First User Program at MLF, J-PARC were Called Internationally.
for 6 Neutron Instruments & 1 Muon Instrument (NNRI is in closed usage)
for 32 Days of User Beamtime

- Call for Proposal: 8 July ~ 3 September, 2008
- Technical Review: ~ October, 2008
- Scientific Review: 31 October, 2008
  by The 1st Neutron Science Proposal Review Committee
  (24 Members (Including 4 Foreign Members))
- User Program will start from 21 December, 2008

Affiliations of Principal Proposers	# of Prop.
University & Institute (inside Japan)	24
University & Institute (outside Japan)	1
Industrial	26
Ibaraki Prefecture Project	32
JAEA	10
KEK	5
Total	98

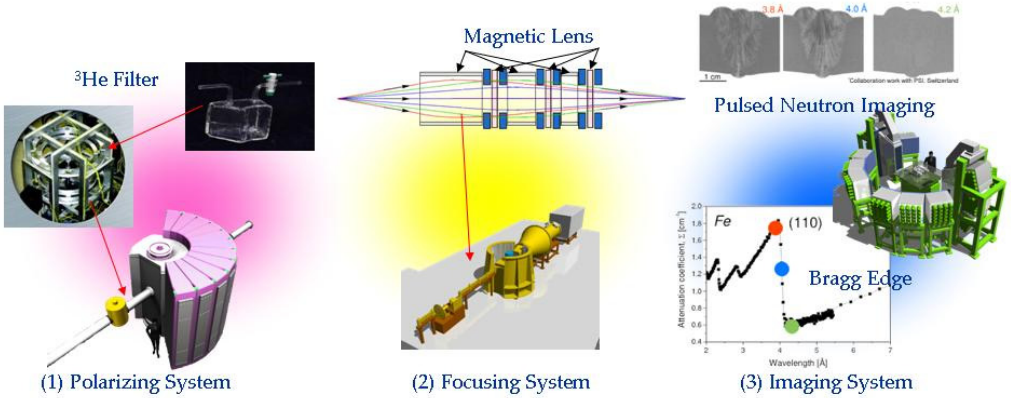
	Total			General Use			Instrumental G./ Project Use		
	# of Prop.	Demand (hours)	Demand (days)	# of Prop.	Demand (hours)	Demand (days)	# of Prop.	Demand (hours)	Demand (days)
BL-01 4SEASONS (High-Efficiency Chopper)	5	1,464	61	3	408	17	2	1,056	44
BL-03 iBIX (Single Crystal Diff.)	10	1,152	48	2	840	35	8	312	13
BL-04 NNRI (Neutron-Nucleus Reaction Instrument)	1	1,008	42	0	0	0	1	1,008	42
BL-08 Super-HRPD	16	2,064	86	14	756	32	2	1,296	54
BL-10 NOBORU	7	2,412	101	4	540	23	3	1,872	78
BL-19 TAKUMI (Engineering Diff.)	6	1,224	51	3	240	10	3	984	41
BL-20 iMATERIA (High Intensity Powder Diff.)	45	729	31	21	420	18	24	309	13
D1 (Muon)	8	1,240	52	5	472	20	3	768	32
Total	**98**	**11,293**	**472**	52	3,676	155	46	7,605	317

JST Program of Development of Advanced Neutron Optics

- The JST* Program for Development of Quantum Beam Technology

*JST: Japan Science and Technology Agency

Principal Investigator: K. Kakurai
Budget: ~100M¥/Year
Period: JFY2008 ~ JFY2012
Subject: Development and Application of Advanced Neutron Optics and Detectors Including Polarizing, Focusing, and Imaging Systems
Member's Institute: JAEA, Hokkaido U., Tohoku U., KEK, Tokyo U., Kyoto U.



Summary

- We have Succeeded in Getting the First Neutron Beam at MLF, J-PARC on 30 May, 2008
- 5 Neutron Instruments have Received the Neutron Beam in Day-1
  iBIX, NNRI, S-HRPD, NOBORU, iMATERIA
- 2 Neutron Instruments Started Commissioning from September, 2008
  4SEASONS, TAKUMI
  and AMATERAS will join soon...
- We have Confirmed the Excellent Performance of the Neutron Source and Commissioning of the Neutron Instruments going well.
- 98 Proposals have been submitted to the First User Program at MLF.
- We will have the First User Program at MLF from 21 December, 2008.
- Other 4 Instruments (NOP, HRC, H-REF, NOVA) will Join in Next Year and we are Expecting to Start the Construction of DNA and HI-SANS.

2.3 Current status of the DNA
Kaoru Shibata (JAEA)

DNA-IAC'08

Current status of the DNA and the actions for comments in the 1st DNA IAC

Kaoru SHIBATA
Neutron Science Section
MLF Division
J-PARC Center

1

Thank you for the Recommendations in the 1st IAC-DNA:2008.Feb.27~29

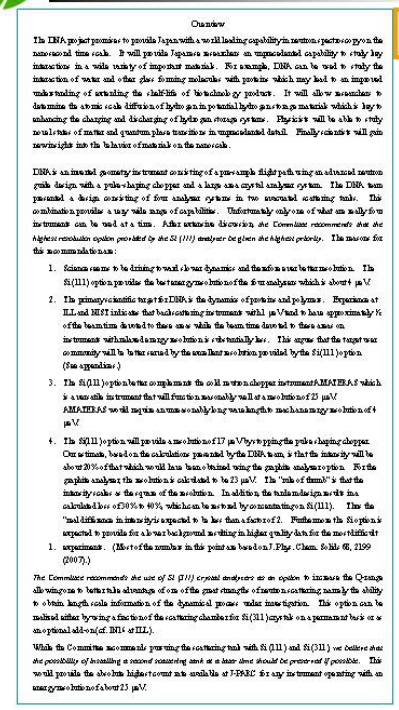
The International Advisory Committee on DNA
The 1st IAC-DNA:2008.Feb.27~29.
chairman: Dr. Dan Neumann (NIST, USA)
Prof. Ferenc Mezei (ISSP, Hungary and LANL, USA)
Dr. Hannu Mutuka (ILL, France)
Dr. Philip Tregenna-Piggott (PSI, Switzerland)

Photos at the 1st IAC-DNA

Recommendations.
/DNA will be a world-leading instrument for the study of nanosecond dynamics using neutron scattering.
/We believe that science is driving demands to ever better energy-resolution.
/It is our opinion that you should try to provide optimized capabilities that are most complementary to those of other instruments at J-PARC.
/It's important for the facility to have a high resolution spectrometer with ~4 μeV resolution.
/We suggest the Si (111) analyzer be given a higher priority while maintaining the possibility of including the graphite chamber as a later option. We believe that this will satisfy user demand in the life sciences.

2

Executive Summary of the International Advisory Committee



Overview

The iBNA project promises to provide Japan with a world leading capability in neutron spectroscopy on the nanosecond time scale. It will provide Japanese researchers an unprecedented capability to study key interactions in a wide variety of important materials. For example, iBNA can be used to study the interaction of water and other glass forming molecules with proteins which may lead to an improved understanding of extending the shelf-life of biotechnology products. It will allow researchers to determine the atomic scale diffusion of hydrogen in potential hydrogen storage materials which is key to enhancing the charging and discharging of hydrogen storage systems. Physicists will be able to study metal-to-take of matter and quantum phase transitions in unprecedented detail. Finally, scientists will gain new insights into the behavior of materials on the nanoscale.

iBNA is an inverted geometry instrument consisting of a pure sample flight path using an advanced neutron guide design with a pulse-shaping chopper and a large area crystal analyzer system. The iBNA team presented a design consisting of four analyzer systems in two truncated scattering tanks. This combination provides a very wide range of capabilities. Unfortunately only one of what are really four instruments can be used at a time. After extensive discussion, *the Committee recommends that the highest resolution option provided by the Si (111) analyzer be given the highest priority.* The reasons for this recommendation are:

1. Science seems to be driving toward slower dynamics and therefore better resolution. The Si(111) option provides the best energy resolution of the four analyzers which is about 4 μeV.
2. The primary scientific target for iBNA is the dynamics of proteins and polymers. Experience at ILL and NIST indicates that backscattering instruments with 1 μeV and 6 have approximately ½ of the beam time devoted to these areas while the beam time devoted to these areas on instruments with relaxed energy resolution is substantially less. This argues that the target user community will be better served by the excellent resolution provided by the Si(111) option (See appendix.)
3. The Si(111) option better complements the cold neutron chopper instrument AMATERAS which is a versatile instrument that will function reasonably well at a resolution of 25 μeV. AMATERAS would require an unreasonably long vacuum flight path mechanical resolution of 4 μeV.
4. The Si(111) option will provide a resolution of 17 μeV by tripping the pulse shaping chopper. Our estimate, based on the calculations presented by the iBNA team, is that the intensity will be about 20% of that which would have been obtained using the graphite analyzer option. For the graphite analyzer the resolution is calculated to be 23 μeV. The "rule of thumb" is that the intensity scales as the square of the resolution. In addition the fundamental gain in flux calculated is of 30% to 40%, which can be traded by concentrating on Si(111). Thus the "real difference in intensity is expected to be less than a factor of 2. Furthermore the Si option is expected to provide for a lower background resulting in higher quality data for the most difficult experiments. (Most of the numbers in this point are based on J. Phys. Chem. Solids 68, 2199 (2007).)

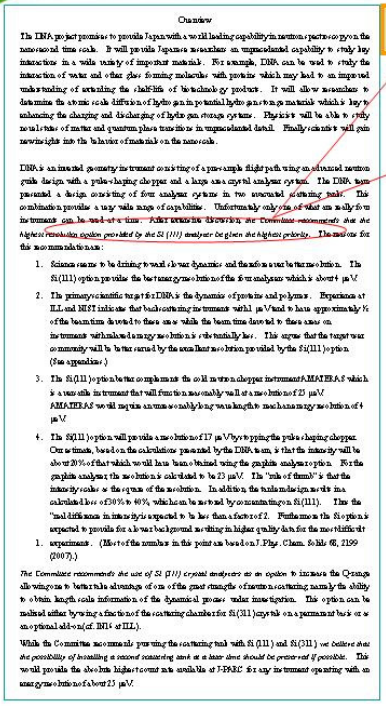
The Committee recommends the use of Si (111) crystal analyzers as an option to increase the Q-range allowing one to better take advantage of one of the great strengths of neutron scattering, namely the ability to obtain length scale information of the dynamical process under investigation. This option can be realized either by using a fraction of the scattering chamber for Si(311) crystals on a permanent basis or as an optional add-on (cf. BL4 at ILL).

While the Committee recommends pursuing the scattering tank with Si(111) and Si(311) *we believe that the possibility of installing a second scattering tank at a later date should be preserved if possible.* This would provide the absolute highest count rate available at J-PARC for any instrument operating with an energy resolution of about 25 μeV.

The most important 2 point in the recommendations

3

Executive Summary of the International Advisory Committee



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While the Committee recommends pursuing the scattering tank with Si(111) and Si(311) *we believe that the possibility of installing a second scattering tank at a later date should be preserved if possible.* This would provide the absolute highest count rate available at J-PARC for any instrument operating with an energy resolution of about 25 μeV.

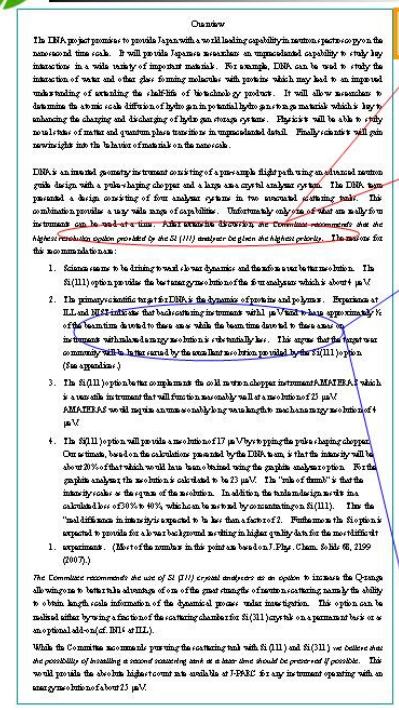
The most important 2 point in the recommendations

the Committee recommends that the highest resolution option provided by the Si (111) analyzer be given the highest priority.

We changed the construction plan that
" the primary spectrometer is Si(111) & Si(311) high energy resolution mode."

4

Executive Summary of the International Advisory Committee



Overview

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DNA is an inverted geometry instrument consisting of a pyrolytic graphite (PG) curved neutron guide with a pulse shaping chopper and a large area crystal analyser system. The DNA team presented a design consisting of four analyser systems in two saw-tooth scattering bank. This combination provides a very wide range of capabilities. Unfortunately only one of these can really be an instrument can be used at a time. After extensive discussion, the Committee recommends that the highest resolution option provided by the Si (111) analyser be given the highest priority. The reasons for this recommendation are:

1. Science seems to be driving towards ever lower dynamics and therefore ever better resolution. The Si(111) option provides the best energy resolution of the four analysers which is about 4 μeV.
2. The primary scientific target for DNA is the dynamics of proteins and polymers. Experience at ILL and NIST indicates that backscattering instruments with 1 μeV tend to have approximately ½ of the beam time devoted to these areas while the beam time devoted to these areas on instruments with relaxed energy resolution is substantially less. This argues that the target user community will be better served by the excellent resolution provided by the Si (111) option. (See appendix.)
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The Committee recommends the use of Si (311) crystal analysers as an option to increase the Q-range allowing one to better take advantage of one of the great strengths of neutron scattering, namely the ability to obtain length scale information of the dynamical process under investigation. This option can be realised either by using a fraction of the scattering chamber for Si(311) crystals on a permanent basis or as an optional add-on (cf. IN1 at ILL).

While the Committee recommends pursuing the scattering bank with Si (111) and Si(311) we believe that the possibility of installing a second scattering bank at a later date should be preserved if possible. This would provide the absolute highest count rate available at J-PARC for any instrument operating with an energy resolution of about 25 μeV.

The most important 2 point in the recommendations

the Committee recommends that the highest resolution option provided by the Si (111) analyzer be given the highest priority.

We changed the construction plan that
" the primary spectrometer is Si(111) & Si(311) high energy resolution mode."

The primary scientific target for DNA is the dynamics of proteins and polymers. Experience at ILL and NIST indicates that backscattering instruments with 1 μeV tend to have approximately ½ of the beam time devoted to these areas while the beam time devoted to these areas on instruments with relaxed energy resolution is substantially less. This argues that the target user community will be better served by the excellent resolution provided by the Si (111) option.

The biophysics group in the DNA science support team agreed with that ***main user demand was an 1 μeV resolution spectrometer.***

5

Report to "J-PARC Neutron Instrument Program Review Committee"

On a Meeting in J-PARC held at Sep.2008
"J-PARC Neutron Instrument Program Review Committee"
It is one of the committees in the J-PARC center.
The role of this committee is the hearing of the construction plans for neutron instrument in MLF at J-PARC

We reported that
the **recommendations** of the 1st DNA-IAC and
the change of construction plan on DNA and these background.

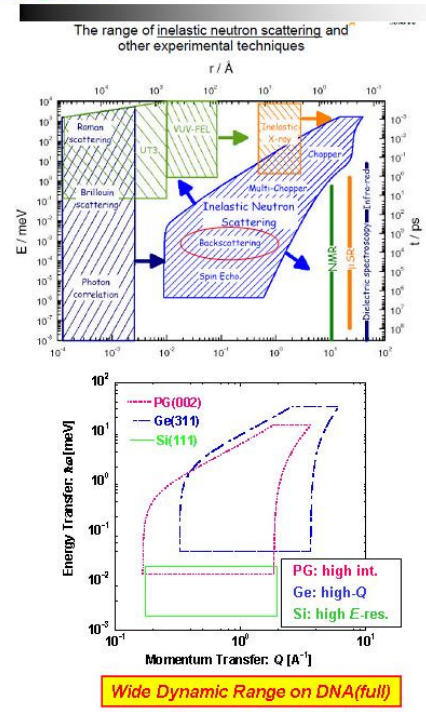
The most important reasons for the change of plan are
the compartmentalization in the Q-E Range of INS in MLF
and
the user demand for an 1 μeV resolution spectrometer

⇩

We changed the construction plan like that;
"Primary spectrometer is
Si(111) & Si(311) high energy resolution mode."

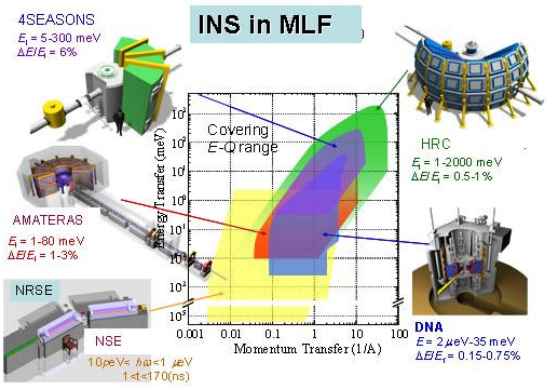
6

Compartmentalization of the Q-E Range Neutron Inelastic Instrument No.1



Wide Dynamic Range on DNA(full)

Q-E range; AMATERAS, DNA(full) & NSE

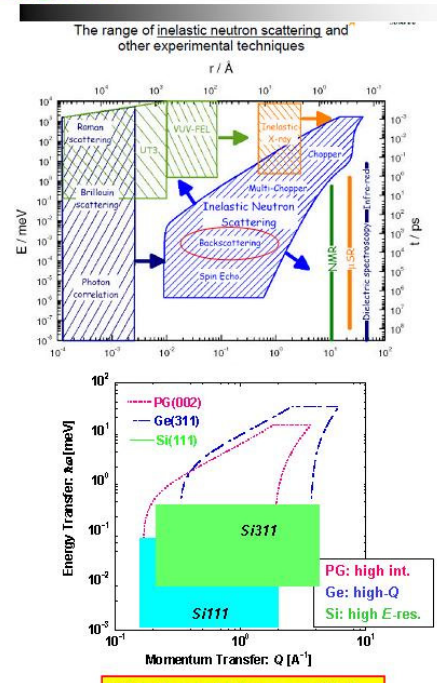


A position of backscattering spectrometer in Q-E range is just between multi-chopper and spin echo spectrometer and unique experimental techniques.

A Q-E range of full spec DNA is widely overlapped with a Q-E range of AMATERAS from several 10 μeV to 10 meV region.

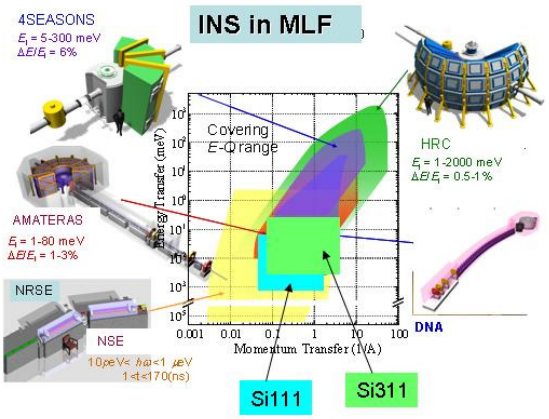
7

Compartmentalization of the Q-E Range Neutron Inelastic Instrument No.2



Wide Dynamic Range on DNA

Q-E range; AMATERAS, DNA(Si) & NSE



An overlapped Q-E range between Si analyzer DNA and AMATERAS and other chopper spectrometer is decreased.

Primary, DNA will concentrate on the study of the nanosecond dynamics.

8

Recommendations of the 1st IAC-DNA:

We are given the 8 comments on instrument functionality

1. Choice of coupled moderator is excellent.
2. Guide design is quite good. Perhaps you can gain a bit by revisiting the horizontal guide profile.
3. It may be possible to gain a little space at the sample for large sample environments such as high-field magnets and high pressure cells. However care must be taken to keep any degradation in resolution to acceptable levels. Provision should be made for orientation of single crystal samples.
4. Analyzer design for Si (111) is good. Si (311) provides a good option to extend the Q-range. The work on the focusing scheme for the analyzer is quite imaginative and thorough.
5. Choice of 1-d position sensitive detectors is robust and allows a simplified analyzer design.
6. We believe that the proposed evacuated scattering chamber is the best choice.
7. Data acquisition system is based on a modern concept offering the desired flexibility and good performance.
8. It's good that data analysis is not an after-thought.

9

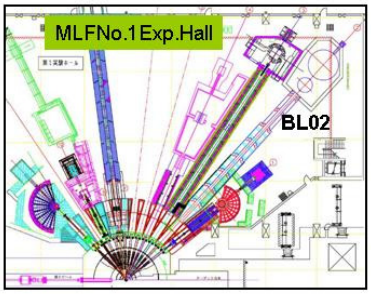
Actions for the 8 Comments on Instrument Functionality No.1

Comments on Instrument Functionality

1. Choice of coupled moderator is excellent.
-> We are continuing DNA construction plan at BL02 beam line seeing a coupled liq.H_2 moderator.
2. Guide design is quite good. Perhaps you can gain a bit by revisiting the horizontal guide profile.
->We are designing the guide system with following specifications;

In vertical section: elliptical shaped guide (gain: 1.5 ~ 2 times)

In horizontal section: Curved guide (m = 3, R = 2200 m, w = 60 mm)



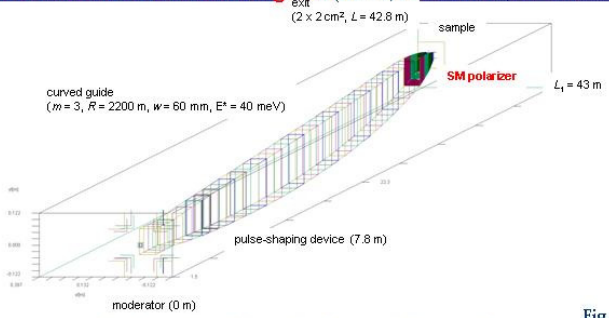


Fig. Geometry of the neutron transportation system

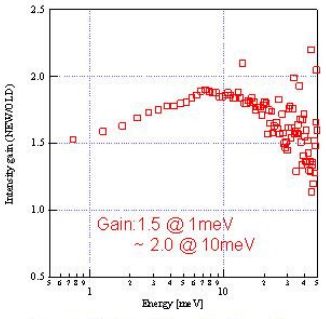


Fig. Intensity gain factor of the elliptic guide, against a commonly used straight guide

10

Actions for the 8 Comments on Instrument Functionality No.2

Comments on Instrument Functionality

3.It may be possible to gain a little space at the sample for large sample environments such as high-field magnets and high pressure cells. However care must be taken to keep any degradation in resolution to acceptable levels. Provision should be made for orientation of single crystal samples.

->Now a design of vacuum chamber have a sample access space with D~400 mm in diameter.
At same time, we are performing a study of E-resolution.

4.Analyzer design for Si (111) is good. Si (311) provides a good option to extend the Q-range. The work on the focusing scheme for the analyzer is quite imaginative and thorough.

->An analyzer mirror study for Si(111) and Si(311) crystals is in progress.
At later, Dr.N.Takahashi will present the study of energy resolution for Si(111) and Si(311)

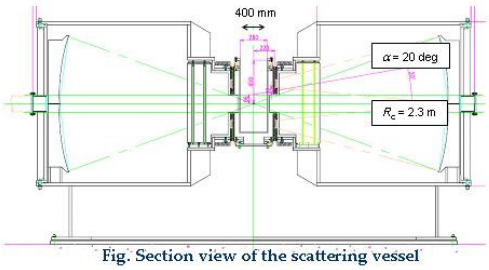


Fig. Section view of the scattering vessel

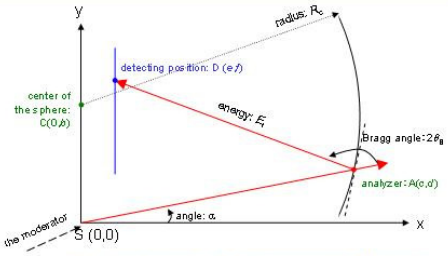


Fig. Design parameters of the components in the vessel

11

Actions for the 8 Comments on Instrument Functionality No.3

Comments on Instrument Functionality

5. Choice of 1-d position sensitive detectors is robust and allows a simplified analyzer design.

->Now, a design of counter banks for U-type 1-D PSD is in progress.

