

**Proceedings of the International Advisory Committee on
“Biomolecular Dynamics Instrument DNA” and the
Workshop on “Biomolecular Dynamics Backscattering
Spectrometers” February 27-29, 2008, J-PARC Center,
Japan Atomic Energy Agency Tokai, Ibaraki, Japan**

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Japan Atomic Energy Agency

日本原子力研究開発機構

JAEA-Review

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Proceedings of the International Advisory Committee on
“Biomolecular Dynamics Instrument DNA”

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“Biomolecular Dynamics Backscattering Spectrometers”

February 27-29, 2008, J-PARC Center, Japan Atomic Energy Agency
Tokai, Ibaraki, Japan

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A workshop entitled “Biomolecular Dynamics Backscattering Spectrometers” was held on February 27th - 29th, 2008 at J-PARC Center, Japan Atomic Energy Agency. This workshop was planned to be held for aiming to realize an innovative neutron backscattering instrument, namely DNA, in the MLF and thus four leading scientists in the field of neutron backscattering instruments were invited as the International Advisory Committee (IAC member: Dr. Dan Neumann (Chair); Prof. Ferenc Mezei; Dr. Hannu Mutka; Dr. Philip Tregenna-Piggott) for DNA from institutes in the United States, France and Switzerland, where backscattering instruments are in-service. It was therefore held in the form of lecture anterior and then in the form of the committee posterior.

This report includes the executive summary of the IAC and materials of the presentations in the IAC and the workshop.

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

国際アドバイザリ委員会
「ダイナミクス解析装置 DNA」

および

J-PARC/MLF 中性子散乱実験装置ワークショップ
「生命科学分子動力学研究のための背面反射型分光器」
講演集

2008 年 2 月 27 日～29 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

(2008 年 5 月 16 日受理)

2008 年 2 月 27 日～29 日に日本原子力研究開発機構 J-PARC センターにおいて、「生命科学分子動力学研究のための背面反射型分光器」に関するワークショップが開催された。本ワークショップは、J-PARC/MLF に建設が計画されている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、米国・フランス・スイスの三国において稼働中の同型の実験装置（背面反射型分光器）に造詣の深い著名な 4 名の研究者を国際アドバイザリ委員（委員：Dan Neumann 博士（委員長）；Ferenc Mezei 教授；Hannu Mutka 博士；Philip Tregenna-Piggott 博士）として招聘し、前半を講演形式、後半を委員会形式で開催された。

本報告書は、国際アドバイザリ委員会の要旨、および委員会・ワークショップで使用された発表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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柴田 薫（原子力機構）、高橋 伸明（原子力機構）、川北 至信（九州大）、佐藤 卓（東京大）

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Group photo



Group photo of the workshop on Biomolecular Dynamics Backscattering Spectrometers held at HENDEL BLDG., JAEA on Feb. 27-29, 2008.

Agenda

J-PARC Workshop on Biomolecular Dynamics Backscattering Spectrometers

Japan Atomic Energy Agency, Tokai Research & Development Center, Tokai, Naka, Ibaraki, JAPAN

February 27-29, 2008

Place: HENDEL BLDG, room310 (3F)

Wednesday, February 27, 2008

09:30 – 09:35	Opening Remark	Masatoshi Arai (JAEA)
09:35 – 09:50	Present Status of J-PARC Neutron Facility	Kazuya Aizawa (JAEA)
09:50 – 10:05	Inelastic Spectrometers at J-PARC	Kenji Nakajima (JAEA)
10:05 – 10:20	Required Spectrometer Specification from Biomolecular Dynamics Studies	Hiroshi Nakagawa (JAEA)
10:20 – 10:50	The Backscattering Spectrometer at NIST	Dan Neumann (NIST)
10:50 – 11:00	Coffee Break	
11:00 – 11:30	The New Spectrometer MARS at PSI	Philip Tregenna-Piggott (PSI)
11:30 – 12:00	Backscattering Spectrometers at ILL	Hannu Mutka (ILL)
12:00 – 13:30	Lunch	
13:30 – 17:45	The J-PARC BS Spectrometer DNA Several times of coffee breaks will be included	DNA construction team
17:45 – 18:00	Issues for homework from the advisory committee	
19:00 – 21:00	Buffet party	