6.We believe that the proposed evacuated scattering chamber is the best choice.

-> A design of vacuum chamber is in progress .

7.Data acquisition system is based on a modern concept offering the desired flexibility and good performance.

->DNA will use the method of event data taking as a data taking system.

8.It's good that data analysis is not an after-thought.

->We are developing the data analysis program.
Dr.Y.Kawakita will present the current status of the data analysis program for DNA.

12

Current General View: DNA: Dynamics Spectrometer

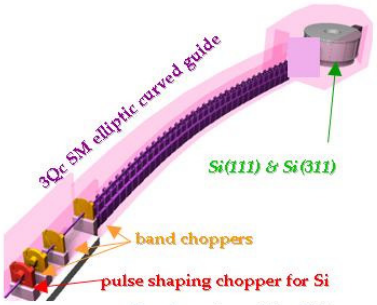


Fig. Overview of the *DNA*

- Si-nBBS spectrometer
  - ✓ Source: Liq.H_2 Coupled Moderator (BL02)
  - ✓ L_1 = 43 m, L_2 = 4.3 m, pulse-shaping device @ L = 7.8 m
  - ✓ Guide: m = 3 SM, elliptic (vertical), curved (horizontal)
- Pulse-shaping device
  - ✓ counter-rotating double-disc chopper: 300~350 Hz
  - ✓ high E-resolution ~ 1 μeV(Si111) & ~ 5 μ eV(Si311)
  - ✓ variable E-resolution 1-17 μeV(Si111) and 5-46 μeV (Si311)
  - ✓ high efficiency by *RRM*
- Si analyzers
  - ✓ Si(111) (ΔE = 1 μeV, Q < 1.9 Å^{-1})
  - ✓ Si(311) (ΔE ~ 5 μeV, Q < 3.8 Å^{-1})
- Polarization devices in future
  - ✓ polarizer: supermirror
  - ✓ analyzer: ^{3}He spin-filters with high-field magnets

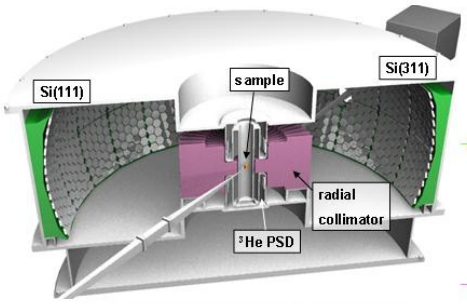


Fig. Inner view of the scattering vessel

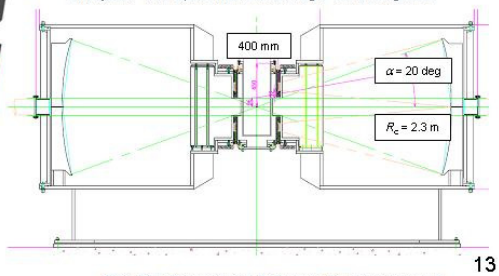
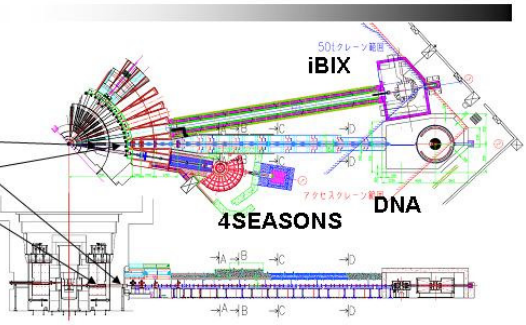


Fig. Section view of the scattering vessel

13

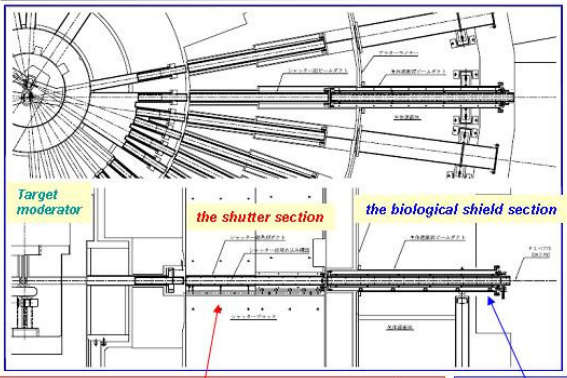
Construction Status :in FY2008 No.1

Budget for the construction on DNA
In FY2008,
>It was founded for the guide systems
in the shutter section (~2 m),
and the biological shield section (~3 m).
Now, we are ordering the guide systems.
(these will be constructed until March 2009)



14

The guide systems in the shutter section and the biological shield section

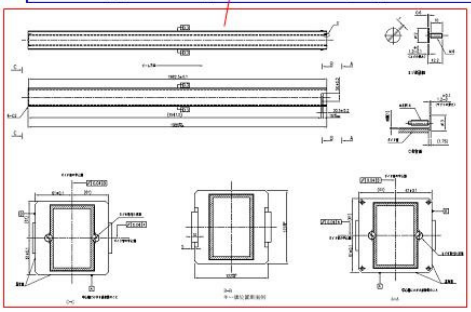


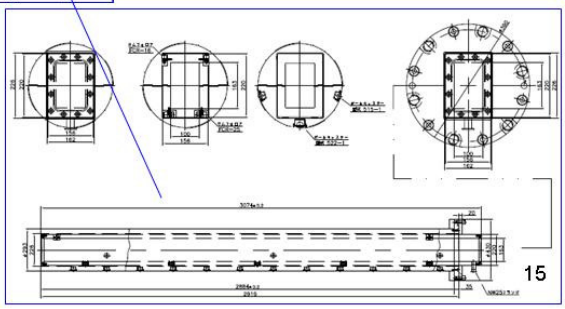
In the shutter section ,

- straight guide
  inner size: W62.0mm × H98.0mm
- total length 1982.5mm
- m = 3.0 Qc
- outer size of support □122mm × 1986.0mm

In the biological shield section

Vertical section: elliptical,
horizontal section: curved (R=2200m)
inner size : W60.0mm × H98.7mm (upper side)
W60.0mm × H132.8mm (lower side)
total length 3028.15mm
m = 3.0 Qc
outer size of support :
W 94 mm × H 157 mm × L 3032 mm

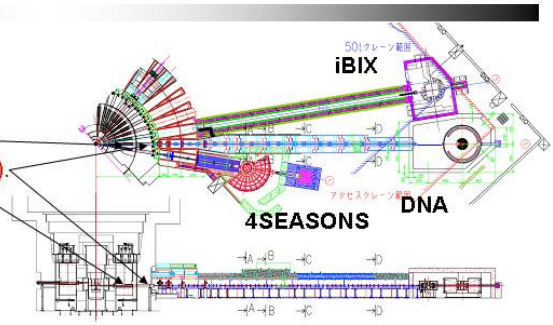




15

Construction Status :in FY2008 No.2

Budget for the construction on DNA
In FY2008,
>It was founded for the guide systems
in the shutter section (~2 m),
and the biological shield section (~3 m).
Now, we are ordering the guide systems.
(these will be constructed until March 2009)



>An analyzer crystal mounting device.
We will construct a prototype of an analyzer crystal mounting device in FY2008.

>A technical design of spectrometer.
We are designing the vacuum chamber for technical reviewing.
Also, we will design the shield for the vacuum chamber including the estimation for radio activities.

A analyzer crystal mounting device in SNS

16

Construction Schedule :from FY2009~

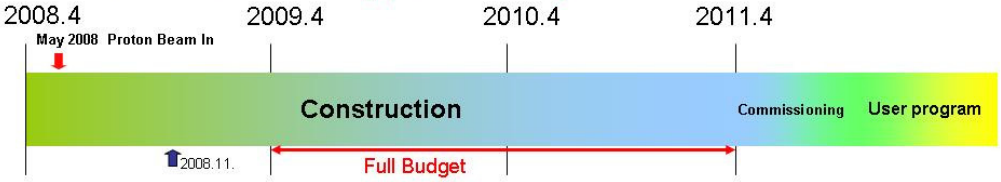
Schedule of the Budget from FY2009
We hope to be founded form FY2009
to FY2010
for total construction of DNA

From the beginning of FY2009, we would like to start the construction of
the guide system in the full beam line,
the vacuum chamber,
the shield for the vacuum chamber,
and the analyzer mirror system and detector system, and etc..

From the beginning of 2011, a part of commissioning study will start.

And from the mid of 2011, an user program will start.

DNA construction schedule (optimistic case)



17

Technical Issues in this Meeting

. Technical issues correspondence to be discussed in this meeting

(1-1). Study of energy resolution [⇐ Recommendation from Dr. D. Neumann] [1], [4]
/Estimation of energy resolution using bent crystal formula
: 1-17 μeV and 5-46 μeV variable for Si111 and Si311 crystal analyzer, respectively.
(1-2).Packaing of vacuum chamber including the design of detector and analyzer bank [3],[5],[6]

(2-1). Study of Repetition Rate Multiplication (RRM)[⇐ Suggestion form Prof. F. Mezei]
/Geometrical study: position of frame separation choppers
/Calculation study: specification of frame separation choppers
/Requirements on choppers
/Verification by McStas
(2-2). Specification of disc choppers [⇐ Comment from Dr. H. Mutka]
(2-3). Specification of guide system [2]

(3). Study of Analyzer crystals [⇐ Comment from Dr. E. Mamontov and Dr. B. Frick]
/Specification of analyser crystal.,
/How to reduce BG from Si crystal wafers.

(4). Developing of the data analysis program [⇐ Comment from Dr. P. Tregenna-Piggott][8]

(5).Other problems

18

3. Main part of the 2nd IAC (technical issues)
3.1. Energy resolution and design of vacuum tank
Nobuaki Takahashi (JAEA)

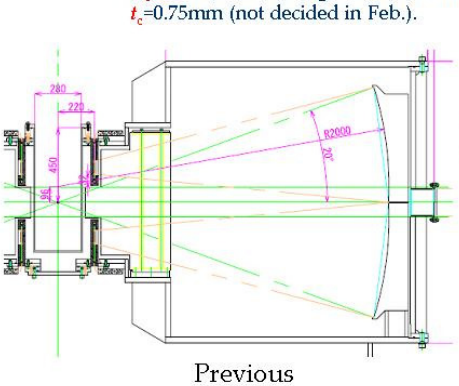
3.1. Energy resolution and Design of vacuum tank

Nobuaki Takahashi (J-PARC)

1

Motivation

- The Committee Dr. D. Neumann recommended that we have to do resolution calculation using bent crystal formula.
- The Committee Dr. H. Mutka recommended to gain a little space at the sample for large sample environments such as high-field magnets and high pressure cells. However care must be taken to keep any degradation in resolution to acceptable levels.
  - Then, we approached logically to decide all parameters of components in the vacuum tank, and also we have tried to expand the diameter for sample area at the same moment.
  - Finally, we have decided the parameters; diameter of the sample space: D_s = 280 mm -> 400 mm. At the same time, the other parameters have gotten decided; radius of analyzer: R_c=2.3m (<- 2.0m); angle in vertical direction: α=±20deg. (no change); thickness of wafers: t_c=0.75mm (not decided in Feb.).



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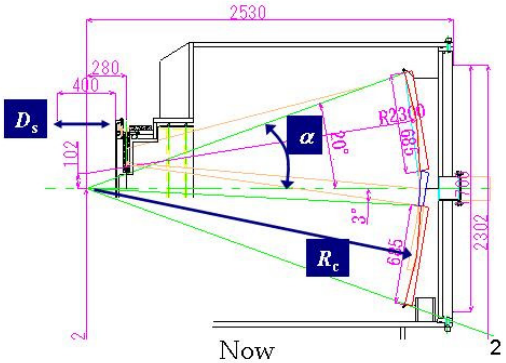

Now

2

Bent perfect crystals

- Treatment of bent Si crystals on energy resolution can be found at [A. Meyer, *et al.*, *Rev. of Sci. Instr.* **74** 2759 (2003)] and [B. Alefeld, *et al.*, *Physica B*, **283** 301, (2000)]. Effective mosaicity of bent perfect crystals; $\Delta d/d$

$$\frac{\Delta d}{d} = \left(\frac{\Delta d}{d}\right)_{\text{Darwin}} + P_{\text{eff}}\left(\frac{t_c}{R_c}\right) \quad \text{(eq. 2)}$$

d: d-spacing
P_{eff}: Poisson ration
R_c: radius of the analyzer bank
t_c: thickness of the crystals

Table 3 Darwin width and Poisson ratio of perfect crystals

Crystals	Darwin width $(\Delta d/d)_{\text{Darwin}}$	Poisson ratio P_{eff}
Si(111)	1.86×10^{-5}	0.442
Si(311)	0.98×10^{-5}	

Table 4 Effective mosaicity of bent perfect crystal Si(111); $\Delta d/d \times 10^4$

R_c[m]	thickness of crystals t_c [mm]					
	0.75	1.0	1.25	1.5	1.75	2.0
2.0	1.66	2.21	2.76	3.32	3.87	4.42
2.3	1.44	1.92	2.40	2.88	3.36	3.80
2.5	1.33	1.70	2.21	2.65	3.09	3.54

HFBS (NIST)

BASIS (SNS)

3

E-resolution of DNA

- *E*-resolution of DNA can be estimated by the following formula.

$$\frac{\Delta E}{E} = 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + (\cot\theta_B \cdot \Delta\theta)^2 + \left(\frac{\Delta t'}{t'}\right)^2} \quad \text{(eq. 5)}$$

Crystal part

Bragg angle and angle ambiguity part

TOF part

4

Crystal part (E-resolution of DNA)

➢ E-resolution of DNA can be estimated by the following formula.

$$\frac{\Delta E}{E} = 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B \cdot \Delta\theta\right)^2 + \left(\frac{\Delta t'}{t'}\right)^2} \quad \text{(eq. 5)}$$

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2.5	1.33	1.70	2.21	2.65	3.09	3.54

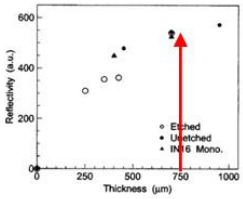


Fig. 11 Plot of neutron reflectivity vs Si {111} wafer thickness (a.u. = arbitrary units). Open circles represent etched wafers, while closed circles represent unetched wafers. The solid triangles refer to the two IN16 monochromators.

Intensity curve shows almost saturation. 5

Bragg angle and angle ambiguity part (E-resolution of DNA)

➢ E-resolution of DNA can be estimated by the following formula.

$$\frac{\Delta E}{E} = 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B \cdot \Delta\theta\right)^2 + \left(\frac{\Delta t'}{t'}\right)^2}$$

✓ Bragg angle θ_B is related to a lot of parameters in tank; R_c, α, D_s.

✓ Ambiguity of the scattering angle; $\Delta\theta$

$$\Delta\theta = \arcsin\left(\frac{w_s}{\sqrt{2}R_c}\right) \quad \text{(eq. 3)}$$

w_s: sample size.

Table 5 Scattering angle ambiguity; $\Delta\theta$ [mrad]

R_c[m]	sample size; w_s [mm]		
	10	20	30
2.0	3.54	7.07	10.6
2.3	3.07	6.15	9.22
2.5	2.83	5.66	8.49

Importance is matching with the other parameters.

Table 7 Products of the Bragg angle and the ambiguity of the scattering angles; $\cot\theta_B \cdot \Delta\theta \times 10^4$

R_c [m]	α [deg]	D_s [mm]	θ_B [deg]	sample size; w_s [mm]		
				10	20	30
2.0	20	280	87.5	1.55	3.09	4.63
		400	87.1	1.79	3.58	5.37
		540	86.5	2.17	4.32	6.48
	30	280	86.9	1.92	3.83	5.74
		400	86.2	2.35	4.70	7.04
2.3	20	280	87.9	1.13	2.26	3.38
		400	87.5	1.34	2.69	4.03
		540	87.1	1.56	3.12	4.67
	30	280	87.3	1.45	2.90	4.35
		400	86.8	1.72	3.44	5.15
2.5	20	280	88.1	0.94	1.88	2.82
		400	87.7	1.14	2.27	3.41
		540	87.3	1.33	2.67	4.00
	30	280	87.6	1.19	2.37	3.56
		400	87.1	1.43	2.87	4.30

TOF part (*E*-resolution of DNA)

➢ *E*-resolution of DNA can be estimated by the following formula.

$$\frac{\Delta E}{E} = 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B \cdot \Delta\theta\right)^2 + \left(\frac{\Delta t'}{t'}\right)^2} \quad \text{(eq. 5)}$$

$\Delta t'$: opening-time in FWHM of pulse-shaping device
t': time-of-flight (pulse-shaping device-to-sample)

✓ Opening-time in FWHM of pulse-shaping device

$$\Delta t' = \arctan\left(\frac{w_{ch}}{2r_{ch}}\right) / 2\pi f \quad \text{(eq. 6)}$$

w_{ch}: slit width at beam center
r_{ch}: radius at beam center
f: rotation frequency

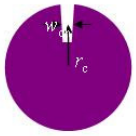



Photo. Pulse-shaping chopper

Table 6 Spec. and the performance of the pulse-shaping device

w_{ch} [cm]	f [Hz]	$\Delta t'$ [μs]	$\Delta t'/t' \times 10^4$
1	350	7.58	1.36
	300	8.84	1.59
	250	10.6	1.90
	200	13.3	2.38
3	350	22.7	4.07
	300	26.4	4.75
	250	31.7	5.70
	200	39.7	7.12
6	350	44.9	8.09
	300	52.4	9.40
	250	62.8	11.3
	200	78.5	14.1

TOF part is variable by choosing slit and/or speed of PS chopper.

7

Conclusion (*E*-resolution of DNA)

Then, the expected *E*-resolution is

good matching

$$\Delta E = E \times 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B \cdot \Delta\theta\right)^2 + \left(\frac{\Delta t'}{t'}\right)^2}$$
$$= 2.085 \times 2\sqrt{\left(1.44\times10^{-4}\right)^2 + \left(1.34\times10^{-4}\right)^2 + \left(1.36\times10^{-4}\right)^2}$$
$$= 1.0\,\mu\text{eV}$$

Optimistic estimation but DNA has a possibility to achieve higher resolution than BASIS.

Instrumental parameters are determined as below;

R_c = 2.3 m (radius of the analyzer bank)
t_c = 0.75 mm (thickness of the crystals)
w_s = 10 mm (sample size)
w_{ch} = 1 cm (slit width at beam center of the pulse-shaping choppers)
f = 350 Hz (frequency of the pulse-shaping choppers)
α = 20 deg (scattering angle in the vertical plane)
D_S = 400 mm (diameter of the sample environmental space)

8

Si(311); expected energy resolution

- *E*-resolution of spallation-source near-BSSs with pulse-shaping device.

$$\frac{\Delta E}{E} = 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B \cdot \Delta\theta\right)^2 + \left(\frac{\Delta t'}{t'}\right)^2} \quad \text{(eq. 5)}$$

$\Delta t'$: opening-time in FWHM of pulse-shaping device
t': time-of-flight (pulse-shaping device-to-sample)

R_c = 2.3 m	(radius of the analyzer bank)
t_c = 0.75 mm	(thickness of the crystals)
w_s = 10 mm	(sample size of on a side)
w_{ch} = 1 cm	(slit width at beam center)
f = 350 Hz	(rotation frequency)
α = 20 deg	(scattering angle in the vertical plane)
D_S = 400 mm	(diameter of the sample environmental space)

- ✓ The geometry of the analyzer should be same as the Si(111) case, then,

$$\cot\theta_B \cdot \Delta\theta_B = 1.34\times10^{-4}$$

- ✓ We assumed the Poisson ratio of Si(311) is not much different from Si (111), then the Δd/d could be as much as that of the Si(111), then,

$$\frac{\Delta d}{d} \sim 1.44\times10^{-4}$$

- ✓ The elastic energy of the Si(311) is 7.64 meV, then the TOF contribution is,

$$\frac{\Delta t'}{t'} = 2.60\times10^{-4}$$

Then, the expected *E*-resolution is

$$\Delta E = E\times2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B\cdot\Delta\theta\right)^2 + \left(\frac{\Delta t'}{t'}\right)^2}$$
$$= 7.64\times2\sqrt{\left(1.44\times10^{-4}\right)^2 + \left(1.34\times10^{-4}\right)^2 + \left(2.60\times10^{-4}\right)^2}$$
$$= 5.0\mu\text{eV}$$

9

Most relaxed resolution (white beam exp.)

highest intensity but long tail, 205 μs at 2 meV, 106 μs at 7.9 meV in FWHM

Si(111)

$$\Delta E = E\times2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B\cdot\Delta\theta\right)^2 + \left(\frac{\Delta t}{t}\right)^2}$$
$$= 2.085\times2\sqrt{\left(1.44\times10^{-4}\right)^2 + \left(1.34\times10^{-4}\right)^2 + \left(3.07\times10^{-3}\right)^2}$$
$$= 13\mu\text{eV}$$

Then, E-resolution is variable between 1 ~ 13 μeV.

Si(311)

$$\Delta E = E\times2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B\cdot\Delta\theta\right)^2 + \left(\frac{\Delta t}{t}\right)^2}$$
$$= 7.64\times2\sqrt{\left(1.44\times10^{-4}\right)^2 + \left(1.34\times10^{-4}\right)^2 + \left(2.97\times10^{-3}\right)^2}$$
$$= 46\mu\text{eV}$$

Then, E-resolution is variable between 5 ~ 46 μeV.

10

Further discussion

- Intensity match-up; *DNA* vs. *BASIS-type* spectrometer (at JSNS, 25 Hz)
  - ✓ Previous result in the paper; intensity difference between the two instruments; × 2.5
    [N. Takahashi et al., *J. Phys. Chem. Sol.* **68**, 2199 (2007)]
  - ✓ Elliptic neutron guide; × 1.7
    Intensity gain at around E ~ 2 meV is about 1.7.
  - ✓ Slit-width of the pulse-shaping device (3 cm -> 1 cm); × 0.29
    opening-time ratio of (w_{ch} = 1 cm, f = 300 Hz)/(w_{ch} = 3 cm, f = 300 Hz)
  - ✓ Fork-type double-slit (1 cm -> 1 cm × 2); × 2
  - ✓ Effect on crystal thickness; × 0.85 ?
    Reflectivity of Si(111) wafers are almost saturated at thickness; t_c ~ 0.75 mm.
    [A. Meyer, *et al.*, *Rev. of Sci. Instr.*, **74** 2759 (2003)].
  - ✓ Total; × 2.0

Table 8 Performance comparison between the *DNA* and *BASIS-type BSS* at JSNS (25 Hz).

BSS	ΔE [μeV]	Intensity/ a.u.	Energy band [μeV]
DNA	1 ~ 13	2	- 35 < $\hbar\omega$ < + 35 (several meV is obtainable using *RRM*)
BASIS-type at JSNS	2.2	1	- 600 < $\hbar\omega$ < + 600

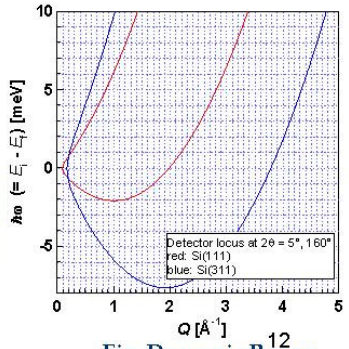
11

Further discussion

- Scattering angle
  - ✓ Horizontal plane: 5° ~ 160° , Vertical Plane: - 20° ~ + 20° then expected ω-Q range is shown in the following Fig. How do you think of it?
  - ✓ For single crystal researcher, good analyzer bank design? (will be reported soon)
- Analyzer-crystals
  - ✓ Hexagonal crystals (D ~ 120 mm) will be glued on the surface (discussions will be done at mounting device part)
  - ✓ How about the thickness of Si(311)? Do you have any idea?
  - ✓ To reduce BG neutron absorbing materials will be spattered on the back side of the crystals. (Dr. K. Shibata reports)

Table Spec. of the Si analyzers

Crystal	d [A]	θ_B [deg]	k_f [A]	E_f [meV]	R_c [m]	L_2[m]	TOF@det	t_c [mm]
Si(111)	3.135	87.5	6.264	2.085	2.3	4.3	74.90	0.75
Si(311)	1.638	87.5	3.272	7.640	2.3	4.3	39.12	0.75



12

Fig. Dynamic Range

Further discussion

- Detectors
  - ✓ U-type ^{3}He PSD for spectrometer, normal PSD for diffraction detectors. Where ?
- Polarization device
  - Sample surrounding space in the scattering vessel will be widely opened (D ~ 400 mm) for some special sample environments and the ^{3}He spin-filters with high-field magnets. Is it enough? K. Andersen shown us PASTIS at ILL. Do you know how much size is sufficient for such kind of devices? (diameter? height?)
  - Spin filter: 4 cm·bar is required at 6A. They can choose 1-2 bar. 2cm is not so difficult.

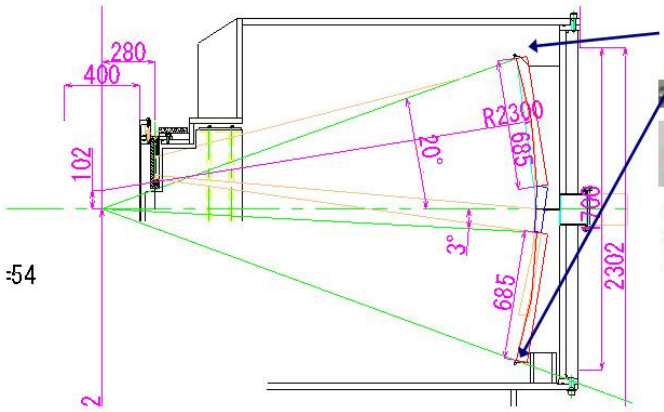


Photo 2. U-type ^{3}He-PSD (Top: 8 mm-ϕ, 20 atm, Toshiba. Bottom: 1/2"-ϕ, 10 atm, GERS)

13

Analyzer bank design

- The Committee recommended to consider about single crystal meas.
  - Dr. K. Shibata has discussed with Dr. K. Herwig (SNS) in March. One of his ideas is to eliminate any space in the horizontal plane for the analyzer bank.
  - A technician of a metal-processing company said that the machining cost become less if the diagonal line of the plate (one unit of the analyzer bank) is less than 800 mm.
- Then, we tried to design analyzer bank and divided into reasonable plates;
  - Scattering angle: -162~162deg.; dividing into 27 units <-> angle=12deg <-> width=481mm (Fig2). The machining area is limited to a circle with D~800, then, the height of the plate has been given about 685 mm (Fig3). The plate with the size can cover from -3deg to 0deg if it is cut (Fig1 blue). Total 68 (= 27x2 + 27/2) plates will be required.
  - One plate will be covered with 40 pieces of Si wafers with D=120mm (Fig3). Then, totally 2720 pieces of Si wafers are required (1360 of Si(111) and Si(311), respectively).

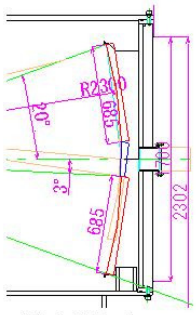


Fig1. Side view

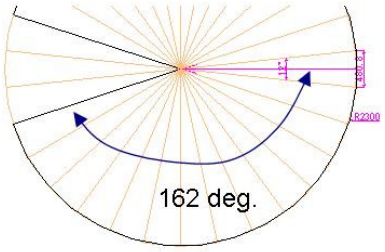


Fig2. Top view

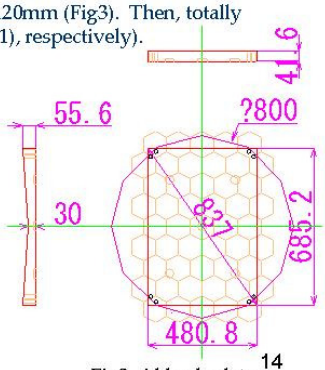


Fig3. Al back plate

14

HFBS (NIST)

➢ *E*-resolution of Reactor-source perfect-BSSs; $\Delta E/E$ [A. Meyer, *et al.*, *Rev. of Sci. Instr.* **74** 2759 (2003)]

$$\frac{\Delta E}{E} = 2\left(\frac{\Delta d}{d} + \frac{1}{8}(\Delta\theta)^2\right) \quad \text{(eq. 1)}$$

✓ Effective mosaicity of bent perfect crystals; $\Delta d/d$
[A. Meyer, *et al.*, *Rev. of Sci. Instr.* **74** 2759 (2003)]

$$\frac{\Delta d}{d} = \left(\frac{\Delta d}{d}\right)_{\text{Darwin}} + P_{\text{eff}}\left(\frac{t_c}{R_c}\right) \quad \text{(eq. 2)}$$

d: d-spacing
P_{eff}: Poisson ration
R_c: radius of the analyzer bank
t_c: thickness of the crystals

✓ Ambiguity of the scattering angle; $\Delta\theta$

$$\Delta\theta = \arcsin\left(\frac{w_s}{\sqrt{2}R_c}\right) \quad \text{(eq. 3)}$$

w_s: sample size. w_s mm on a side.

✓ For example, a HFBS-type BSS (NIST)

$$\Delta E = E\times 2\left(\left[1.86\times10^{-5} + 0.442\times\left(\frac{0.75}{2000}\right)\right] + \frac{1}{8}\left(7.07\times10^{-3}\right)^2\right)$$
$$= 2.08\times2\times(1.84\times10^{-4} + 6.25\times10^{-6})$$
$$= 0.79\,\mu\text{eV}$$

R_c = 2.0 m
t_c = 0.75 mm
w_s = 20 mm

Table 3 Darwin width and Poisson ratio of perfect crystals

Crystals	Darwin width $(\Delta d/d)_{\text{Darwin}}$	Poisson ratio P_{eff}
Si(111)	1.86×10^{-5}	0.442
Si(311)	0.98×10^{-5}	

[B. Alefeld, *et al.*, *Physica B*, **263** 301, (2000)]

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R_c[m]	thickness of crystals t_c [mm]					
	0.75	1.0	1.25	1.5	1.75	2.0
2.0	1.66	2.21	2.76	3.32	3.87	4.42
2.3	1.44	1.92	2.40	2.88	3.36	3.80
2.5	1.33	1.70	2.21	2.65	3.09	3.54

Table 5 Scattering angle ambiguity; $\Delta\theta$ [mrad]

R_c[m]	sample size; w_s [mm]		
	10	20	30
2.0	3.54	7.07	10.6
2.3	3.07	6.15	9.22
2.5	2.83	5.66	8.49

$\frac{\Delta d}{d} >> \frac{1}{8}(\Delta\theta)^2$

Bending has much adverse affect on the *E*-resolution rather than the other component.

15

BASIS (SNS)

➢ *E*-resolution of spallation-source near-BSSs; $\Delta E/E$ [B. Frick, *Neutron and X-ray Spectroscopy*, Springer, 483 (2006)]

$$\frac{\Delta E}{E} = 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + (\cot\theta_B\cdot\Delta\theta)^2 + \left(\frac{\Delta t}{t}\right)^2} \quad \text{(eq. 4)}$$

θ_B: Bragg angle
Δt: time-width of pulsed-source
t: time-of-flight (moderator-to-sample)

✓ For example, a BASIS-type BSS (SNS)

$$\Delta E = E\times2\left(\left[1.86\times10^{-5} + 0.442\times\left(\frac{2.0}{2500}\right)\right]^2 + \left(\cot 88^\circ\times8.49\times10^{-3}\right)^2 + \left(\frac{31\times10^{-3}}{133}\right)^2\right)$$
$$= 2.085\times2\sqrt{\left(3.72\times10^{-4}\right)^2 + \left(2.96\times10^{-4}\right)^2 + \left(2.33\times10^{-4}\right)^2}$$
$$= 2.21\,\mu\text{eV}$$

R_c = 2.5 m
t_c = 2.0 mm
w_s = 30 mm
θ_B = 88°
Δt: 31 μs (poisoned, thin side)
t: 133 ms (L_1 = 84 m)

$\frac{\Delta d}{d} > \frac{\Delta t}{t} > \cot\theta_B\cdot\Delta\theta$

Bending thick crystals have the worst adverse affect on the *E*-resolution rather than the other two components.

✓ How to achieve ~ 1 μeV *E*-resolution

ΔE = 1μeV

$$= 2.085\times2\sqrt{\left(1.38\times10^{-4}\right)^2 + \left(1.38\times10^{-4}\right)^2 + \left(1.38\times10^{-4}\right)^2}$$

$\frac{\Delta d}{d} \approx \frac{\Delta t}{t} \approx \cot\theta_B\cdot\Delta\theta \approx 1.38\times10^{-4}$

Match these three components to be ~ 1.38 × 10^{-4}

$\frac{\Delta t}{t} = 1.38\times10^{-4} \Leftrightarrow L_1 = 206\text{m}$

Nonsense → **pulse-shaping device** is necessary

16

Spectroscopic Principle

- near-backscattering geometry
  - ✓ Bragg angle (θ_B) is less than 90 deg.
  - ✓ Analyzer surface is a sphere with radius of R_c. The same spheres are above and below the equatorial. Centers of the spheres are on the Y-axis.
  - ✓ Detectors are not on the Y-axis, because of sufficient sample environment space.
  - ✓ TOF of neutrons reaching at a pixel of a detector is different with each other, and thus, PSD will be used and obtained TOF will be treated with the pixel.
    Private communication with Dr. E. Mamontov, who is the responsible of the BASIS @ SNS.
  - ✓ Analytical calculations have been done to get most suitable design parameters. Positions of C and D got decided from a certain R_c and α.
- Two contradictory parameters
  - ✓ Small X-coordinates of the detector (e) is good for E-resolution, on the other hand, bad for the sample environment space.
    See Table 7.
  - ✓ High scattering angle (α) is good for wider covering solid angle of the analyzer, on the other hand, bad for E-resolution.
    See Table 7.

  And also short-blind-section-detector is necessary.
  See Photo 2.

Photo 2. U-type ^{3}He-PSD (Top: 8 mm-ϕ, 20 atm, Toshiba. Bottom: 1/2"-ϕ, 10 atm, GERS)

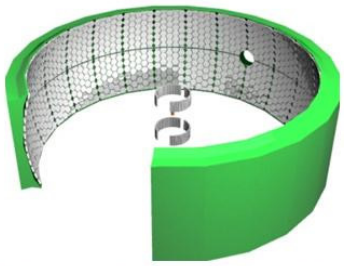


Fig. Inner view of the vessel (analyzers and detectors)

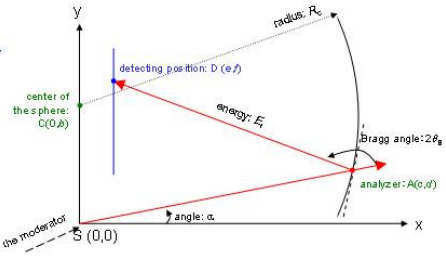


Fig. Design parameters of the components in the vessel

17

Calculation has been done by Excel macro.

3.2. Repetition Rate Multiplication: RRM
Nobuaki Takahashi (JAEA)

3.2. RRM: Repetition Rate Multiplication for the DNA
(partly discussions about guide and chopper are included)

Nobuaki Takahashi (J-PARC)

1

Motivation

- We have already started to study RRM for DNA in 2005 (NT et al., J, Neutron Res. (2007)), but
  - ✓ It was just conceptual study. We did not consider leakage from long tail of pulse shape at that time. Moreover we did not know how to check the leakage nor how to study frame separation.
  - ✓ And also situation for DNA has almost changed; L_1: 32m -> 43m, L_{ch}: 7.5m ->7.8m, source: decoupled -> coupled...

- Then, we have asked Prof. F. Mezei about how we design frame separation choppers after the previous meeting in March 2008. This discussion had been continued by e-mail.

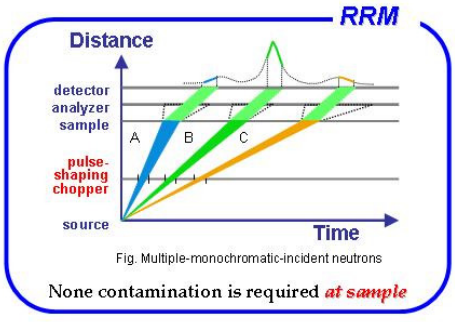
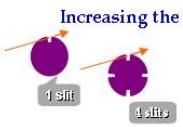
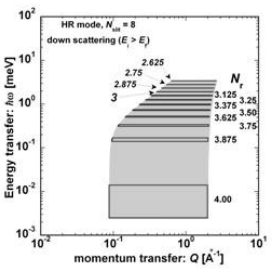


Fig. Multiple-monochromatic-incident neutrons

None contamination is required *at sample*

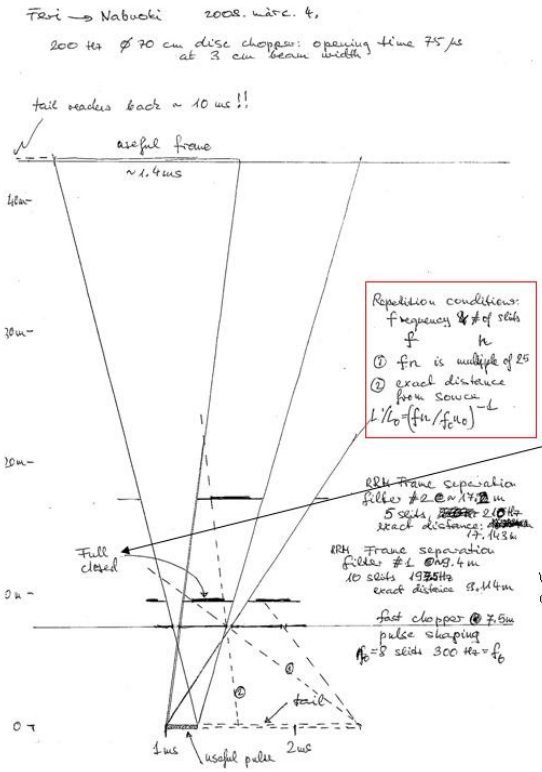




N. Takahashi *et al.*,
J. Nentron Res., **15**, 61 (2007).

Geometrical Study; Where to put frame sep. choppers

3



Prof. F. Mezei's suggestion (May '08 at Tokai)

Suggestion 0:

frame separation choppers should be opened as much as possible. All neutrons in the useful pulse passing through pulse-shaper must not have been cut off by the RRM frame separation choppers.

w=30mm
opening time = 53μs(full), 26.5μs(FWHM, counter rotate)

4

Definition for the frame separation

- Pulse-shape of the coupled moderator, E ~ 2 meV
  - ✓ **Peak intensity** is at 120 μs in the TOF spectrum.
  - ✓ **Useful-frame** is defined as the TOF band between the ½ of the peak intensities; 40 μs ~ 260 μs. The width t_{use} = 220 μs.
  - ✓ **Useless-frame** which we have to avoid when applying the RRM technique is the long tail in the TOF spectrum. We have defined the TOF band less than × 10^{-3} to be cut out. Then the long tail to be avoid is 2 ms at least.

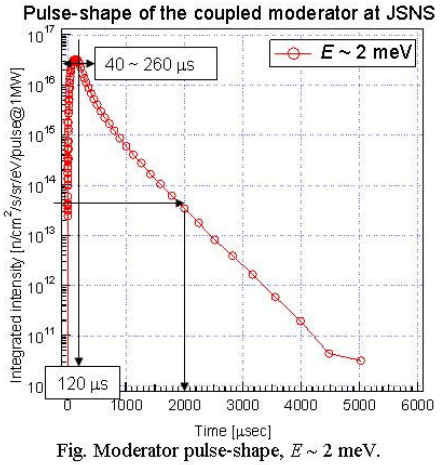


Fig. Moderator pulse-shape, E ~ 2 meV.

Table. Useful and useless frames in the TOF spectrum when applying the RRM technique.

	width [μs]	start [μs]	end [μs]
peak intensity	-	120	-
useful frame; t_{use}	220	40	260
useless frame	-	-	2000

5

How to obtain spec. of Frame Sep. Choppers?

- 1. Deciding tentatively spec. of pulse-shaper, L_0 = 7.8 m, f_0 = 300 Hz, n_0 = ?.
- 2. Calculation of spec. of frame sep. chopper, according to the following eqs. (L, f, n)

$$f \cdot n = 25 \cdot m \ (m = 1,2,3,...)$$

$$L = \frac{f_0 \cdot n_0}{f \cdot n} L_0$$

n: number of slits on discs
f: frequency
L: where to put the chopper

- 3. Drawing TOF diagram.
  According to Feri's suggestion (right figure).
- 4. Checking the leakage. If good, finished. If bad, go to 5.
- 5. Adding the next frame sep. chopper, then go to 2.

- xxx. Trial and error again and again.
  BUT if no-win situation, go to 1.

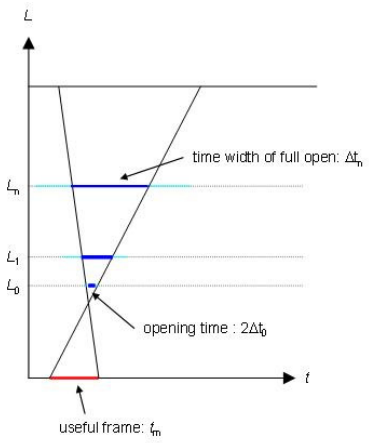


Figure: schematic TOF diagram, which indicates frame separation concept

6

Finally, we found one of the good solutions...

Table 1: Spec of the pulse-shaper

	Length L_0 [m]	Frequency f_0 [Hz]	slit width w_0 [cm]	number of slits n_0	opening-time in FWHM Δt_0 [μs]
Pulse-shaping chopper	7.8	300	3	8	26.44

Table 2: Spec. of the frame-separation choppers (all of them are counter-rotating double-disc type)

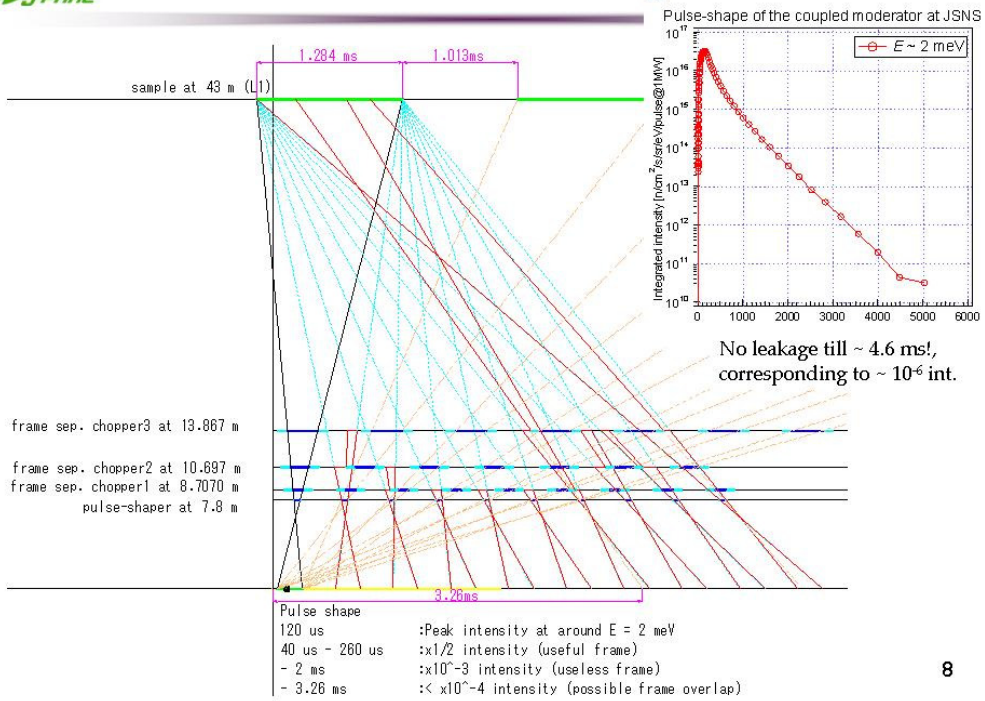
	Length L_n [m]	Frequency f_n [Hz]	number of slits n_n
frame sep. #3	13.867	270	5
frame sep. #2	10.697	250	7
frame sep. #1	8.7070	268.75	8

Expected E-resolution, Si(111)

$$\Delta E = E \times 2\sqrt{\left(\frac{\Delta d}{d}\right)^2 + \left(\cot\theta_B \cdot \Delta\theta\right)^2 + \left(\frac{\Delta t}{t}\right)^2}$$
$$= 2.085 \times 2\sqrt{\left(1.44\times10^{-4}\right)^2 + \left(1.34\times10^{-4}\right)^2 + \left(4.75\times10^{-4}\right)^2}$$
$$= 2.1\mu\text{eV}$$

7

Result: TOF diagram



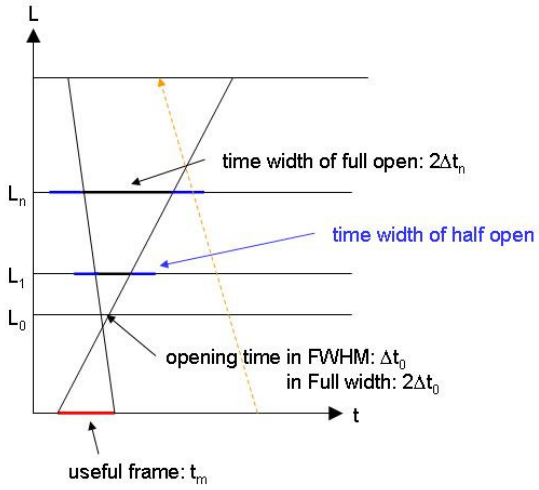
8

Calculation of spec. of Frame-Sep. Choppers

9

Motivation: slit angle?; single-disc? double?;...

- Actually, when checking leakage on TOF diagrams,
  - Definite opening-time of frame sep. choppers are required; half-open -> full-open -> half-open. Length of half-open is very important.
  - If the half-open time is so long, leakage occurs easily.