Thursday, February 28, 2008

09:30 – 09:50	R&D at J-PARC	Kazuhiko Soyama (JAEA)
09:50 – 10:10	DAQ and software developments at J-PARC	Takeshi Nakatani (JAEA)
10:10 – 12:00	Answers to the issues	DNA construction team
12:00 – 13:30	Lunch	
13:30 – 15:30	Closed meeting of the advisory committee	Advisory committee
15:30 – 16:00	Advice from the advisory committee	Dan Neumann (NIST)
16:00 – 17:50	Preparing report	Advisory committee
17:50 – 18:00	Receiving the report and closing remark	Masatoshi Arai (JAEA)
19:00	Dinner	

Friday, February 29, 2008

09:30 – 12:30	J-PARC + JRR-3 tour	
13:30 – 18:00	Preparing report	Advisory committee

List of attendees

<u>Name</u>	<u>Affiliation</u>
Dan Neumann, chair	NIST
Feri Mezei, member	LANL and BNC
Hannu Mutka, member	ILL
Philip Tregenna-Piggott, member	PSI
Kaoru Shibata	J-PARC, JAEA
Nobuaki Takahashi	J-PARC, JAEA
Yukinobu Kawakita,	Kyushu University
Taku J. Sato,	Univ. of Tokyo
Hiroshi Nakagawa,	QuBS, JAEA
Satoru Fujiwara	QuBS, JAEA
Masatoshi Arai	J-PARC, JAEA
Kazuya Aizawa	J-PARC, JAEA
Kenji Nakajima	J-PARC, JAEA
Kazuhiko Soyama	J-PARC, JAEA
Takeshi Nakatani	J-PARC, JAEA
Mitsutaka Nakamura	J-PARC, JAEA
Yasuhiro Inamura	J-PARC, JAEA
Naohito Metoki	ASRC, JAEA
Kazuhisa Kakurai	QuBS, JAEA
Dai Yamazaki	J-PARC, JAEA
Kentaro Suzuya	J-PARC, JAEA
Shinichi Takata	J-PARC, JAEA

1. Executive Summary of the International Advisory Committee

International Advisory Committee (Chair: Dan Neumann)

Overview

The DNA 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, DNA 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 novel states of matter and quantum phase transitions in unprecedented detail. Finally scientists will gain new insights into the behavior of materials on the nanoscale.

DNA is an inverted geometry instrument consisting of a pre-sample flight path using an advanced neutron guide design with a pulse-shaping chopper and a large area crystal analyzer system. The DNA team presented a design consisting of four analyzer systems in two evacuated 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 ever 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 DNA is the dynamics of proteins and polymers. Experience at ILL and NIST indicates that backscattering instruments with 1 μeV tend to have approximately $\frac{1}{2}$ 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 appendices.)
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 wavelength to reach an energy resolution of 4 μeV .
4. The Si(111) option will provide a resolution of 17 μeV by stopping the pulse shaping chopper. Our estimate, based on the calculations presented by the DNA 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 tandem design results in a

calculated loss of 30% to 40%, which can be restored 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 (311) 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. IN16 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 time 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 rest of the report deals primarily with components of DNA.

1. Moderator

The choice of the coupled cold moderator for a high resolution spectrometer is an innovative and very advantageous solution. The coupled moderator, in particular with the special pre-moderator concept at J-PARC provides much higher peak flux than de-coupled moderators. Pulse shaping allows one to take advantage of the higher peak flux and also secure perfect symmetric pulse shapes with sharp edges. This advantageous pulse shape enhances the data collection rate compared to the common, exponentially decaying decoupled moderator line shapes at equal resolution. For DNA the length of the coupled moderator pulses is sufficient to achieve $\pm 40 \mu\text{eV}$ scan dynamic range, which is adequate for the instrumental resolution of about 4 μeV . The combination of the coupled moderator and pulse shaping choppers also opens up the possibility to maximize the intensity (albeit at the expense of resolution and a degraded line shape) by selecting lower chopper speeds or by stopping the chopper all together. This flexibility to trade intensity for resolution and vice versa to best meet the requirements of each experiment is an important advantage of the use of pulses from coupled moderators. This novel opportunity for pulsed sources is fully taken advantage of in the DNA instrument project.