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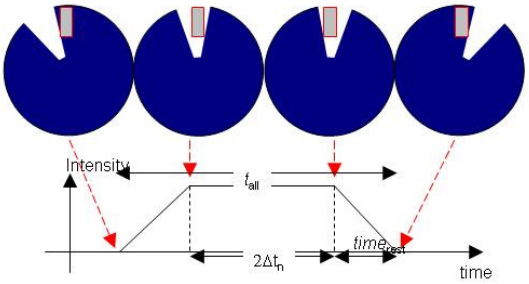
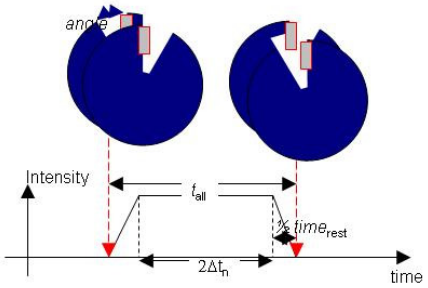
Motivation, CONT.

- Actually, when we check leakage on TOF diagrams,
  - So type of choppers are important; single disc or counter-rotating double-discs. Then, we checked both type on every TOF diagram. And finally, we found the solution which we presented previously. In that situation, double disc case only can work well, nor single disc case.

half-open is much less for double disc.



Single Disc case



Double disc case

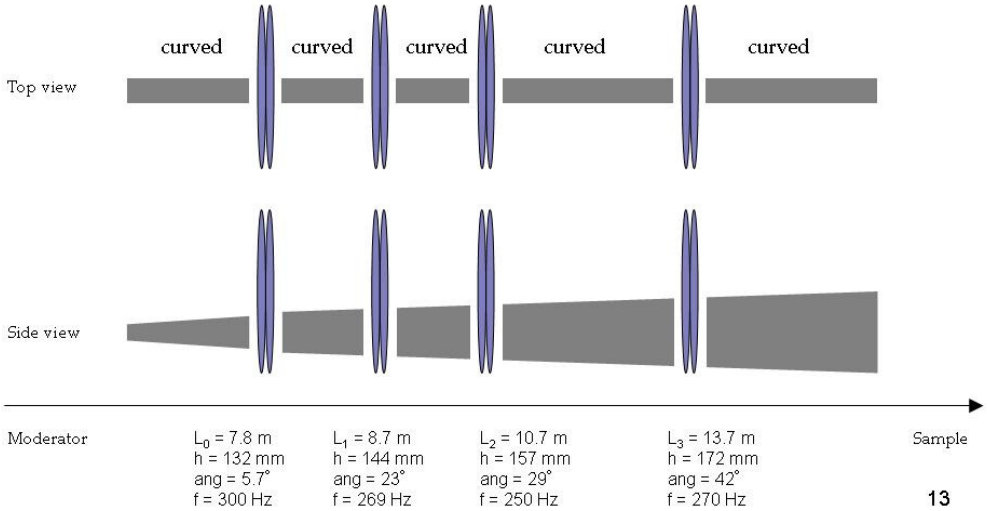
11

Requirements on Choppers

12

Requirements on Choppers

- We are proposing elliptic (V) + curved (H) geometry for the neutron transportation system, then
  - Tall slit is required on some discs with relatively high freq.
  - We have asked spec. of choppers of IN5 at the ILL last month by Dr. H. Mutka and Dr. J. Ollivier. One of them is 690 mm disc with tall slit (170mm). It has been operated with high freq. (283Hz = 17000rpm).



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Conclusion; complete spec. of choppers

Table 1: Spec of the pulse-shaper

	Length L_0 [m]	Frequency f_0 [Hz]	slit width w_0 [cm]	# of slits n_0	opening-time in FWHM Δt_0 [μs]
Pulse-shaping chopper	7.8	300	3	8	26.44

Table 2: Spec. of the frame-separation choppers (all of them are counter-rotating double-disc type)

	Length L_n [m]	Frequency f_n [Hz]	# of slits n_n	slit angle $angle_n$ [deg]	opening-time of full-open Δt_n [μs]	whole opening-time t_{all} [μs]	width of guide w_g [mm]	height of guide h_g [mm]
frame sep. #3	13.867	270	5	41.73	265.12	429.36	60.0	172.1
frame sep. #2	10.697	250	7	29.30	154.23	325.60	60.0	156.9
frame sep. #1	8.7070	268.75	8	23.17	84.61	239.50	60.0	143.8

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Verification by McStas

15

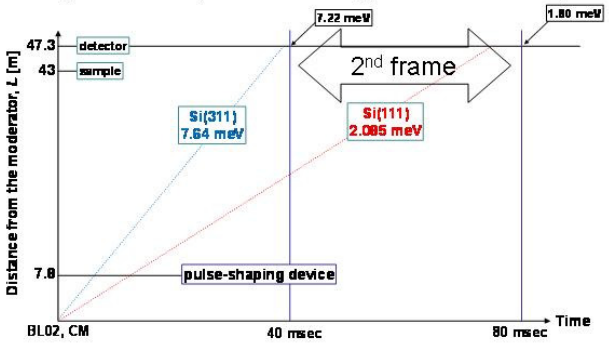
discussion with Dr. Emmanuel Farhi at the ILL

Oct. 2008

- We did not know how to check the designed frame separation choppers work successfully or not by McStas, till last months. Then when we visited the ILL I asked Dr. Emmanuel Farhi.
- He had an answer. We should use some components which he made and supplied to the McStas package.
  - ✓ Use "PreMonitor_nD.comp" and "Monitor_nD.comp".
  - ✓ **We can check "record of neutrons".** In our case, we can check which neutron have passed each chopper, i.e., pulse-shaper, #1 frame-sep. chopper, #2 frame-sep. chopper and #3 frame-sep. chopper.

Simulation parameters

Using 2nd frame (incident energy: 1.8 ~ 7.22 meV)



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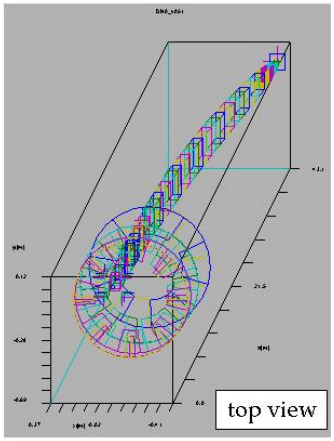
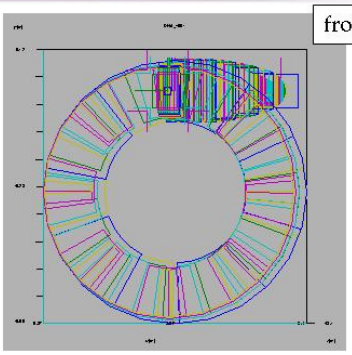
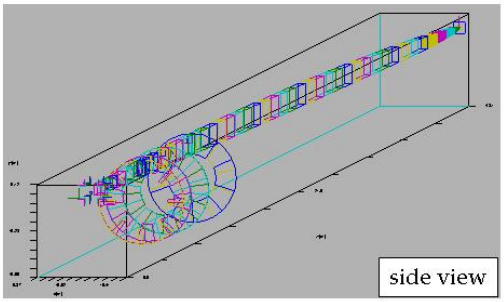
Simulation System

MC display







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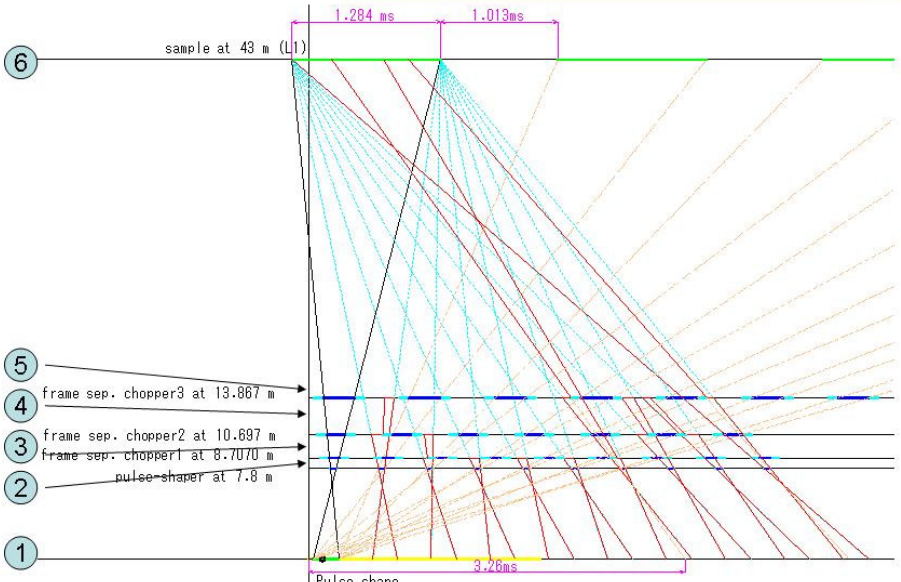
Position of PreMonitors

" record of neutrons": We will show you TOF at each point, but it ONLY counted neutrons which reached sample!



Pulse shape

120 us	:Peak intensity at around E = 2 meV
40 us - 260 us	:x1/2 intensity (useful frame)
- 2 ms	:x10^-3 intensity (useless frame)
- 3.26 ms	:< x10^-4 intensity (possible frame overlap)

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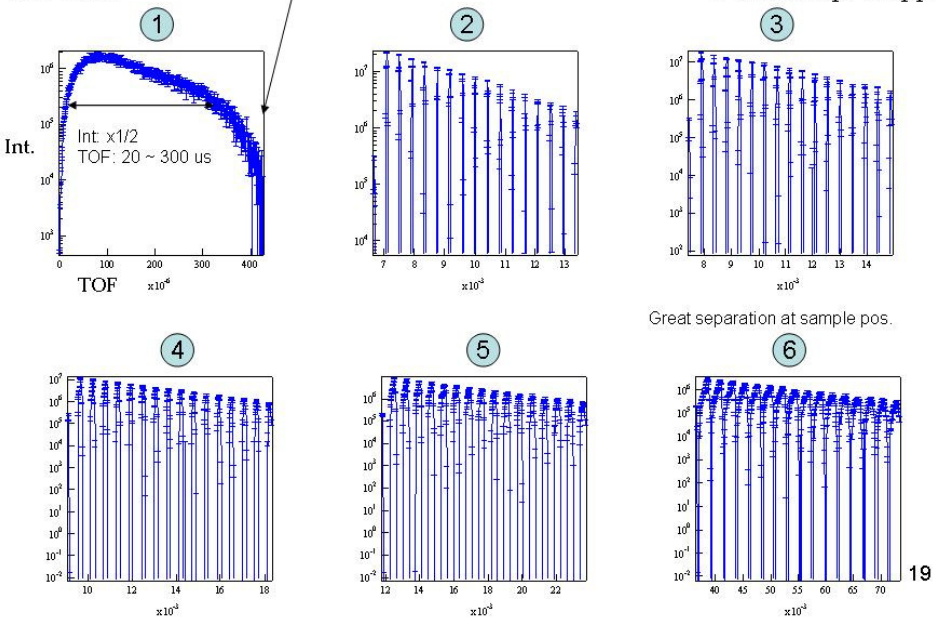
Beautiful frame-separation

ON: PS, #1, #2. #3
Off: none

beautiful cut off at about 430 us

Good case
3 frame-sep. choppers



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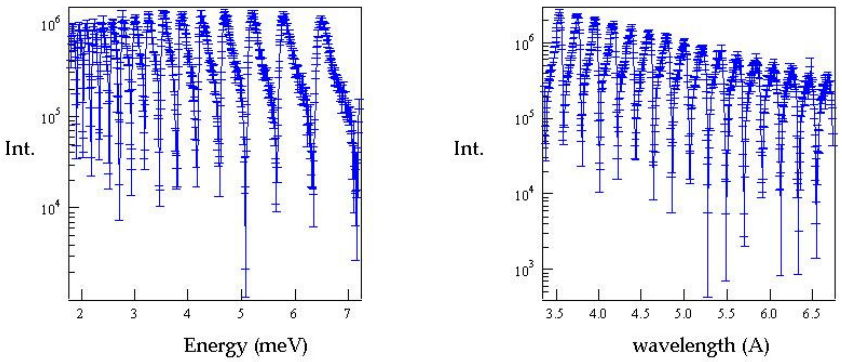
Wide energy-band obtainable by the RRM

- Broad E-band (left), wavelength-band (right) measurements can be obtained at once.



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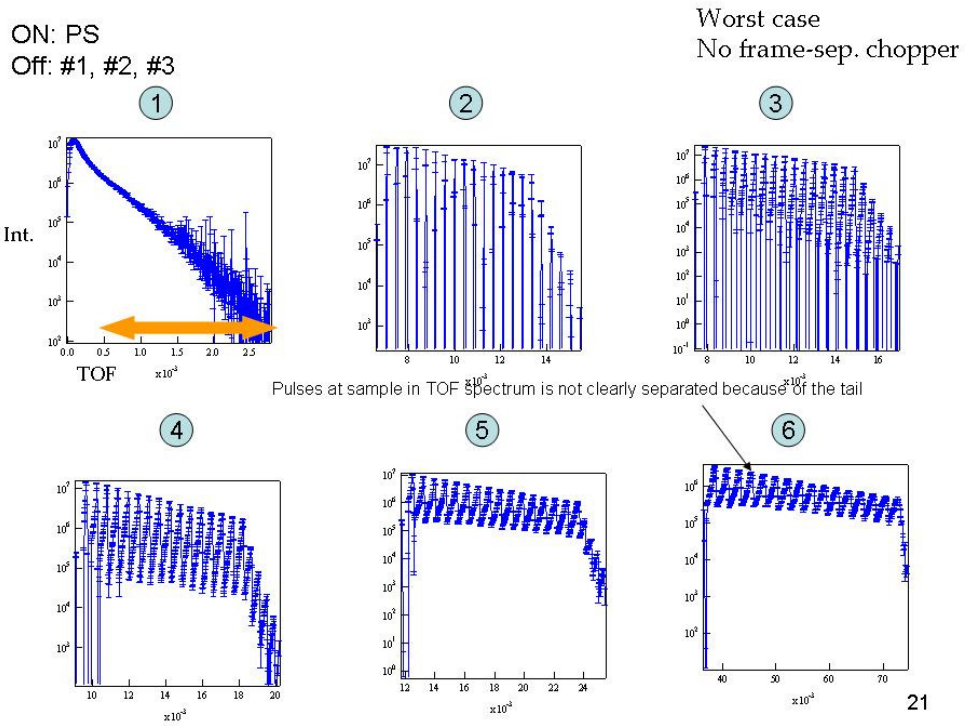
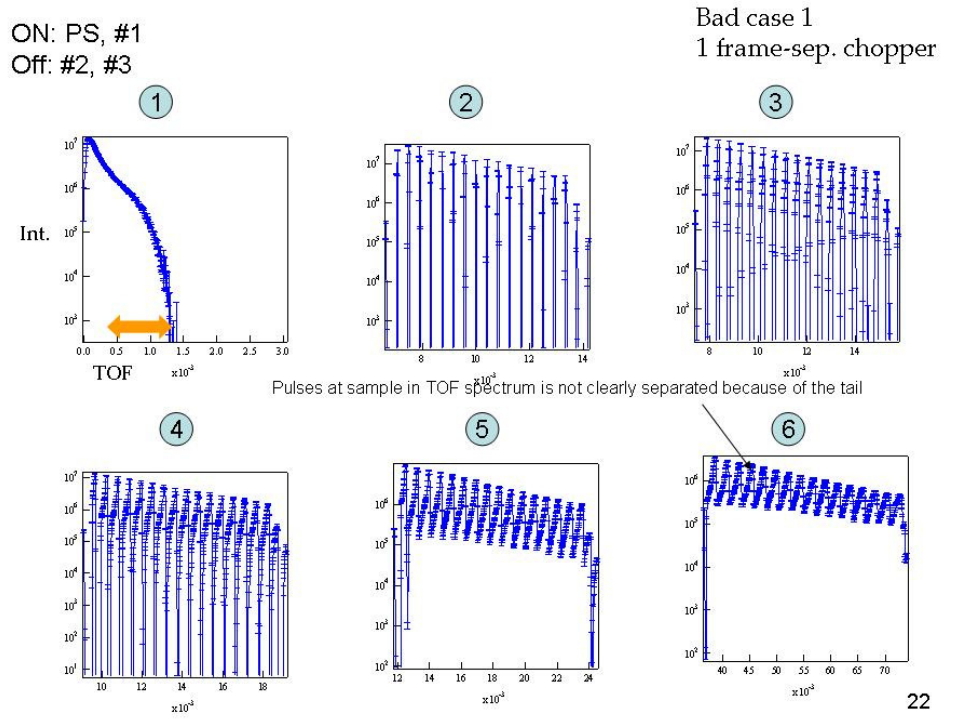
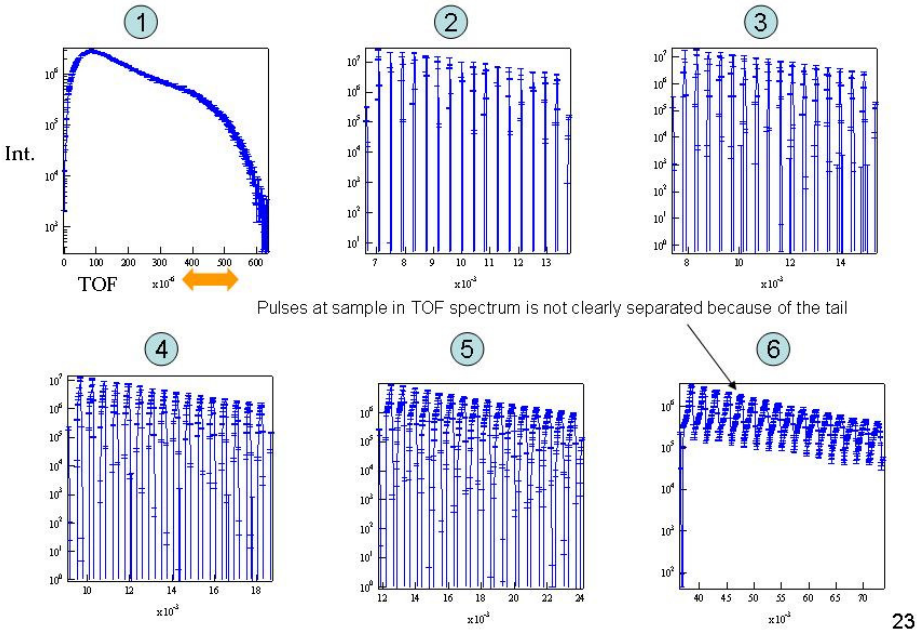

ON: PS
Off: #1, #2, #3
Worst case
No frame-sep. chopper
1
2
3
Int.
TOF
Pulses at sample in TOF spectrum is not clearly separated because of the tail
4
5
6
21


ON: PS, #1
Off: #2, #3
Bad case 1
1 frame-sep. chopper
1
2
3
Int.
TOF
Pulses at sample in TOF spectrum is not clearly separated because of the tail
4
5
6
22

ON: PS, #1, #2
Off: #3

Bad case 2
2 frame-sep. chopper



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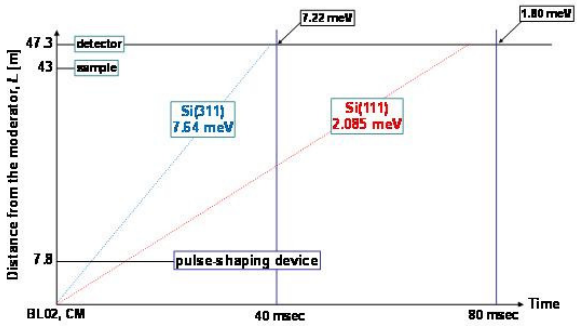
Further discussion

- Discussion is necessary about
  - When using second frame another band-chopper(s) are required. Where to be put and What spec.?
  - How about the Si(311) case?



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Further discussion

- Discussion is necessary about
  - The guide width is 60 mm. While the slit width is 30 mm when applying RRM. For normal meas. we will use other disc, ex. triple slit of 1cm, 3cm, 6cm. Do you think we have to consider about the eye-of-the-needle type neutron guide or double-elliptical shape guide? (Dr. P. Böni is planning for MARS.) While we do not think so. They are good for efficiency but loss of intensity will occur.

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Appendix (double-elliptical guide for MARS by Dr. P. Böni)

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New concepts for neutron instrumentation

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Available online 8 December 2007

Abstract

With the progress made in establishing new coating and grinding techniques and the availability of new simulation tools significant progress has been made in increasing the performance of optical components being used for neutron instrumentation. These include passive components like honeycomb lenses, focusing collimators, devices using supermirror coatings as well as active phase space transformers. In this contribution I shall discuss various possibilities of how the phase space of neutron beams can be adapted to match the needs of neutron beam lines and how to transport the neutrons efficiently from the moderator to the sample and detector. It is shown that elliptic guides can lead to significant flux gains while improving the resolution of spectrometers. The power of the new focusing techniques will be demonstrated for triple axis, time of flight and spin-echo spectroscopy as well as for imaging with neutrons.
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PACS: 03.75.Be; 28.41.Rc; 29.27.Eg; 29.25.Dz

Keywords: Neutron optics; Guides; Focusing; Supermirror; Polarization analysis

Appendix (double-elliptical guide for MARS by Dr. P. Böni)

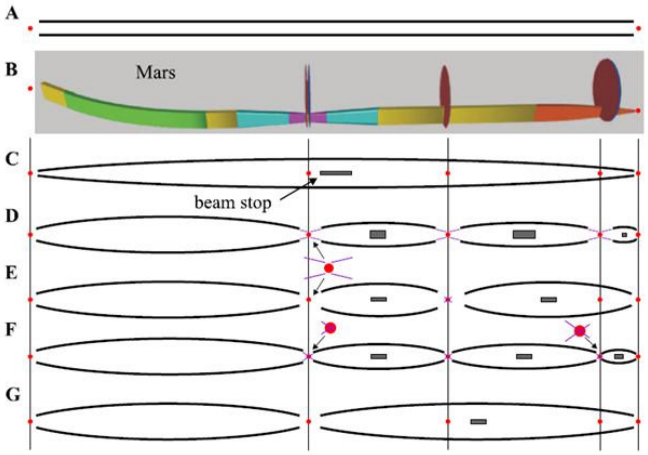

Fig. 6. Various options for transporting neutrons between the time-determining devices in a ToF-spectrometer. Solution B is realized for the backscattering spectrometer MARS at SINQ [20]. The beam stops interrupt the direct line of sight between the choppers and the sample thus improving the time resolution.

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Appendix (double-elliptical guide for MARS by Dr. P. Böni)

Table 2
Definition of various guide geometries for the backscattering spectrometer MARS at SINQ [20]

Item	Length (m)	Type of focusing	Entrance (mm^2)	Exit (mm^2)	Remarks	Gain
Linear (A)	74.5	all linear	30 × 120	30 × 120	M-S	1.0
Present	36	linearly tapered	30 × 120	15 × 60	M-C1	2.9
Design	0.308	straight	15 × 60	15 × 60	C1-C2	
(SINQ)	15.6	linearly tapered	15 × 60	30 × 120	C2-C3	
(B)	18.4	linear/parabolic	30 × 120	30 × 58	C3-C4/5	
	4	parabolic	30 × 58	8 × 15	C4/5-S	
1 elliptic (C)	74.5	elliptic	30 × 120	11 × 44	M-S	14
4 elliptic	36	elliptic	30 × 120	15 × 59	M-C1	4.5
Configuration (D)	14.55	elliptic	30 × 100	30 × 100	C2-C3	
(beam size matched)	17.20	elliptic	30 × 100	30 × 100	C3-C4/5	
	3.95	elliptic	30 × 100	18 × 61	C4/5-S	
3 elliptic	36	elliptic	30 × 120	15 × 59	M-C1	5.3
Configuration (E)	14.35	elliptic	29 × 118	29 × 118	C2-C3	
(beam size matched)	17.65	elliptic	22 × 88	50 × 199	C3-C4/5	
	3.95	elliptic	50 × 199	12 × 48	C4/5-S	
4 elliptic	36	elliptic	30 × 120	15 × 59	M-C1	1.8
Configuration (F)	15.5	elliptic	6 × 24	6 × 24	C2-C3	
(divergence matched)	18.1	elliptic	7 × 29	7 × 29	C3-C4/5	
	3.96	elliptic	1.6 × 6.5	3.6 × 15	C4/5-S	
2 elliptic (G)	36	elliptic	30 × 120	15 × 59	M-C1	7.6
($m = 3.6$)	38.2	elliptic	15 × 59	11 × 45	C2-S	

M: moderator, Ci: choppers, S: sample. Note that the beam size at the focal points is smaller than the size of the openings of the guides. The gains are normalized to a configuration with a straight guide with coating $m = 2$.