The DNA team also introduced an innovative enhancement for the use of pulse shaping choppers for instruments on coupled moderators or long pulse sources: the generalization of the repetition rate multiplication (RRM) technique to inverted geometry spectrometers. By this new method up to 8 shaped pulses can be extracted for simultaneous data collection from each source pulse, instead of just one. Each pulse covers a different incoming neutron energy range. The new method accelerates 8 fold the data collection in a particular class of experiments, when the scattering spectrum is explored over a broader energy range by scanning the incoming energy window with the help of shifting or slewing the phasing of the pulse shaping chopper. The first implementation of this technique will be a particular strength of this

instrument.

Overall, the innovative design of DNA allows it to fully exploit the characteristics of the coupled, cold moderator at J-PARC opening up the opportunity to utilize the pulsed source power with unprecedented efficiency and will make this instrument the best in its class worldwide.

2. Guides

Advanced supermirror neutron guide systems allow us to deliver a higher fraction of the neutrons emitted by the moderator to the sample. The DNA design takes advantage of these capabilities. In the vertical plane the elliptic shape of the guide employs the ballistic beam delivery concept. The large beam cross section over most of the guide lowers the number of reflections and keeps the reflection angles small thereby reducing reflection losses. The compression of the large cross section beam to the smaller sample area enhances the flux at the expense of higher beam divergence. In the horizontal plane the guide design is governed by the need to filter out fast neutrons and to provide for short chopper pulses. A fine-tuning of the guide design, in particular in the horizontal plane, might result in a small additional gain in flux. J-PARC is a world leader in the development of very high cut-off angle supermirrors, and this could be used to good advantage at DNA by employing these supermirrors at the few critical locations in the focussing guide in order to optimize the focussing features of the guide system.

The concept of having two sample positions one behind the other with guides focussing on both sample positions would incur substantial beam intensity losses at the downstream sample position. The Committee recommends that the Si(111) analyzer option should have an optimized, no-compromise neutron guide providing the highest possible flux on the sample for this option. This requires examining alternative mechanical solutions which avoid focussing the beam twice along the beam line. This will be straightforward to realize in the recommended staged implementation of the instrument, in which only the Si (111) analyzer chamber is built in the first stage.

3. Choppers

Few technical details were presented concerning the DNA choppers. Therefore we assume that the DNA team expects no difficulties in the production and/or procurement of these items. We note that choppers are needed on most of the instruments and therefore the Committee doesn't foresee any potential problems in this area.

4. Sample Area

The sample flange for DNA is only 25 cm. This is not particularly surprising as the requirement of approaching a scattering angle of 180° from the analyzer necessitates having the detectors near the sample position. Thus backscattering instruments such as DNA tend to have more compact sample areas than other instruments. However, the proposed sample area is considerably smaller than the J-PARC standard of 40 cm. Moreover it is almost certainly too small to mount a high-field superconducting magnet or a very high pressure device. The desirability of having as many sample environments as possible on DNA

means that any deviation from the sample area standard should be very carefully considered. Thus we encourage the DNA team to lay out the performance (by this we primarily mean resolution) consequences of matching the J-PARC standard. If it is determined that DNA won't have a resolution of 4 μeV or better with the larger sample area, then we believe the sample area standard should be relaxed for DNA.

The DNA team should consider providing for the alignment of single crystal samples. Rotation of the sample can be provided via the sample stick as is being done at other facilities. However, tilting the sample may require some type of external device. Note that the arcs only have to move a few degrees as users typically bring their samples well-aligned. This would be a unique capability to DNA and J-PARC.

5. Analyzer

The Committee appreciated the imaginative and elegant work concerning the time and space focusing optics of the analyzer banks. This is a truly original contribution to the neutron scattering community. The analytical calculations and simulation work have provided a solid base for optimizing the analyzer design. The use of position sensitive detectors alleviates the drawback of not applying the full focusing operation for the Si(111) option and accordingly we can state that analyzer design for Si (111) is good. In our opinion Si (311) provides a good option to extend the Q-range.

6. Detectors

The Committee fully endorses the proposed use of position-sensitive, 16 mm diameter ^3He 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. Note that the possible expansion of the sample area would involve moving the detectors and thus some of these issues may need to be revisited.