Further discussion

- Discussion is necessary about
  - The guide width is 60 mm. While the slit width is 30 mm when applying RRM. For normal meas. we will use other disc, ex. triple slit of 1cm, 3cm, 6cm. Do you think we have to consider about the eye-of-the-needle type neutron guide or double-elliptical shape guide? (Dr. P. Böni is planning for MARS.) While we do not think so. They are good for efficiency but loss of intensity will occur.

  - Intensity gain of 2 elliptic/ 1 elliptic is 0.54, then,
    - 1 elliptic is the best solution.
    - If it will be appeared that the chopper spec. is unrealistic, at that moment, we should reconsider the guide design.

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Further discussion

- Discussion is necessary about
  - Measuring inelastic part will be achievable while high BG (low S/N) is remaining as a big issue for BSS, then reducing BS idea will be important. (Dr. K. Shibata's part and anyone have idea?)

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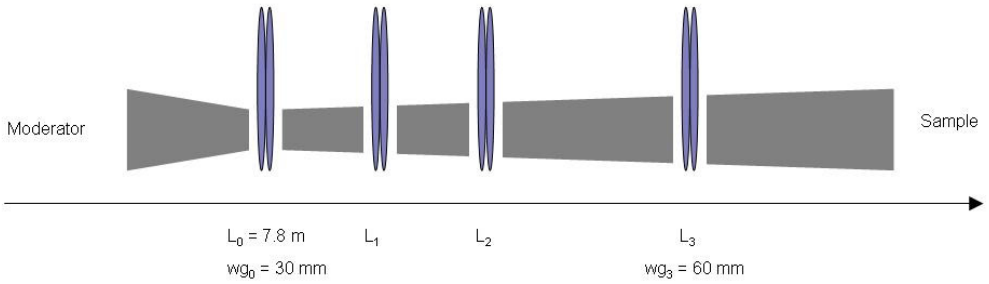
“eye-of-the-needle” guide design

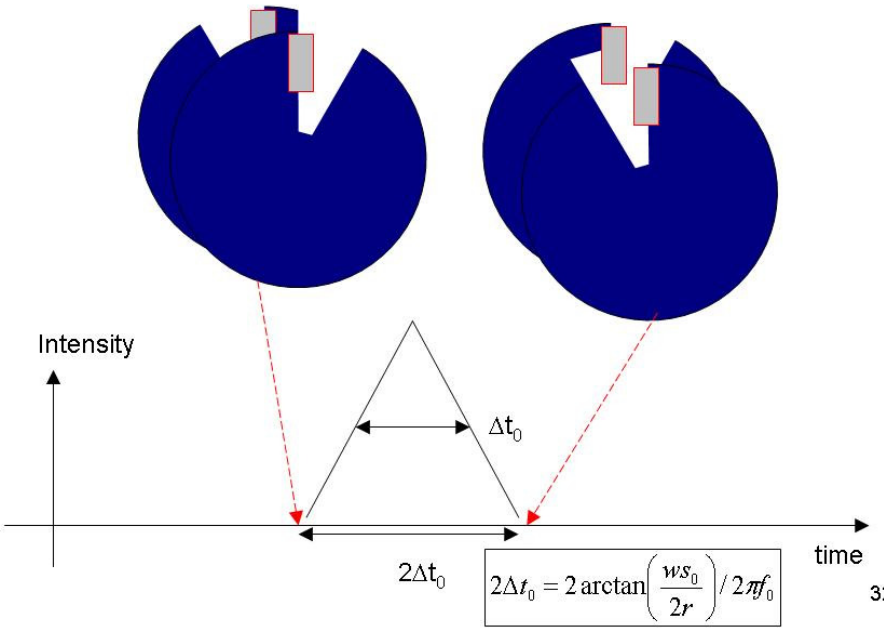


guide width; wg

$$wg_n = wg_0 + (wg_3 - wg_0) \times \frac{L_n - L_0}{L_3 - L_0} \quad (n = 1,2)$$

31

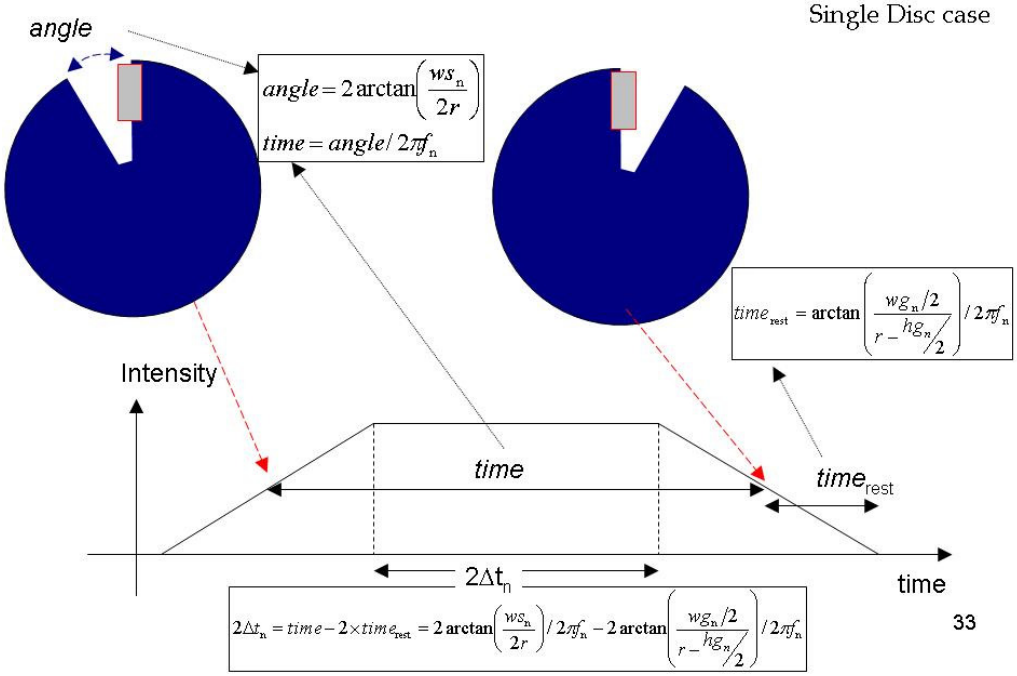
Appendix: Opening-time of the Pulse-shaper



32

Calculation of full opening-time of Frame-Sep. Chopper

Single Disc case



33

CONT.

Single Disc case

$$2\Delta t_n = time - 2 \times time_{rest} = 2\arctan\left(\frac{ws_n}{2r}\right) / 2\pi f_n - 2\arctan\left(\frac{wg_n/2}{r - hg_n/2}\right) / 2\pi f_n$$

$$\Delta t_n \times 2\pi f_n = \arctan\left(\frac{ws_n}{2r}\right) - \arctan\left(\frac{wg_n/2}{r - hg_n/2}\right)$$

$$ws_n = \tan\left(\Delta t_n \times 2\pi f_n + \arctan\left(\frac{wg_n/2}{r - hg_n/2}\right)\right) \times 2r$$

ws_n: slit width at beam center of each disc (n)
r: disc radius at beam center of each disc
f_n: frequency of each disc (n)
wg_n: width of guide at each chopper position
hg_n: height of guide at each chopper position

$2\Delta t_n$: Full-open time-width
time: time-width shown in the previous slide
$time_{rest}$: time-width shown in the previous slide

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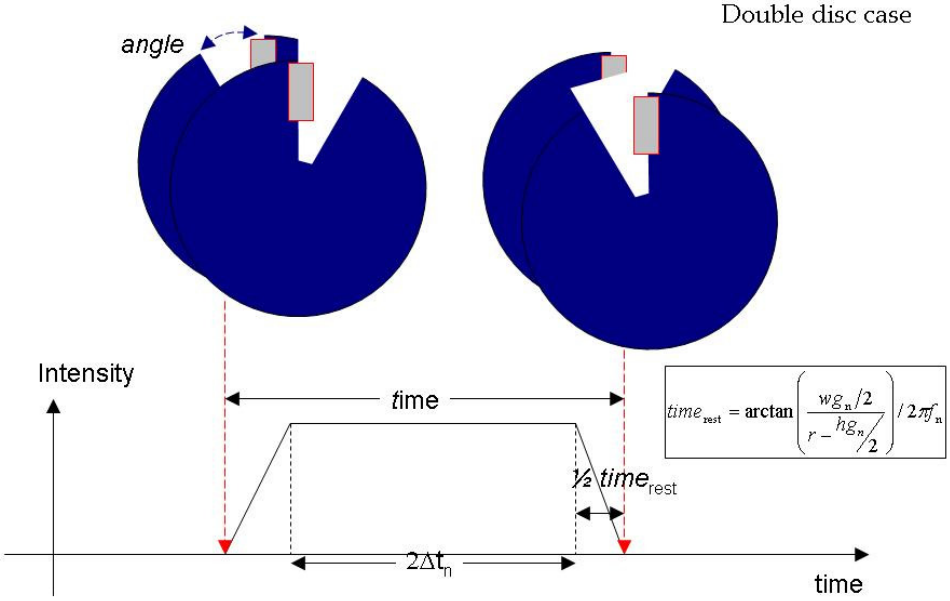
Calculation of full opening-time of Frame-Sep. Chopper

Double disc case



$$time_{rest} = \arctan\left(\frac{wg_n/2}{r - hg_n/2}\right) / 2\pi f_n$$

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CONT.

Double disc case

$$2\Delta t_n = time - 2\times\frac{1}{2}time_{rest} = 2\arctan\left(\frac{ws_n}{2r}\right)/2\pi f_n - \arctan\left(\frac{wg_n/2}{r - hg_n/2}\right)/2\pi f_n$$

$$2\Delta t_n \times 2\pi f_n = 2\arctan\left(\frac{ws_n}{2r}\right) - \arctan\left(\frac{wg_n/2}{r - hg_n/2}\right)$$

$$ws_n = \tan\left[\frac{1}{2}\left\{2\Delta t_n \times 2\pi f_n + \arctan\left(\frac{wg_n/2}{r - hg_n/2}\right)\right\}\right]\times 2r$$

ws_n: slit width at beam center of each disc (n)
r: disc radius at beam center of each disc
f_n: frequency of each disc (n)
wg_n: width of guide at each chopper position
hg_n: height of guide at each chopper position

$2\Delta t_n$: Full-open time-width
time: time-width shown in the previous slide. In this case this indicates whole opening time.
$time_{rest}$: time-width shown in the previous slide

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3.3. Analyzer system
Kaoru Shibata (JAEA) and Nobuaki Takahashi (JAEA)

3.3. Analyzer system
Analyzer mounting device (NT)
Analyzer alignment system (NT)
Reducing BG (KS)

Kaoru Shibata (J-PARC) & Nobuaki Takahashi (J-PARC)

Analyzer bank design

- The Committee recommended to consider about single crystal meas.
  - Dr. K. Shibata has discussed with Dr. K. Herwig (SNS) in March. One of his ideas is to eliminate any space in the horizontal plane for the analyzer bank.
  - A technician of a metal-processing company said that the machining cost become less if the diagonal line of the plate (one unit of the analyzer bank) is less than 800 mm.
- Then, we tried to design analyzer bank and divided into reasonable plates;
  - Scattering angle: -162~162deg.; dividing into 27 units <-> angle=12deg <-> width=481mm (Fig2). The machining area is limited to a circle with D~800, then, the height of the plate has been given about 685 mm (Fig3). The plate with the size can cover from -3deg to 0deg if it is cut (Fig1 blue). Total 68 (= 27x2 + 27/2) plates will be required.
  - One plate will be covered with 40 pieces of Si wafers with D=120mm (Fig3). Then, totally 2720 pieces of Si wafers are required (1360 of Si(111) and Si(311), respectively).

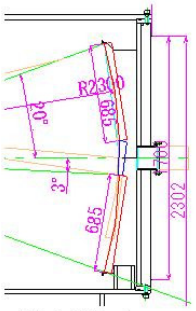


Fig1. Side view

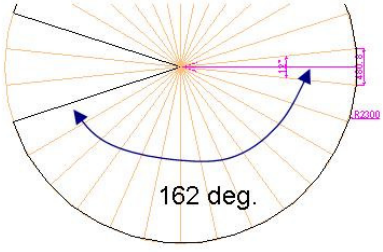


Fig2. Top view

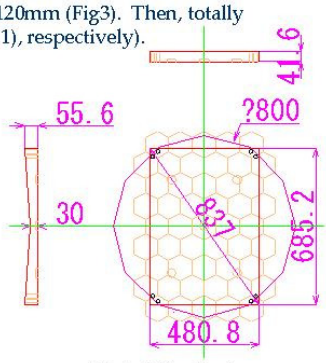
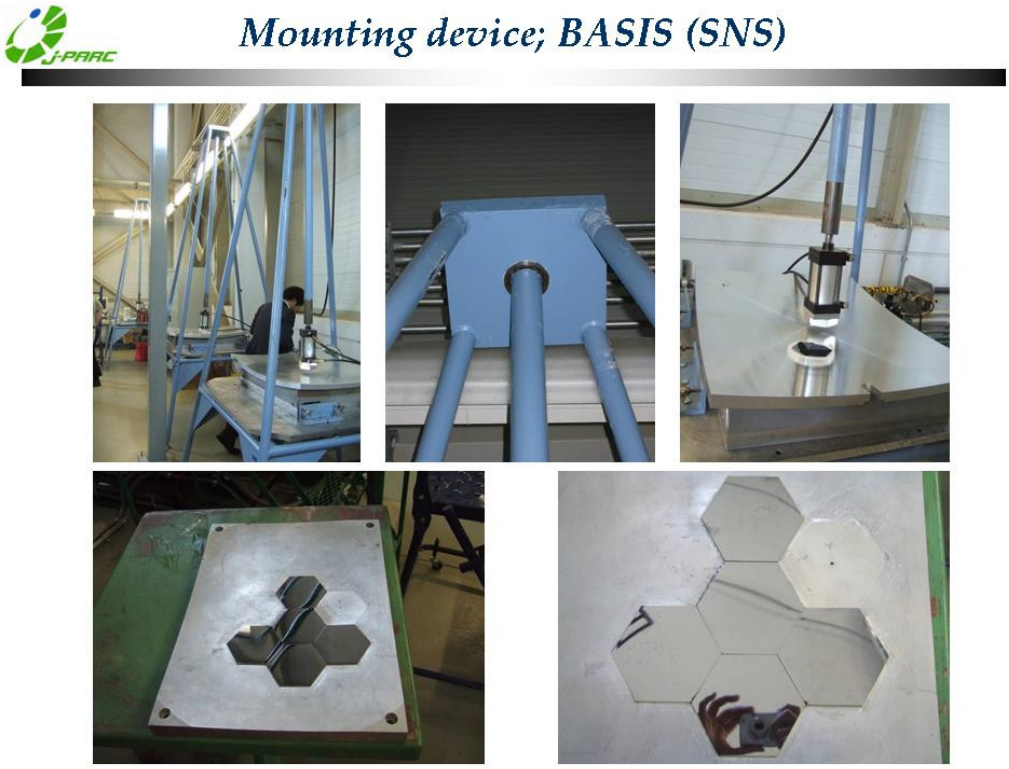


Fig3. Al back plate

Analyzer mounting device

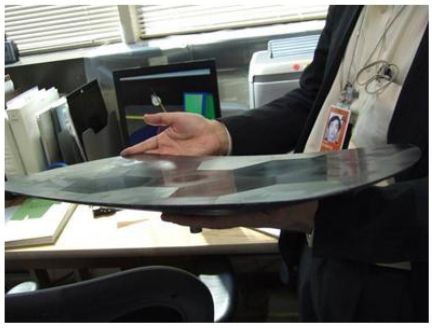
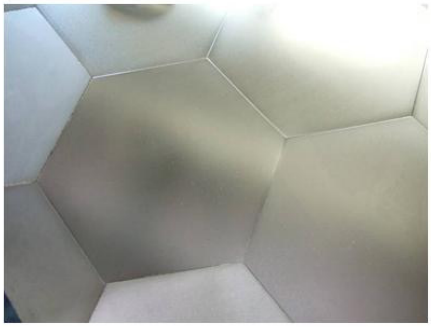
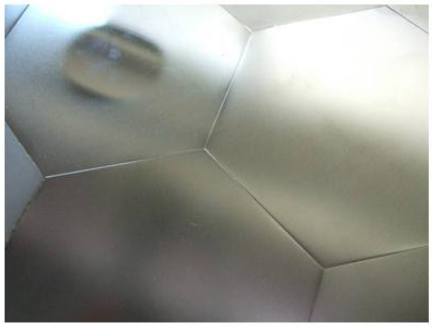


Mounting device; HFBS (NIST)



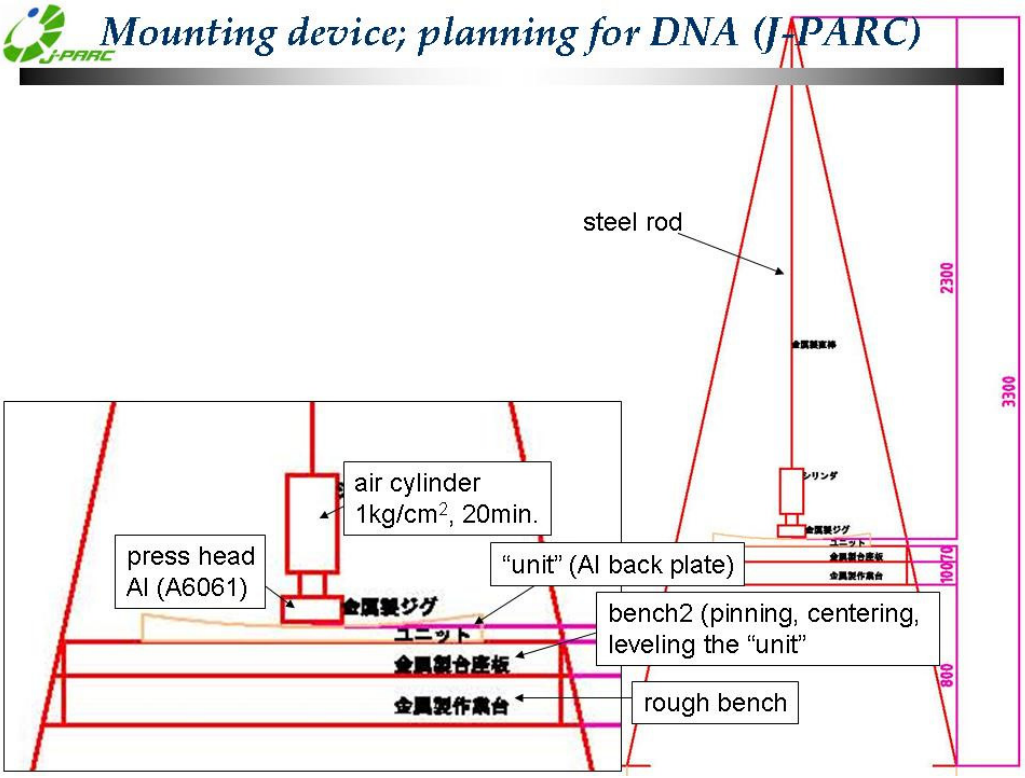


App. Doppler monochromator; HFBS (NIST)

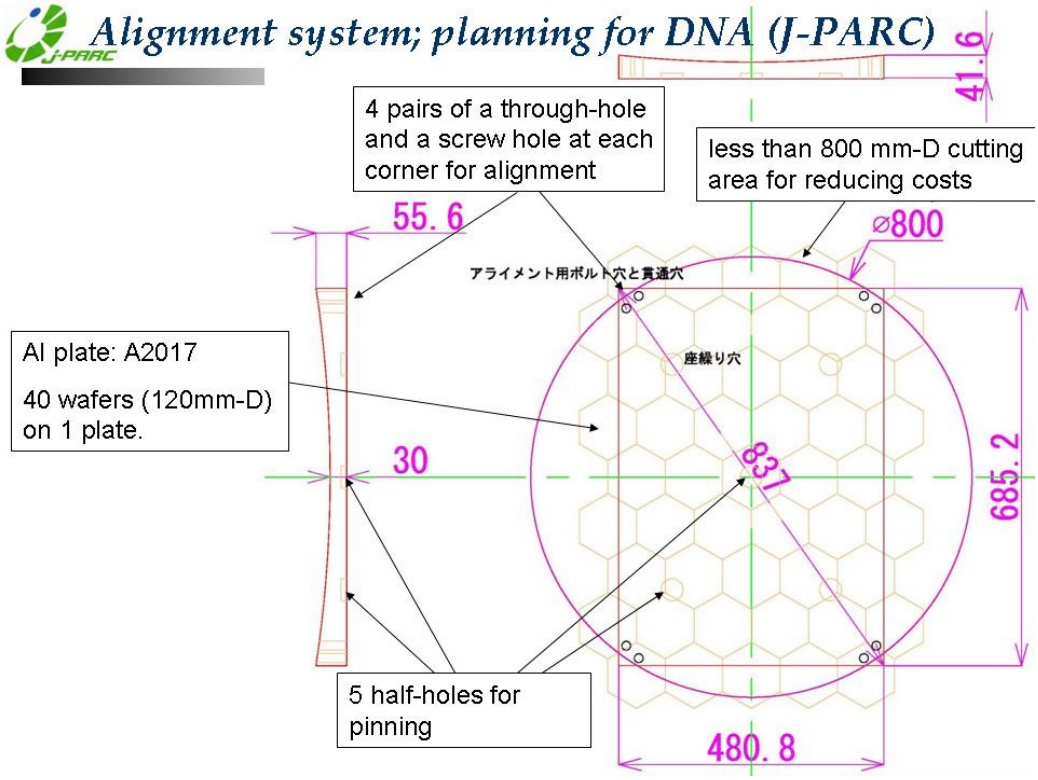





Mounting device; IN16 (ILL)

Mounting device; planning for DNA (J-PARC)

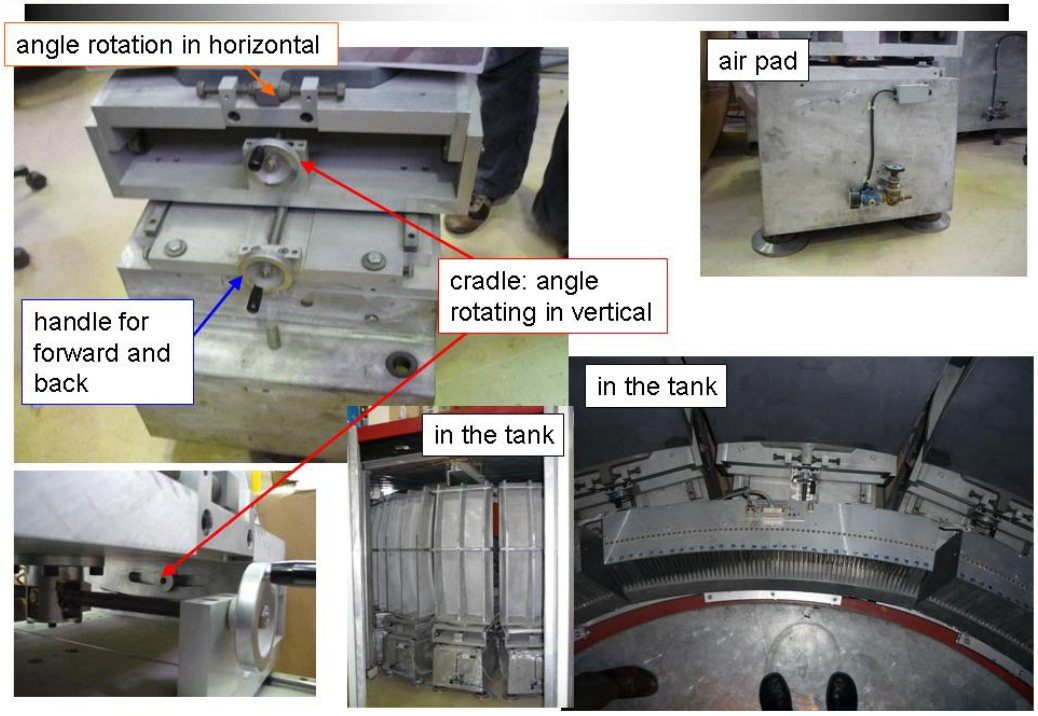


Analyzer alignment system

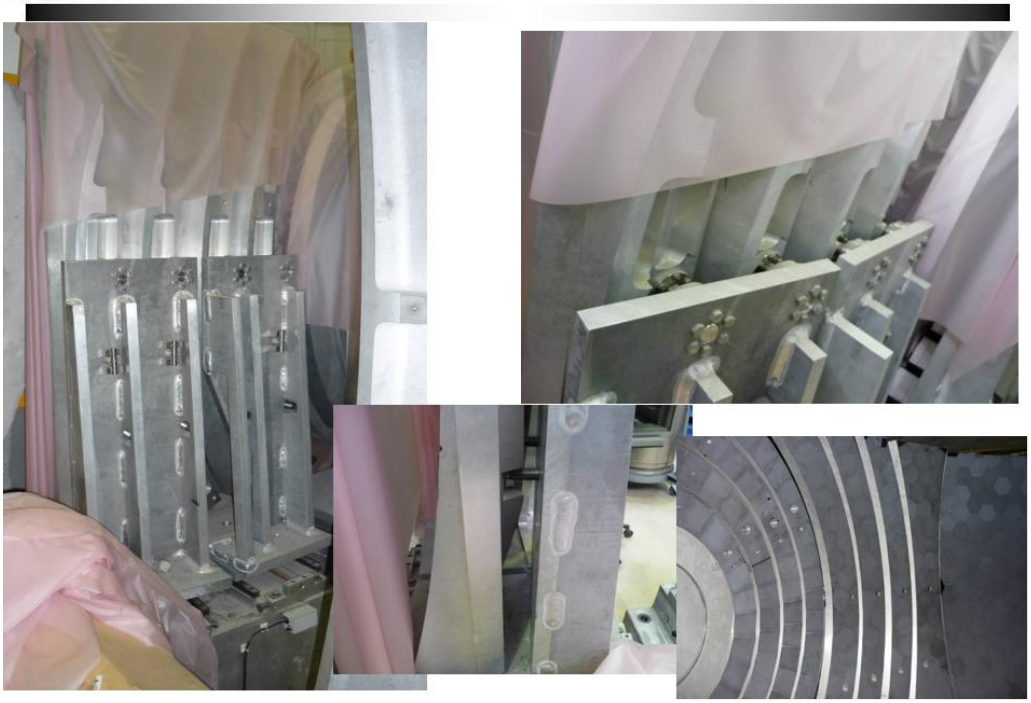


Alignment system; IN16

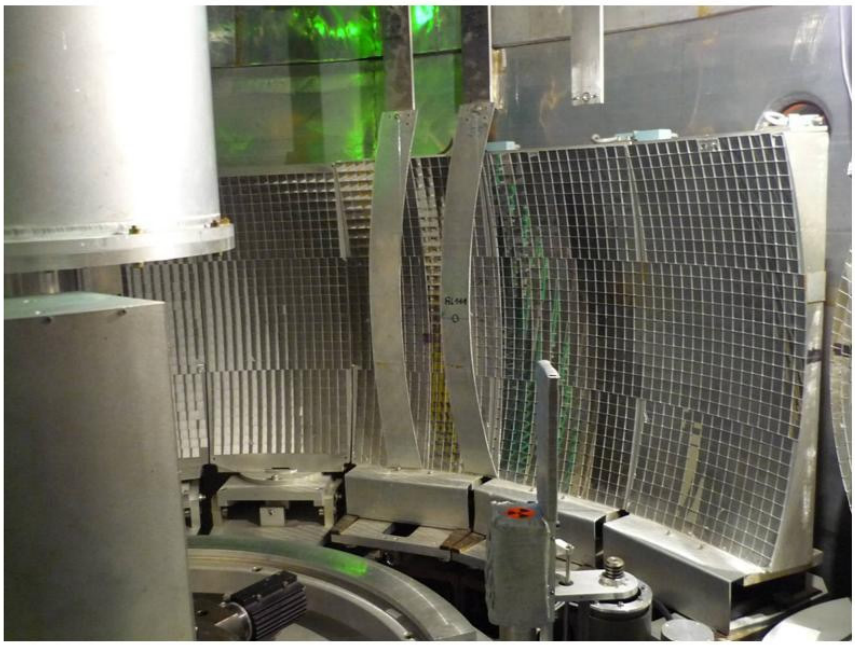
Alignment system; IN16 (normal bank)



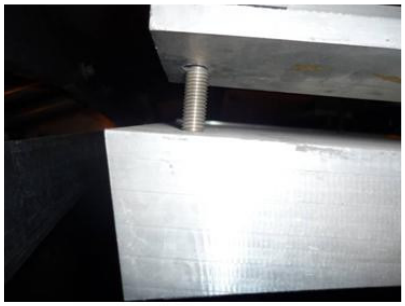
Alignment system; IN16 (small angle bank)

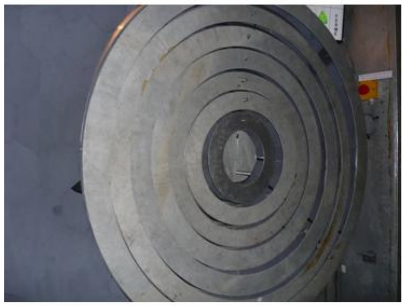


Alignment system; IN13



Alignment system; IN10






Reducing BG

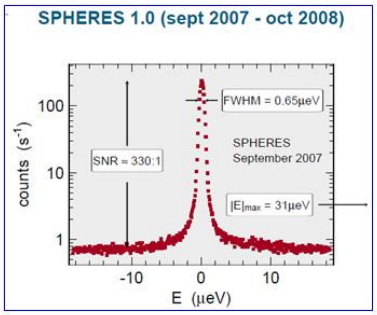
Status of BG on BS Spectrometer and User Demand for S/N ratio

On BS spectrometers S/N ratio: 1/300 ~ 1/1000

Friendly Comparison by Christian Breunig„

	IN16	HFBS	SPHERES
resolution fwhm (μeV)	0.8–0.9	0.93	0.65
flux at sample (10^5/s)	<12	<12	>6
signal-to-noise ratio	excellent ~ 1000	>400	330

BASIS@SNS ~ 1000



User demand for S/N ratio

On a spectrometer around elastic with narrow E scan range

-> elastic and quasi elastic scattering measurements

demand for S/N ratio :10^{-2}~10^{-3}

On a spectrometer around elastic with wide E scan range

->+ Inelastic mode measurements

demand for S/N ratio :10^{-4}~10^{-5} (~10^{-6})

When the scan E range is expanded, we need more low background spectrum for the inelastic measurements.

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How to reduce BG No.1

Background Origins

Measures to reduce BG

External BG origins:	air scattering week shield around detectors electric noise etc.
Internal BG origins:	H- incoherent scattering from resin on the backside of Si crystal Bragg scattering from crystal analyzer Al back bone plate TDS from Si, (PG) crystal etc.

Neutron absorber (B, B_4C, Gd, Gd_2O_3) coating on the backside of Si crystal

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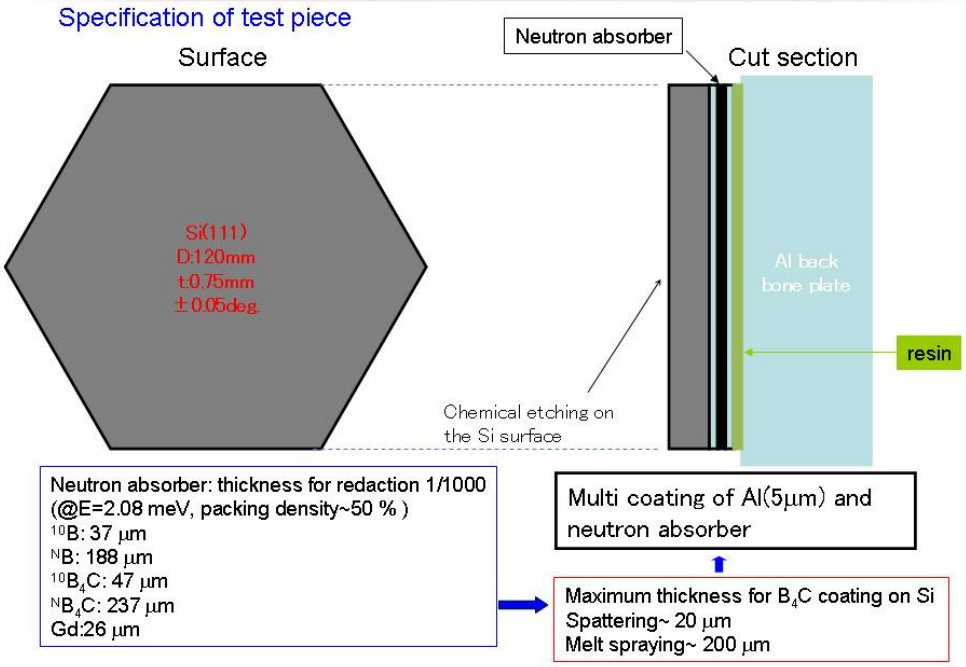
Neutron absorber (^{10}B, B_4C, Gd, Gd_2O_3) coating on Si surface



How to reduce BG No.2

Background Origins — **Measures to reduce BG**

External BG origins:	air scattering week shield around detectors electric noise etc.
Internal BG origins:	H- incoherent scattering from resin on the backside of Si crystal Al Bragg scattering from crystal analyzer back bone plate TDS from Si, (PG) crystal → Experimental results to estimate the intensity form TDS etc.

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Introduction of *Thermal Diffuse Scattering (TDS) around Near Back Scattering TOF Configuration*

Theory

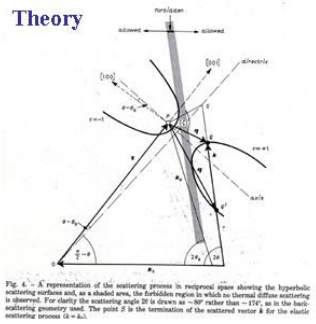
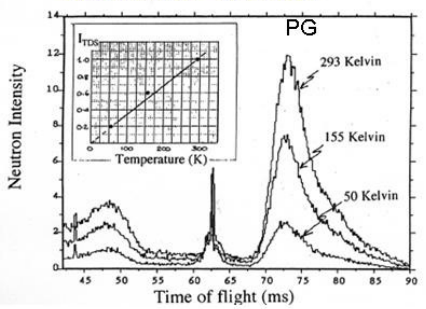
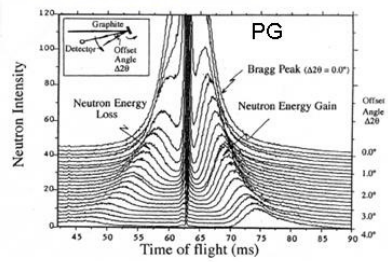


Fig. 4. – A representation of the scattering process in reciprocal space showing the hyperbolic scattering surfaces and, as a shaded area, the forbidden region in which no thermal diffuse scattering is observed. For clarity the scattering angle 2θ is drawn as ~ 80° rather than ~ 174°, as in the back-scattering geometry used. The point S is the termination of the scattered vector k for the elastic scattering process (k = k_0).

Temperature Dependence



Off Set Angle Dependence



This type TDS had been reported by the group of IRIS at ISIS in 1980's. (by Prof. B.T.M.Willis)

Experiments on LAM-80ET_D for DNA
For PG(002), Si(111), Mica(006)

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TOF measurements : Analyzer Crystals

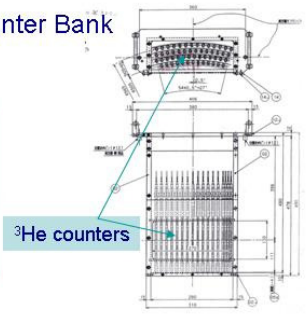
On LAM-80D at KENS;

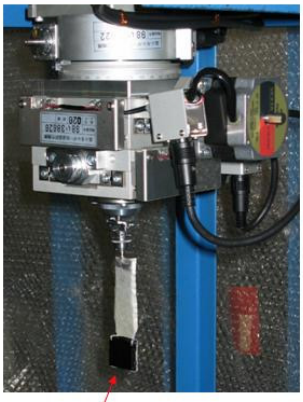
The diffraction counter bank on LAM-80ET

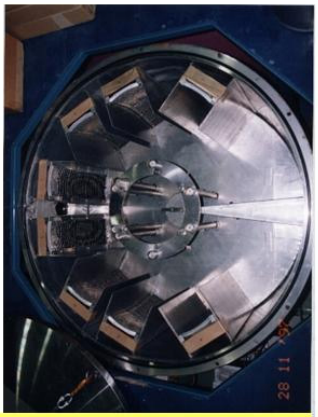
Specification

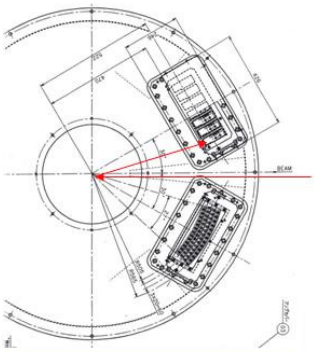
N.P. CH_4 Solid Cold Moderator ; L_1=26.m, L_2=505~565mm
Incident Neutron Wave Length: λ…= 2.5 ~ 30 Å
Scattering Angles: 2θ =163.5 ~ 136.5° Δ θ =0.5°
Number of ^{3}He counters : 55.

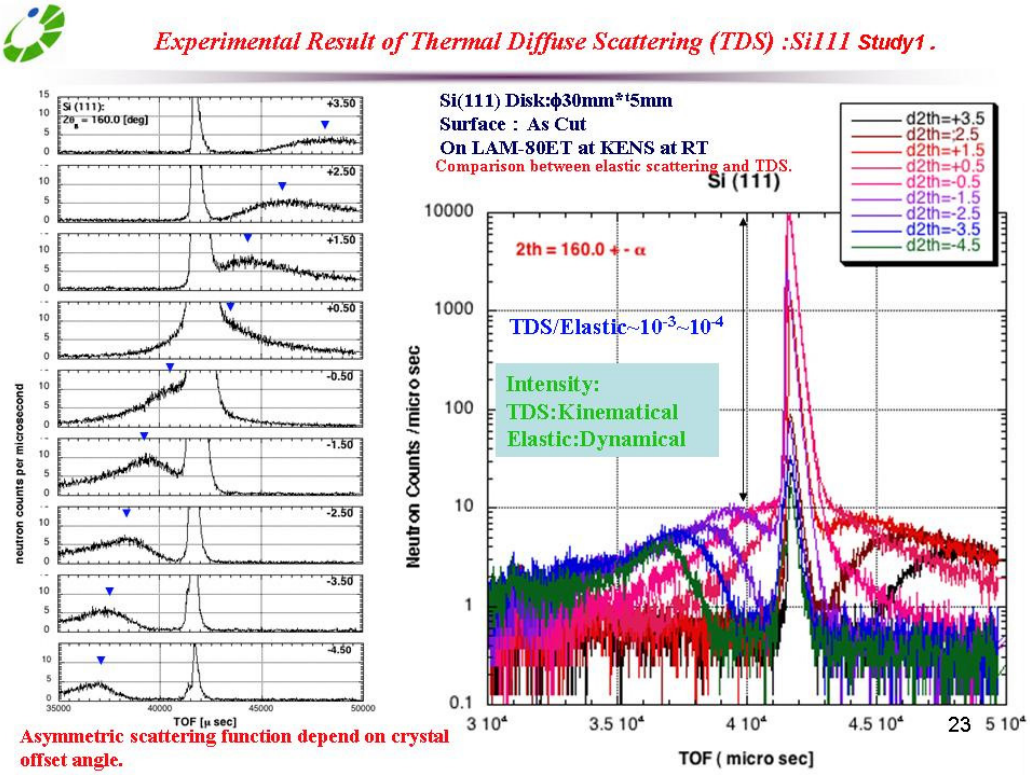
Counter Bank

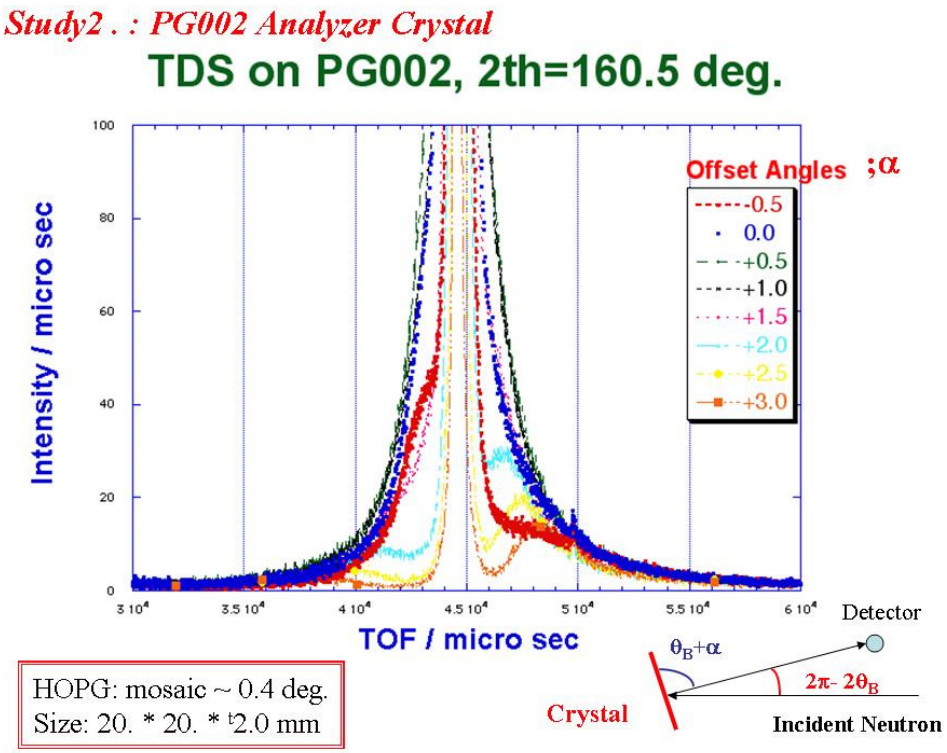








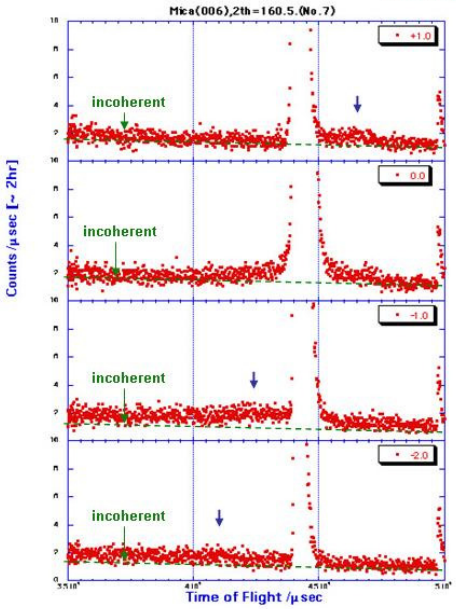

Experimental Result of Thermal Diffuse Scattering (TDS) :Si111 Study1 .
Si(111) Disk:ϕ30mm*t5mm
Surface : As Cut
On LAM-80ET at KENS at RT
Comparison between elastic scattering and TDS.
Si (111)
2th = 160.0 + - α
TDS/Elastic~10-3~10-4
Intensity:
TDS:Kinematical
Elastic:Dynamical
d2th=+3.5
d2th=+2.5
d2th=+1.5
d2th=+0.5
d2th=-0.5
d2th=-1.5
d2th=-2.5
d2th=-3.5
d2th=-4.5
Neutron Counts /micro sec
TOF (micro sec)
neutron counts per microsecond
TOF [μ sec]
Asymmetric scattering function depend on crystal offset angle.


Study2 . : PG002 Analyzer Crystal
TDS on PG002, 2th=160.5 deg.
Offset Angles ;α
-0.5
0.0
+0.5
+1.0
+1.5
+2.0
+2.5
+3.0
Intensity / micro sec
TOF / micro sec
Detector
θB+α
2π- 2θB
Crystal
Incident Neutron
HOPG: mosaic ~ 0.4 deg.
Size: 20. * 20. * t2.0 mm

Study 3. : Mica006 Analyzer Crystal

Natural Green Mica(006)
Size: 20. * 20. * t2.0 (stacked)

α: offset angle



NEUTRON INVESTIGATION OF MICA SPECIMENS in PSI
P. Allenspach (PSI), D. Engberg (ISIS, UK)

Slabs of single crystalline mica are - due to their large lattice spacing - used as monochromators or analysers in high resolution spectrometers. For a specific choice of mica a survey of all available types of mica and their thermal diffuse scattering (TDS) was needed. It turned out that there is almost no temperature dependence observable. Hence, an improvement of the signal-to-background ratio cannot be achieved by cooling as in pyrolytic graphite.

1.Annite with strong 002 and 006 but missing 004 and a background comparable to Muscovite.
2.Phlogopite with all reflections consistently strong and a background similar to Muscovite.
3.Fluor-Phlogopite with strong 002 and 006, weak 004 but very low background.

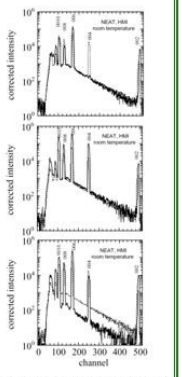


Fig. 1: Time-of-Flight diffraction pattern of Annite (top), Phlogopite (middle), and Fluor-Phlogopite (bottom) compared to Muscovite (dashed lines).

Thermal Diffuse Scattering (TDS) :Discussion

- TDS would be one of background origin in a spectrum on nBSS with wide dynamic range.

- Si(111) ; Comparison between TDS and Elastic scattering.

  TDS: **Kinematical scattering process**

  Elastic.: **Dynamical scattering process**
  + Kinematical scattering process
  (on the surface, as cut condition)

  Intensity ratio (TDS/Elastic.) ~ 10^{-4}~10^{-5} (t=0.75 mm)

  If the Si111 crystal with chemical etched surface was used,

  Intensity ratio (TDS/Elastic.) > 10^{-4}~10^{-5}

To Reduce TDS (B.G.)