The Committee was also pleased by the provision of diffraction detectors which can be very useful to monitor the sample. Since the bandwidth for Si (111) is quite small, the simultaneous measurement of inelastic scattering and diffraction would require 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. Scattering chamber

The analyzer system will be mounted inside an evacuated scattering chamber. This option is now standard practice for time-of-flight instruments. The Committee believes that the proposed evacuated scattering chamber is the best choice for DNA serving to reduce the background and avoid losses at long wavelengths. The Committee notes that its recommendation to give the highest priority to the Si(111) option means building a single chamber. This will not only substantially reduce the cost of the instrument, but will also result reduce the construction time, allowing DNA to produce science more quickly.

8. Data acquisition

The event recording approach is an excellent choice for DNA. (In high energy physics, where it has long been the standard data acquisition method, it is known as “list mode” data collection.) In particular, it provides great flexibility and is sufficiently robust to efficiently handle the complexities of this highly sophisticated instrument. The standard data acquisition of the MFL facility will be employed. Thus the Committee does not foresee any problems in this area.

9. Data Analysis

The DNA team is already considering how they will analyze the data that DNA produces. This is particularly commendable since software is an afterthought in most instrument development projects around the world. The forethought given to the primary resolution function and how one can deconvolute the resolution from $S(Q, \omega)$ using maximum entropy is equally commendable. The time invested to this problem will ensure that the most science is obtained from the data. It is also highly commendable that work has already begun on user-friendly software to visualize and reduce the data. It is a pity that the international collaboration foreseen in this endeavor between the facilities of J-PARC, the NCNR and ISIS came to nothing. Nevertheless we recommend that the following principle be maintained: the source code should be freely available and written in a transparent way such that the user can see how the raw data is transformed to the scattering function. The topic of data reduction on inverted-geometry TOF instruments is a contentious, non-trivial issue. (See B. Dorner, *J. Neutron Res.* **13**, 267 (2005); P.L.W. Tregenna-Piggott *et al.*, *J. Neutron Res.* (submitted)).

Cost and Schedule

The instrument design is not mature enough to have a reliable cost estimate. The schedule for completion in 2010 is quite optimistic, particularly in light of the fact that construction funding is not in hand.

Acknowledgements

The committee would like to extend their gratitude to the DNA team for their clear, carefully prepared presentations that demonstrated an excellent grasp of topics spanning neutron instrumentation, biology and computer science. We have every confidence that the pride and motivation that they evidently feel for their work will result in the realization of the premier inverted-geometry TOF instrument that will be available to the Japanese scientific community. We emphasize that the discussions were of great benefit to the committee members, and we eagerly anticipate the next meeting.

2. Proceedings of the International Advisory Committee
2.1. General Review of the BS Spectrometer DNA at J-PARC
Kaoru Shibata (JAEA)

DNA-IAC:2008. 02. 27. @HENDEL 310

J-PARC Workshop
on
Backscattering Spectrometers
DNA
[The DNA Advisory Meeting]

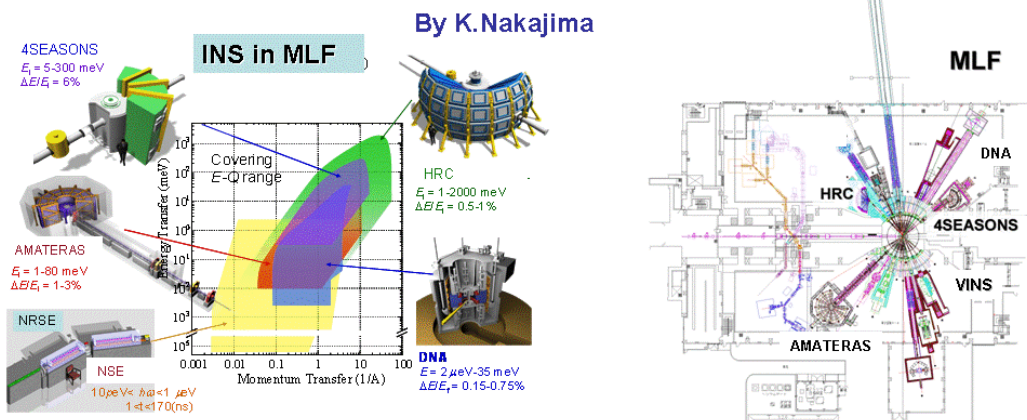
Japan Atomic Energy Agency, Tokai Research &
Development Center, Tokai, Naka, Ibaraki, JAPAN
February 27-29, 2008