1. To Reduce the thickness of Si crystal -> t=2.5-> 0.75 mm(1/3)
2. Cooling analyzer crystal -> Big analyzer cooling
3. Change Si -> Ge, 1/M -> Int(TDS) small,

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How to reduce BG (***Summary***)

Background Origins		Measures to reduce BG
External BG origins:	air scattering week shield around detectors electric noise etc.	→ Depend on the design
Internal BG origins:	H- incoherent scattering from resin on the backside of Si crystal S/N ratio~ 10^{-3}~10^{-4}	→ Neutron absorber (B, B4C, Gd, Gd3O2) coating on the backside of Si crystal
	Al Bragg scattering from crystal analyzer back bone plate	
	TDS from Si, (PG) crystal S/N ratio~ 10^{-4}~10^{-5} etc.	→ Experimental results to estimate the intensity form TDS

User demand for S/N ratio

Elastic and quasi elastic scattering measurements	demand for S/N ratio :10^{-2}~10^{-3}
Inelastic mode measurements	demand for S/N ratio :10^{-4}~10^{-5} (~10^{-6})

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3.4. Neutron transportation system
Nobuaki Takahashi (JAEA)

3.4. Neutron transportation system

Nobuaki Takahashi (J-PARC)

Studies about the neutron transportation system

- Low energy neutrons should be transported to the sample as much as possible.
  - ✓ elliptical shaped SM guide is much better rather than straight type in vertical direction. The expected intensity gain is more than 1.5 ~ 2 times. See Fig. 6 [N. Takahashi *et al.*, *Proc. ICANS-XVIII*, 373 (2007)]
- Background from higher order reflections of Si(311) (933, and higher) should be avoided. The elastic energy of the Si(933) is about 70 meV, then
  - ✓ Curved guide with cut-off energy of 40 meV is planned. (m = 3, R = 2200 m, w = 60 mm)
- Polarization devices will be installed before the sample position. This instrument is normally used for elastic scans and/or quasi-elastic measurements. The elastic energy of the Si analyzers are 7.640 meV and 2.085 meV. Such a long wavelength neutrons SM type polarizer would be better.
  - ✓ SM polarizer

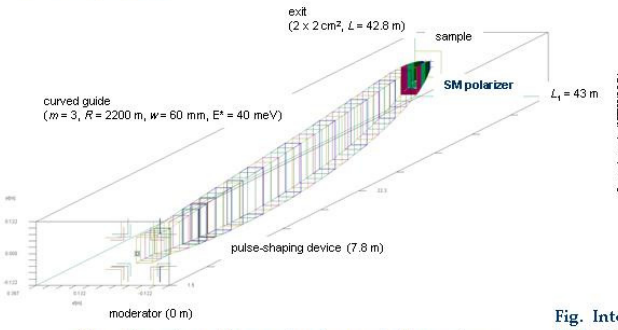


Fig. Geometry of the neutron transportation system

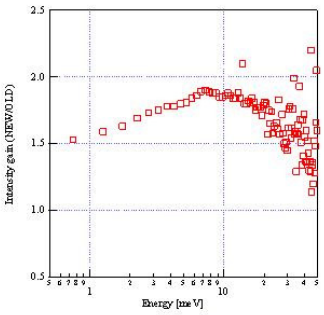
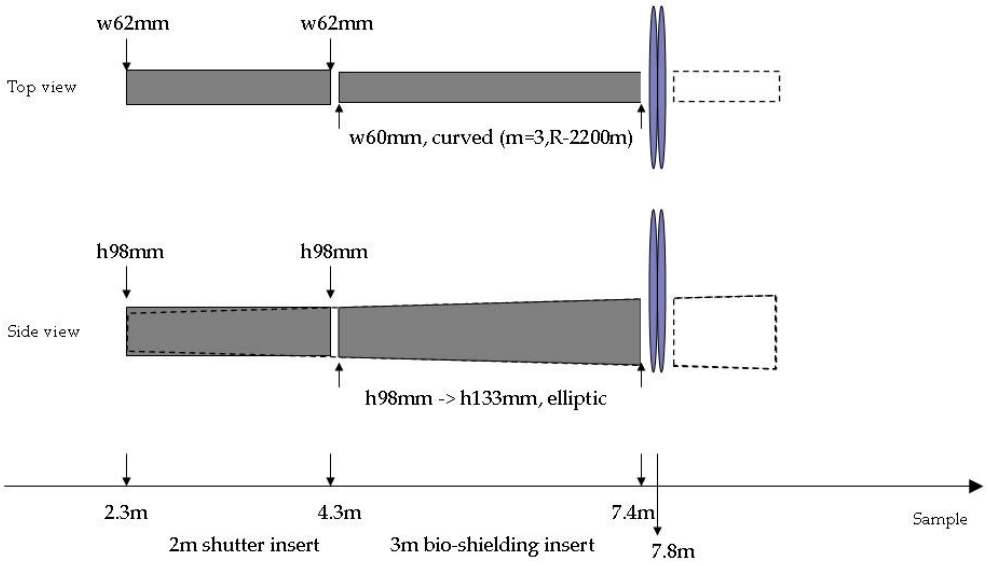


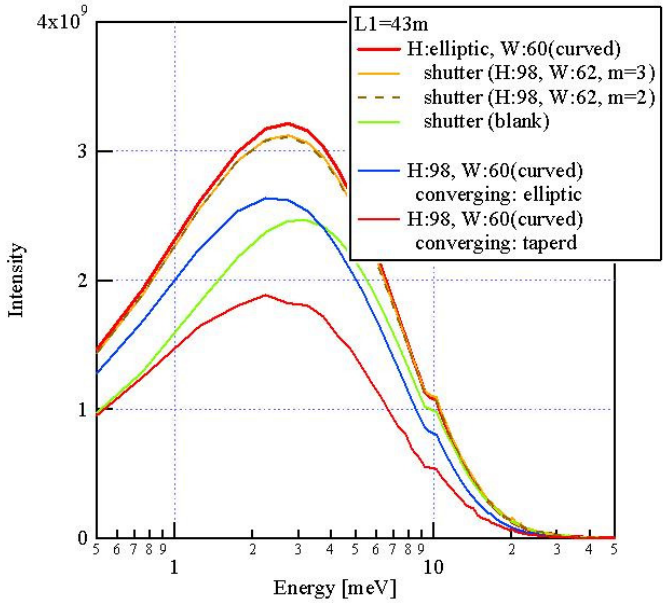
Fig. Intensity gain factor of the elliptic guide, against a commonly used straight guide

Fabrication is partly started (JFY2008)

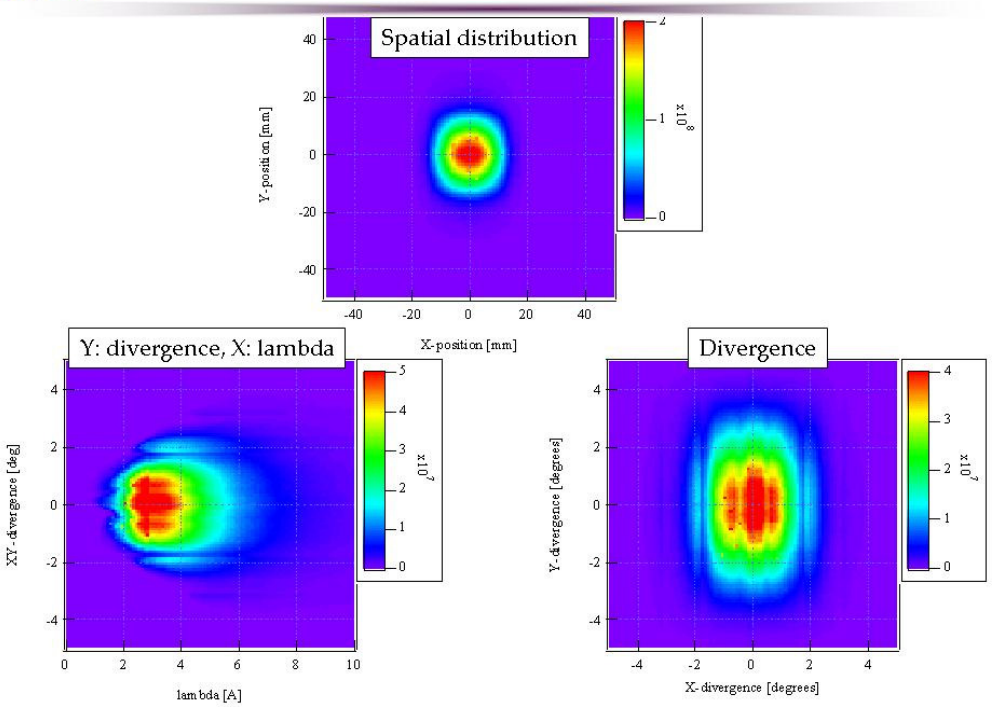
- Fabrication of the neutron guide is started in this JFY for 2m-shutter-insert and 3m-bio-shielding-insert.



Intensity comparison



Spatial distribution & divergence

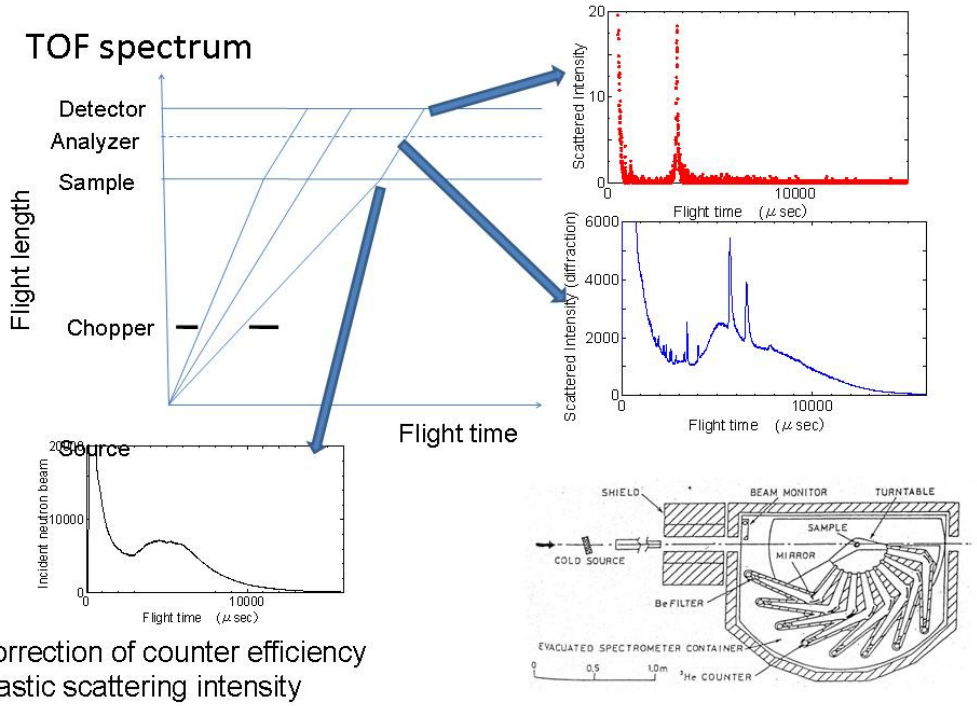


3.5. Data analysis software
Yukinobu Kawakita (Kyushu U.)

Data processing from TOF data

Faculty of Sciences, Kyushu University
Yukinobu Kawakita

1. TOF spectra
2. Normalization by wavelength distribution of the incident beam
   & counter efficiencies
3. Window correction
   TOF of the elastic scattering should be defined.
   Binning
   TOF -> energy transfer (flight length)
   Constant Δt -> constant ΔE
4. Subtraction of container and background, Absorption correction
5. Detailed balance factor
6. Resolution decoupling
7. Surface interpolation + Multiple scattering correction



Correction of counter efficiency
Elastic scattering intensity
from an incoherent standard sample (V)

Window correction

This procedure depends on how store the scattering counts.

If we measure TOF with constant time interval,
we have to transform the step to constant energy interval.

Count at each time step should be multiplied by $\left|\frac{dE}{dt}\right|$.

Detailed balance factor

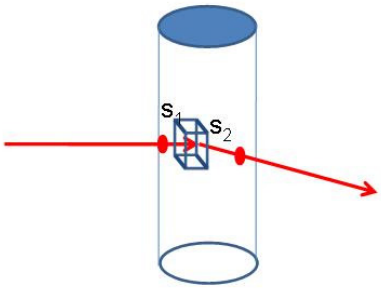
To obtain symmetrical S(Q,E),

$$\bar{S}(Q,E) = S^{obs}(Q,E)\exp(-E/2k_BT)$$

Absorption correction

Energy dependence of absorption cross sections
$1/\lambda$ law or theoretical calculation

Each pixel of energy transfer should be dealt independently.



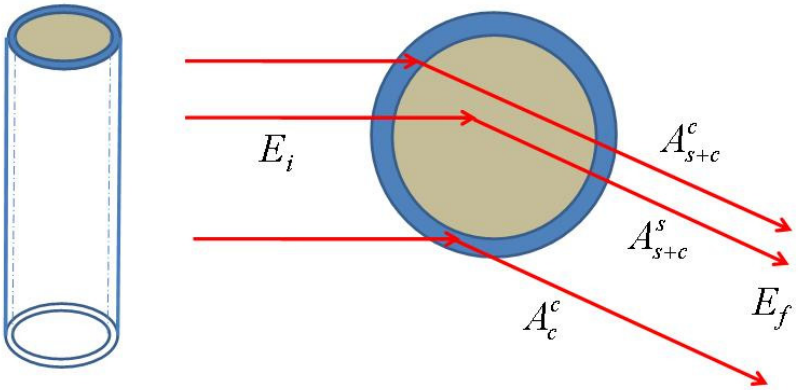
Dependency on incident neutron energy,
direction of detector,
and sample shape

$$A(E;\theta,\varphi) = \iiint_V \exp(-\sigma(E_i)ns_1)\exp(-\sigma(E_f)ns_2)dxdydz$$

$$E = E_i - E_f$$

for each detector

Subtraction of container and background contributions



$$I_s(E) = \frac{1}{A^s_{s+c}} \left\{ \left[I^{obs}_{s+c}(E) - I^{obs}_b(E) \right] - \frac{A^c_{s+c}}{A^c_c} \left[I^{obs}_c(E) - I^{obs}_b(E) \right] \right\}$$

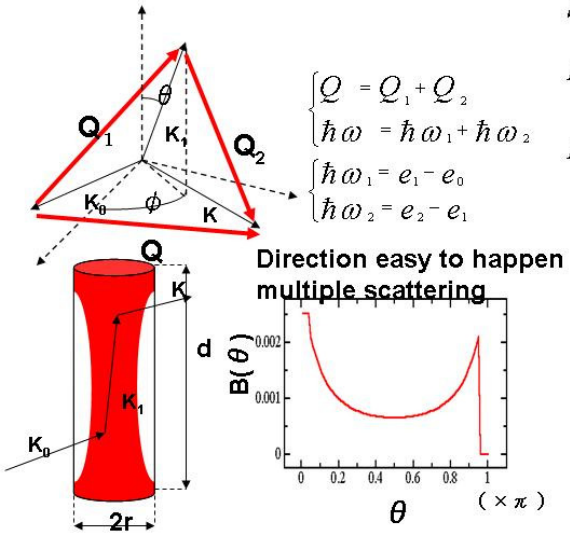
A^j_i Absorption coefficient of neutron scattered from matter j and absorbed by i material
function of E, θ and φ

Multiple scattering correction

Approximation V.F. Sears

Monte Carlo simulation
MSCAT J.R.D. Copley

Method by V.F. Sears



$$\begin{cases} Q = Q_1 + Q_2 \\ \hbar\omega = \hbar\omega_1 + \hbar\omega_2 \end{cases}$$

$$\begin{cases} \hbar\omega_1 = e_1 - e_0 \\ \hbar\omega_2 = e_2 - e_1 \end{cases}$$

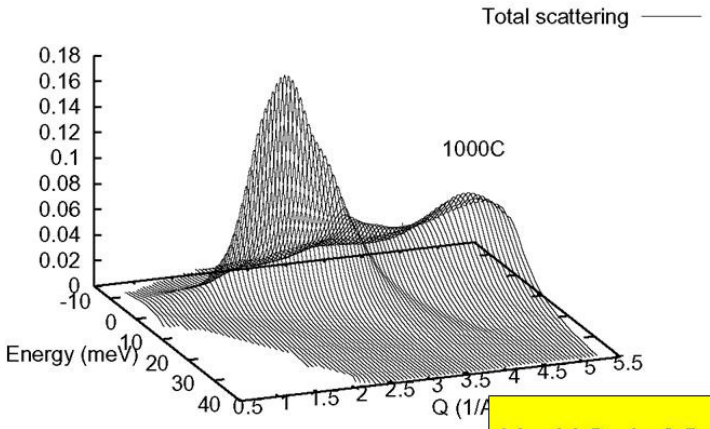
Direction easy to happen multiple scattering

$$S(k_0,k) = H_1(k_0,k)\{S(Q,\omega) + \Delta R_2(k_0,k)\}$$

$$R_2(k_0,k) = \frac{1}{\delta}\int_0^{\pi} R(k_0,\theta,k)B(\theta_1)d\theta$$

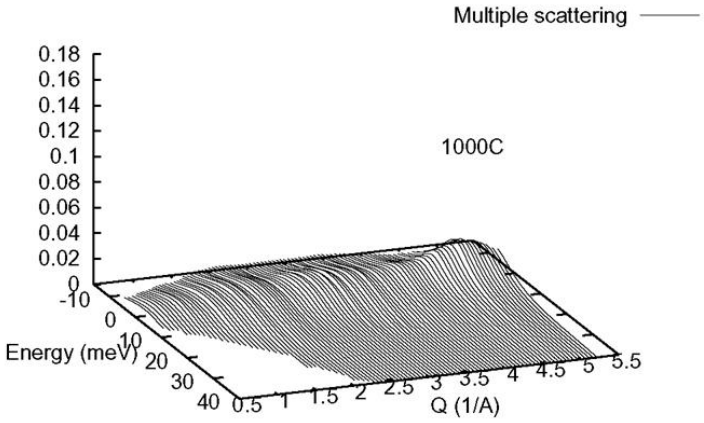
$$R(k_0,\theta,k) = \frac{1}{2\pi}\int_0^{2\pi} d\phi_1 \int_0^{\infty} d\varepsilon_1 S(Q_1,\omega_1)S(Q_2,\omega_2)$$

Case of liquid Ge

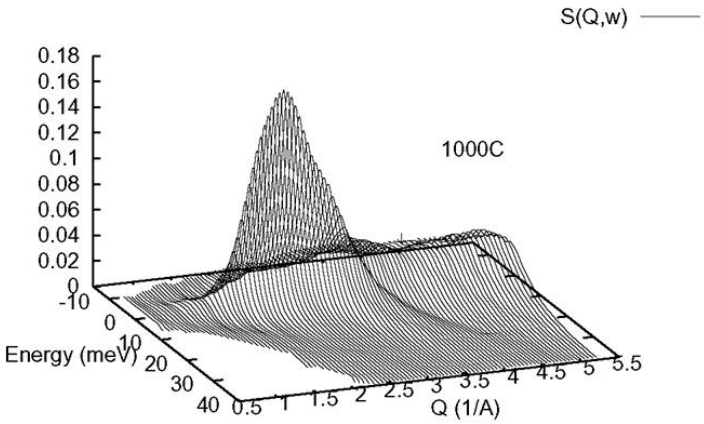


Liquid Ge (r=0.5cm, d=5cm)	
Mean free path	2.0985 cm
Single scattering	82.81%
Double scattering	15.15%
Multiple scattering	17.18%

Case of liquid Ge

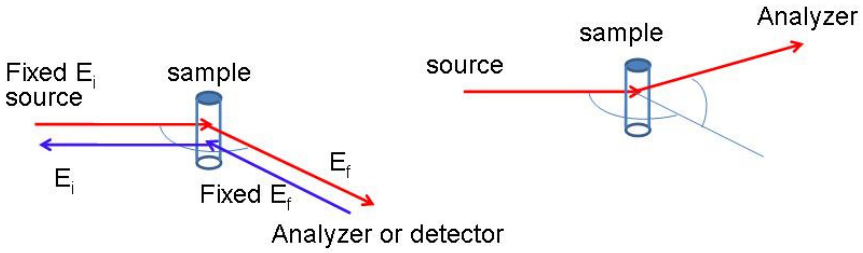


Case of liquid Ge



Monte Carlo simulation MSCAT85

Software generates 1000 neutrons injected to the sample at first and simulates elastic and inelastic scattering process. In further run, it simulates only elastic component instead of the full calculation and automatically attaches inelastic part using the results of the first run.



All code assumes a fixed single energy of incident neutron.
We need a new code to calculate multiple scattering for BS instruments, because of geometrically asymmetry .

Iteration

Predictor function of S(Q,E) including single scattering

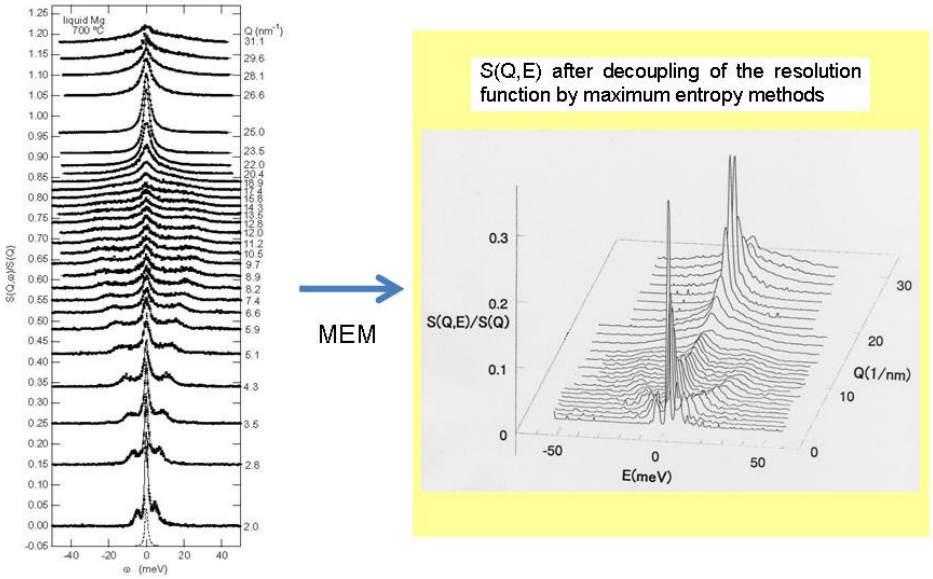
Calculate or simulate multiple scattering contribution

Compare the observed S(Q,E) and calculated one

Taking into account the deviation, new function of single S(Q,E)

This process perhaps can include absorption correction.

Decoupling of energy resolution function using by MEM



N. Takahashi, et al., J. Phys. Chem. Sol. (2007)

III. *moderator* possibilities; 2. expected performances

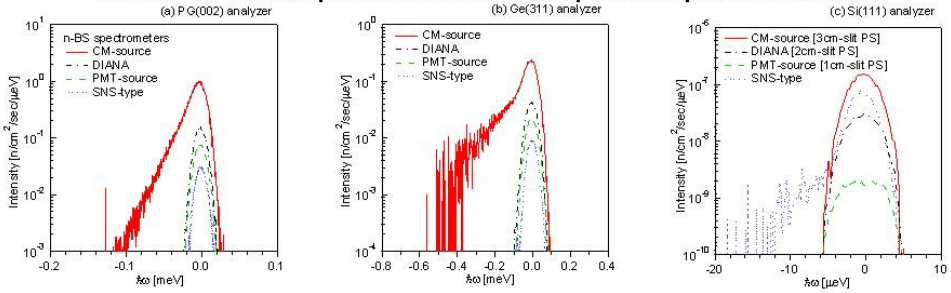


Fig. E-resolution of PG analyzer　Fig. E-resolution of Ge analyzer　Fig. E-resolution of Si analyzer

Table: performance comparisons

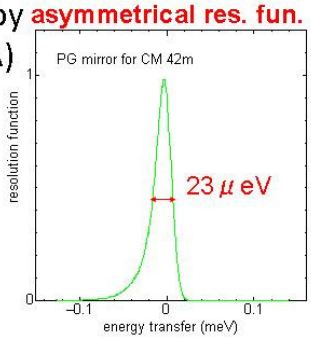
source (name of n-BS)	L_1 [m]	main guide section	analyzer	E_{ef} [meV]	$\hbar\omega$-range (one frame) [meV]	slit-width of PS [cm]	$\Delta\lambda$ [Å]	$\Delta\hbar\omega$ [μeV]	sample-position intensity at E_{ef} [10⁴ n/cm²/μeV/sec]	merit	demerit
★CM (CM-source)	42	curved w60xh98 R2200m	PG (002)	1.87	$-0.3 < \hbar\omega < 4.3$	-	3.6	23	160	×5 ~ 9 intensity (PG, Ge, SI [PS])	30 ~ 35 % worse resolution (PG, Ge)
			Ge (311)	7.25	$-1.1 < \hbar\omega < E^*$	-	3.6	82	66	21 % better resolution (SI [PS])	asymmetric resolution function (PG, Ge)
			SI(111)	2.09	± 0.04 [PS]	3	3.6	3.8	7.1	×3 wider band (SI [PS])	
DM (DIANA)	32	curved w46xh98 R1650m	PG (002)	1.87	$-1.0 < \hbar\omega < 1.8$	-	4.7	17	17		
			Ge (311)	7.25	$-3.6 < \hbar\omega < E^*$	-	4.7	63	7.4		
			SI(111)	2.09	± 0.014 [PS]	2	4.6	4.8	1.4		
PMT (PMT-source)	21.5	straight + T0-chopper w98xh98 0.5m-gap for T0-chopper	PG (002)	1.87	$-0.2 < \hbar\omega$	-	6.9	17	8.6	wide band (PG, Ge)	×1/2 intensity (PG, Ge)
			Ge (311)	7.25	$-5.5 < \hbar\omega$	-	6.9	64	4.1		×1/7 intensity (SI [PS])
			SI(111)	2.09	± 0.014 [PS]	1	6.7	6.2	0.20		
PMt (SNS-type)	84	curved w60xh98 R2200m	PG (002)	1.87	$-0.4 < \hbar\omega < 0.8$	-	1.9	15	3.2	10 ~ 12 % better resolution (PG, Ge)	×1/5 intensity (PG, Ge)
			Ge (311)	7.25	$-1.3 < \hbar\omega < 17$	-	1.9	57	1.5	×2 intensity (Si)	narrow band (PG, Ge)
			SI(111)	2.09	$-0.6 < \hbar\omega < 0.6$	-	1.8	3.6	2.7	×3 wider band (Si)	

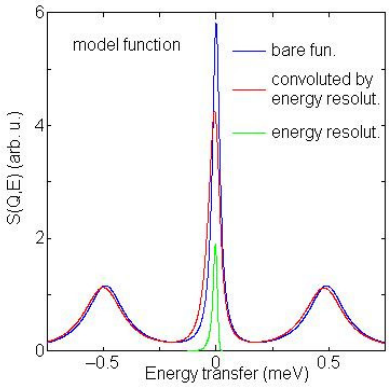
Curved guide: E^* = 40 meV

De-convolution of energy resolution function by asymmetrical res. fun.
Maximum entropy method (PG mirror for DNA)

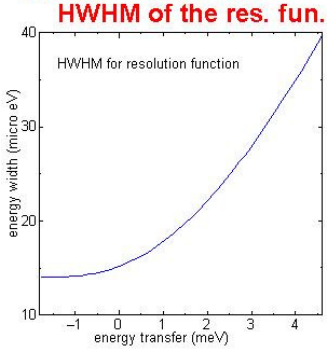
Model function

center FWHM 20 μeV relative intensity 0.5
excitation FWHM 100 μeV relative intensity 0.5
excitation energy ± 500 μeV





Energy dependence of HWHM of the res. fun.

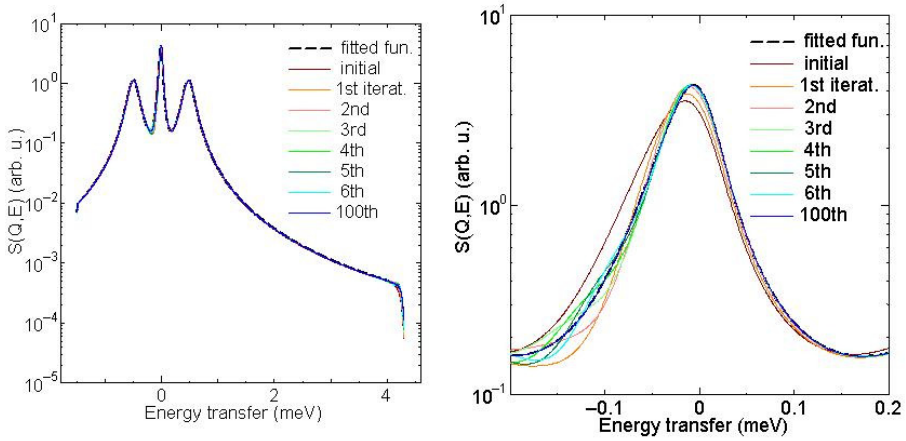


MEM results for PG mirror

We propose that a experimental data should be used as a initial function. easy & convenient for users

Initial fun. = observed data ⊗resolution fun.

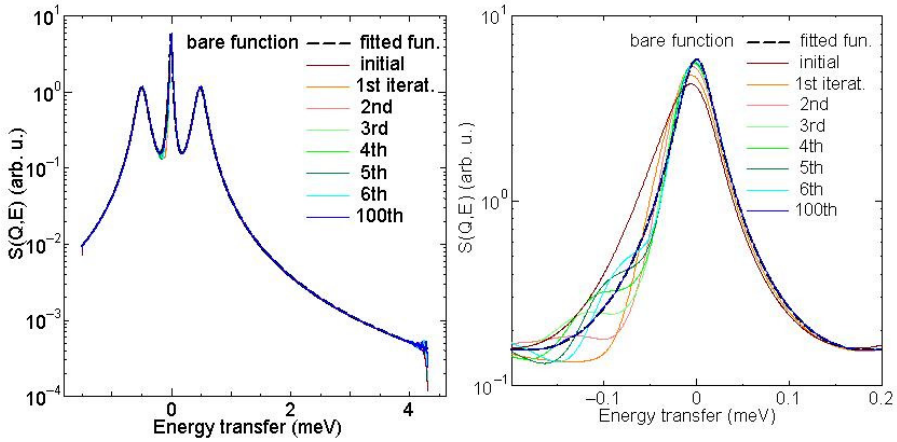
Logarithmic scale



reproduce well even a tail part with lowest intensity

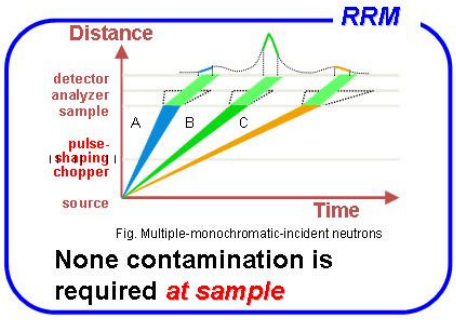
MEM results for PG mirror

Bare function without convolution of res. fun.
Logarithmic scale



almost perfect reproduction
by a hundred of iterations in MEM procedure

Resolution decoupling for Si analyzer ?



Resolution function of Si analyzer has a quite good symmetrical shape.
Decoupling of resolution function for Si analyzer is much easier than for PG.

In RRM (Repetition Rate Multiplication) mode, each energy range has a different energy resolution. Resolution decoupling still can be a powerful tool to compare different scattering regimes.

4. Summary
International Advisory Committee (Chair: Dan Neumann)

4. Summary

IAC

DNA will be a world-leading instrument for the study of ns dynamics using neutron scattering

The work since the last meeting is excellent and should lead to a high resolution spectrometer with an energy resolution of ~1 μeV.

The current layout is imaginative and well-considered. The performance will be excellent with the ability to trade resolution for intensity. The RRM scheme would be the first of a kind and we believe it should work well.

The current design will be expensive to realize, but we see no way to significantly reduce the cost without compromising performance.

Comments on Instrument Layout

1. Choice of coupled moderator is excellent.
2. Guide design has improved from last time. We encourage you to continue your efforts to optimize the coatings for cost savings.
3. The RRM chopper set-up is very good.
   a) More detailed analysis of the precision of positioning and phasing would be helpful.
   b) Develop a scheme for "evening" out the "monitor" in the RRM mode.
4. We were pleased to see that considerable effort has went into optimizing the size of the sample area. The diameter of 40 cm adds considerable flexibility for sample environments. Please keep in mind the ability to align single crystal samples.

Comments on Instrument Layout

4. Analyzer design for Si (111) is good. Some issues:
   a) The thickness of the Si (111) crystals might need to be increased slightly to account for strain relief at the edges of the crystals
   b) The same care needs to be applied to Si(311) as to Si (111)
   c) Absorber backing needs to be established to achieve the ambitious goal of 10,000 to 1 signal to noise (which would allow qualitatively new science.
5. Choice of 1-d position sensitive detectors is appropriate.
6. Data acquisition system is the MLF standard.

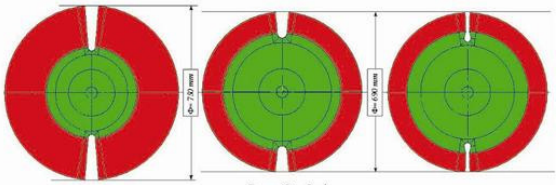
Appendix A - Disc choppers of IN5
courtesy of J. Ollivier & IN5 project Team (ILL)

Appendix; Disc choppers of IN5

2 SPECIFICATIONS

DISKS	1 and 2	3 and 4	5 and 6
Diameter (mm)	750	690	690
Windows angular aperture (°)	9	9.5	3.25
Beam height (mm)	170	82	72
Gd_2O_3 height (mm)	180	92	82
Useful window height (mm)	180	92	82
Fillet radius (mm)	15	20	15
Total window height with fillet (mm)	195	112	127
Maximum peripherical linear speed	668 $m.s^{-1}$	614 $m.s^{-1}$	614 $m.s^{-1}$

Operating speed : 7000/17000 rpm
2 windows per disk

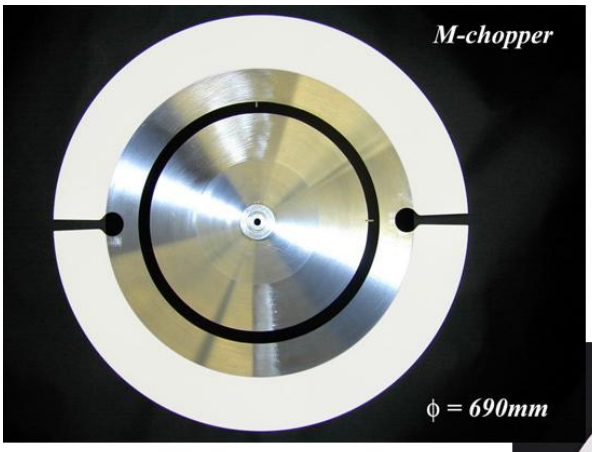


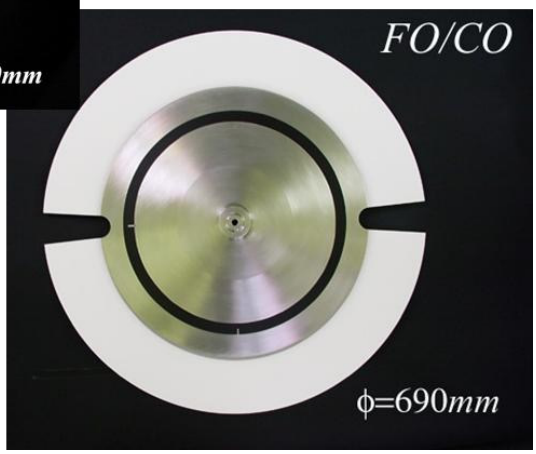
Pulsing choppers Disks 1 and 2 | *Frame Overlap/ Contaminant Order choppers Disks 3 and 4* | *Monochromating choppers Disks 5 and 6*

3 CHOICE OF MATERIAL AND BEHAVIOUR LAW

3.1 STRUCTURAL MATERIAL = ALUMOLD

- Chemical composition : Zn 6% Mg 2.4% Cu 1.6%





国際単位系（SI）

表１．SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd

表２．基本単位を用いて表されるSI組立単位の例

組立量	SI 基本単位	
	名称	記号
面積	平方メートル	m^2
体積	立法メートル	m^3
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s^2
波数	毎メートル	m^{-1}
密度，質量密度	キログラム毎立方メートル	kg/m^3
面積密度	キログラム毎平方メートル	kg/m^2
比体積	立方メートル毎キログラム	m^3/kg
電流密度	アンペア毎平方メートル	A/m^2
磁界の強さ	アンペア毎メートル	A/m
量濃度[(a)]，濃度	モル毎立方メートル	mol/m^3
質量濃度	キログラム毎立法メートル	kg/m^3
輝度	カンデラ毎平方メートル	cd/m^2
屈折率[(b)]	（数字の） 1	1
比透磁率[(b)]	（数字の） 1	1

(a) 量濃度（amount concentration）は臨床化学の分野では物質濃度（substance concentration）ともよばれる。
(b) これらは無次元量あるいは次元１をもつ量であるが、そのことを表す単位記号である数字の１は通常は表記しない。

表３．固有の名称と記号で表されるSI組立単位

組立量	SI 組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン[(b)]	rad	1[(b)]	m/m
立体角	ステラジアン[(b)]	sr[(c)]	1[(b)]	m^2/m^2
周波数	ヘルツ[(d)]	Hz		s^{-1}
力	ニュートン	N		m kg s^{-2}
圧力，応力	パスカル	Pa	N/m^2	m^{-1} kg s^{-2}
エネルギー，仕事，熱量	ジュール	J	N m	m^2 kg s^{-2}
仕事率，工率，放射束	ワット	W	J/s	m^2 kg s^{-3}
電荷，電気量	クーロン	C		s A
電位差（電圧），起電力	ボルト	V	W/A	m^2 kg s^{-3} A^{-1}
静電容量	ファラド	F	C/V	m^{-2} kg^{-1} s^4 A^2
電気抵抗	オーム	Ω	V/A	m^2 kg s^{-3} A^{-2}
コンダクタンス	ジーメンス	S	A/V	m^{-2} kg^{-1} s^3 A^2
磁束	ウエーバ	Wb	Vs	m^2 kg s^{-2} A^{-1}
磁束密度	テスラ	T	Wb/m^2	kg s^{-2} A^{-1}
インダクタンス	ヘンリー	H	Wb/A	m^2 kg s^{-2} A^{-2}
セルシウス温度	セルシウス度[(e)]	℃		K
光束	ルーメン	lm	cd sr[(c)]	cd
照度	ルクス	lx	lm/m^2	m^{-2} cd
放射性核種の放射能[(f)]	ベクレル[(d)]	Bq		s^{-1}
吸収線量，比エネルギー分与，カーマ	グレイ	Gy	J/kg	m^2 s^{-2}
線量当量，周辺線量当量，方向性線量当量，個人線量当量	シーベルト[(g)]	Sv	J/kg	m^2 s^{-2}
酸素活性	カタール	kat		s^{-1} mol

(a)SI接頭語は固有の名称と記号を持つ組立単位と組み合わせても使用できる。しかし接頭語を付した単位はもはやコヒーレントではない。
(b)ラジアンとステラジアンは数字の１に対する単位の特別な名称で、量についての情報をつたえるために使われる。実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号である数字の１は明示されない。
(c)測光学ではステラジアンという名称と記号srを単位の表し方の中に、そのまま維持している。
(d)ヘルツは周期現象についてのみ、ベクレルは放射性核種の統計的過程についてのみ使用される。
(e)セルシウス度はケルビンの特別な名称で、セルシウス温度を表すために使用される。セルシウス度とケルビンの単位の大きさは同一である。したがって、温度差や温度間隔を表す数値はどちらの単位で表しても同じである。
(f)放射性核種の放射能（activity referred to a radionuclide）は、しばしば誤った用語で"radioactivity"と記される。
(g)単位シーベルト（PV,2002,70,205）についてはCIPM勧告2（CI-2002）を参照。

表４．単位の中に固有の名称と記号を含むSI組立単位の例

組立量	SI 組立単位		
	名称	記号	SI 基本単位による表し方
粘度	パスカル秒	Pa s	m^{-1} kg s^{-1}
力のモーメント	ニュートンメートル	N m	m^2 kg s^{-2}
表面張力	ニュートン毎メートル	N/m	kg s^{-2}
角速度	ラジアン毎秒	rad/s	m m^{-1} s^{-1}=s^{-1}
角加速度	ラジアン毎秒毎秒	rad/s^2	m m^{-1} s^{-2}=s^{-2}
熱流密度，放射照度	ワット毎平方メートル	W/m^2	kg s^{-3}
熱容量，エントロピー	ジュール毎ケルビン	J/K	m^2 kg s^{-2} K^{-1}
比熱容量，比エントロピー	ジュール毎キログラム毎ケルビン	J/(kg K)	m^2 s^{-2} K^{-1}
比エネルギー	ジュール毎キログラム	J/kg	m^2 s^{-2}
熱伝導率	ワット毎メートル毎ケルビン	W/(m K)	m kg s^{-3} K^{-1}
体積エネルギー	ジュール毎立方メートル	J/m^3	m^{-1} kg s^{-2}
電界の強さ	ボルト毎メートル	V/m	m kg s^{-3} A^{-1}
電荷密度	クーロン毎立方メートル	C/m^3	m^{-3} sA
表面電荷	クーロン毎平方メートル	C/m^2	m^{-2} sA
電束密度，電気変位	クーロン毎平方メートル	C/m^2	m^{-2} sA
誘電率	ファラド毎メートル	F/m	m^{-3} kg^{-1} s^4 A^2
透磁率	ヘンリー毎メートル	H/m	m kg s^{-2} A^{-2}
モルエネルギー	ジュール毎モル	J/mol	m^2 kg s^{-2} mol^{-1}
モルエントロピー，モル熱容量	ジュール毎モル毎ケルビン	J/(mol K)	m^2 kg s^{-2} K^{-1} mol^{-1}
照射線量（X線及びγ線）	クーロン毎キログラム	C/kg	kg^{-1} sA
吸収線量率	グレイ毎秒	Gy/s	m^2 s^{-3}
放射強度	ワット毎ステラジアン	W/sr	m^4 m^{-2} kg s^{-3}=m^2 kg s^{-3}
放射輝度	ワット毎平方メートル毎ステラジアン	W/(m^2 sr)	m^2 m^{-2} kg s^{-3}=kg s^{-3}
酵素活性濃度	カタール毎立方メートル	kat/m^3	m^{-3} s^{-1} mol

表５．SI 接頭語

乗数	接頭語	記号	乗数	接頭語	記号
10^{24}	ヨタ	Y	10^{-1}	デシ	d
10^{21}	ゼタ	Z	10^{-2}	センチ	c
10^{18}	エクサ	E	10^{-3}	ミリ	m
10^{15}	ペタ	P	10^{-6}	マイクロ	μ
10^{12}	テラ	T	10^{-9}	ナノ	n
10^{9}	ギガ	G	10^{-12}	ピコ	p
10^{6}	メガ	M	10^{-15}	フェムト	f
10^{3}	キロ	k	10^{-18}	アト	a
10^{2}	ヘクト	h	10^{-21}	ゼプト	z
10^{1}	デカ	da	10^{-24}	ヨクト	y

表６．SIに属さないが、SIと併用される単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h =60 min=3600 s
日	d	1 d=24 h=86 400 s
度	°	1°=(π/180) rad
分	’	1’=(1/60)°=(π/10800) rad
秒	”	1”=(1/60)’=(π/648000) rad
ヘクタール	ha	$1ha=1hm^2=10^4m^2$
リットル	L，l	$1L=11=1dm^3=10^3cm^3=10^{-3}m^3$
トン	t	$1t=10^3$ kg

表７．SIに属さないが、SIと併用される単位で、SI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位で表される数値
電子ボルト	eV	$1eV=1.602\ 176\ 53(14)\times10^{-19}J$
ダルトン	Da	$1Da=1.660\ 538\ 86(28)\times10^{-27}kg$
統一原子質量単位	u	1u=1 Da
天文単位	ua	$1ua=1.495\ 978\ 706\ 91(6)\times10^{11}m$

表８．SIに属さないが、SIと併用されるその他の単位

名称	記号	SI 単位で表される数値
バール	bar	$1 bar=0.1MPa=100kPa=10^5Pa$
水銀柱ミリメートル	mmHg	1mmHg=133.322Pa
オングストローム	Å	$1 Å=0.1nm=100pm=10^{-10}m$
海里	M	1 M=1852m
バーン	b	$1 b=100fm^2=(10^{-12}cm)2=10^{-28}m^2$
ノット	kn	1 kn=(1852/3600)m/s
ネーパ	Np	SI単位との数値的な関係は、対数量の定義に依存。
ベル	B	
デジベル	dB	

表９．固有の名称をもつCGS組立単位

名称	記号	SI 単位で表される数値
エルグ	erg	$1 erg=10^{-7}$ J
ダイン	dyn	$1 dyn=10^{-5}$N
ポアズ	P	$1 P=1 dyn\ s\ cm^{-2}=0.1Pa\ s$
ストークス	St	$1 St=1cm^2\ s^{-1}=10^{-4}m^2\ s^{-1}$
スチルブ	sb	$1 sb=1cd\ cm^{-2}=10^4cd\ m^{-2}$
フォト	ph	$1 ph=1cd\ sr\ cm^{-2}\ 10^4lx$
ガル	Gal	$1 Gal=1cm\ s^{-2}=10^{-2}ms^{-2}$
マクスウェル	Mx	$1 Mx = 1G\ cm^2=10^{-8}Wb$
ガウス	G	$1 G=1Mx\ cm^{-2}=10^{-4}T$
エルステッド[(c)]	Oe	$1 Oe \triangleq (10^3/4\pi)A\ m^{-1}$

(c) ３元系のCGS単位系とSIでは直接比較できないため、等号「 ≙ 」は対応関係を示すものである。

表10．SIに属さないその他の単位の例

名称	記号	SI 単位で表される数値
キュリー	Ci	$1 Ci=3.7\times10^{10}Bq$
レントゲン	R	$1 R = 2.58\times10^{-4}C/kg$
ラド	rad	$1 rad=1cGy=10^{-2}Gy$
レム	rem	$1 rem=1 cSv=10^{-2}Sv$
ガンマ	γ	1γ=1 nT=10-9T
フェルミ		1フェルミ=1 fm=10-15m
メートル系カラット		1メートル系カラット = 200 mg = 2×10-4kg
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリー	cal	1cal=4.1858J（「15℃」カロリー），4.1868J（「IT」カロリー）4.184J（「熱化学」カロリー）
ミクロン	μ	1 μ =1μm=10^{-6}m

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