0.General Review by K.Shibata (J-PARC)

Outline

0.General Review

- 0.1 About J-PARC, MLF, DNA
- 0.2 Back Ground of Development
- 0.3 Neutron Sources, E – Resolutions and MEM
- 0.4 Analyzer Mirror, Transport System and Scattering Vessel
- 0.5 Device Development
- 0.6 Schedule and Cost
- 0.7 DNA Proposal Group



Pulsed-source in MLF at J-PARC

MLF/J-PARC will have 4 kinds of pulsed neutron sources

Liq.H₂ Coupled Moderator (ϕ 15 cm x 10^H cm) : CM

Liq.H₂ Decoupled Moderator (13^W x 12^H x 6.2^T cm³) : DM

(Liq.H₂, Poisoned Decoupled Moderator thin side (13^W x 12^H x 2.5/(6.2)^T cm³) : PM-thick

Liq.H, Poisoned Decoupled Moderator thick side ($13^W \times 12^H \times 3.7/(6.2)^T$ cm³) : PIV-thin

The world n-BS spectrometers

IRIS, OSIRIS @ ISIS: source = DM, L1 = 36.4, 34 m
Si n-BS (BASIS) @ SNS:

Si n-BS (BASIS) @ SNS:

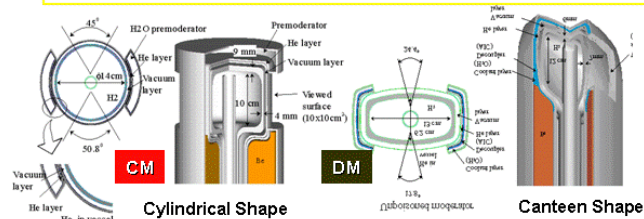
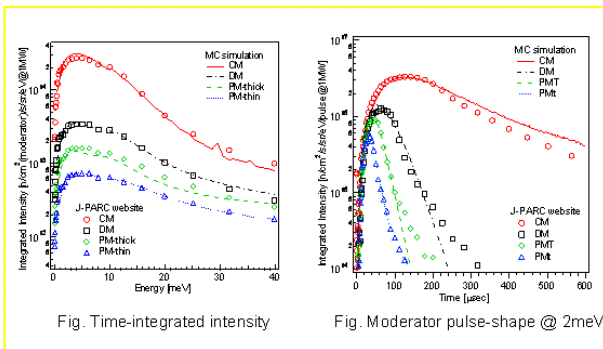
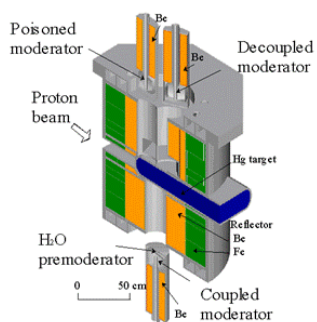
source = poisoned moderator (PM), L1 = 84 m

Question:

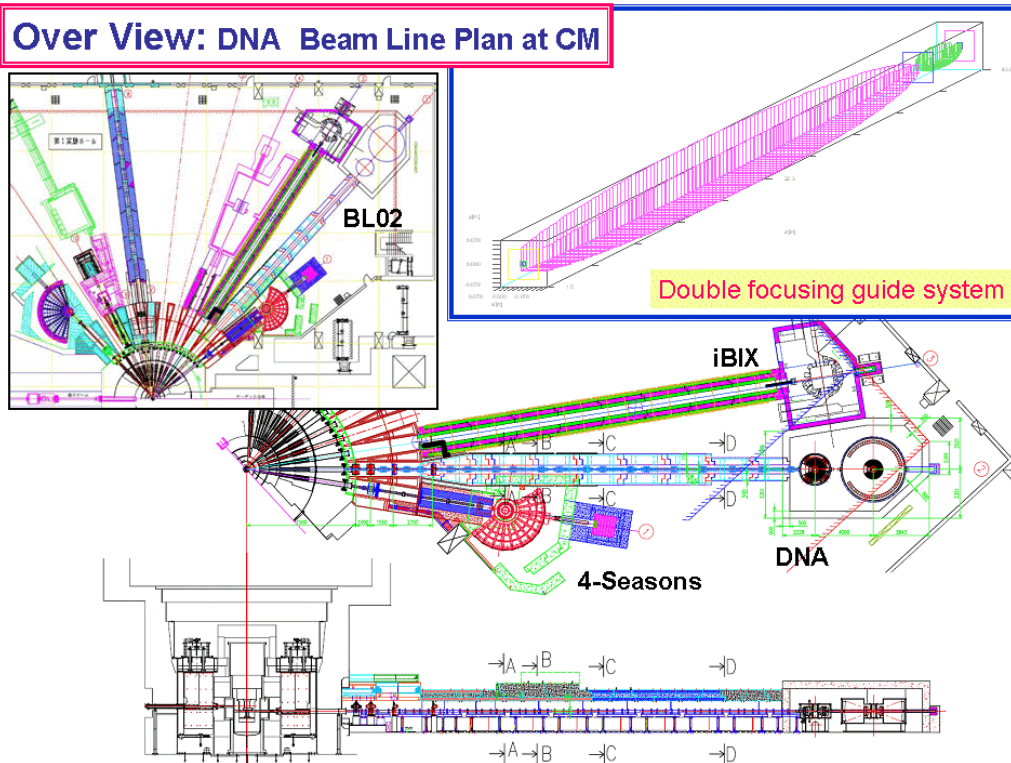
Decoupled moderator is the best neutron Source for n-BS spectrometers ? or !

CM, L1 = 39 & 43 m $\rightarrow$ **CM-source n-BS**

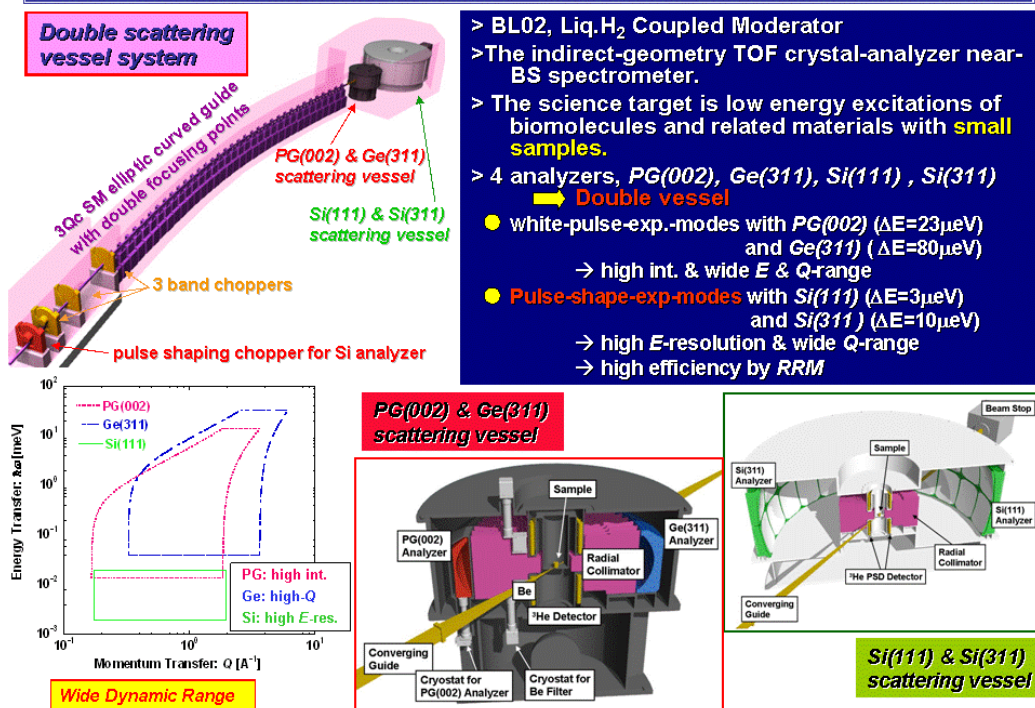
DM, L1 = 32 m $\rightarrow$ DNA Old Plan



Over View: DNA Beam Line Plan at CM



(Back ground development) DNA: Biomolecular Dynamics Spectrometer

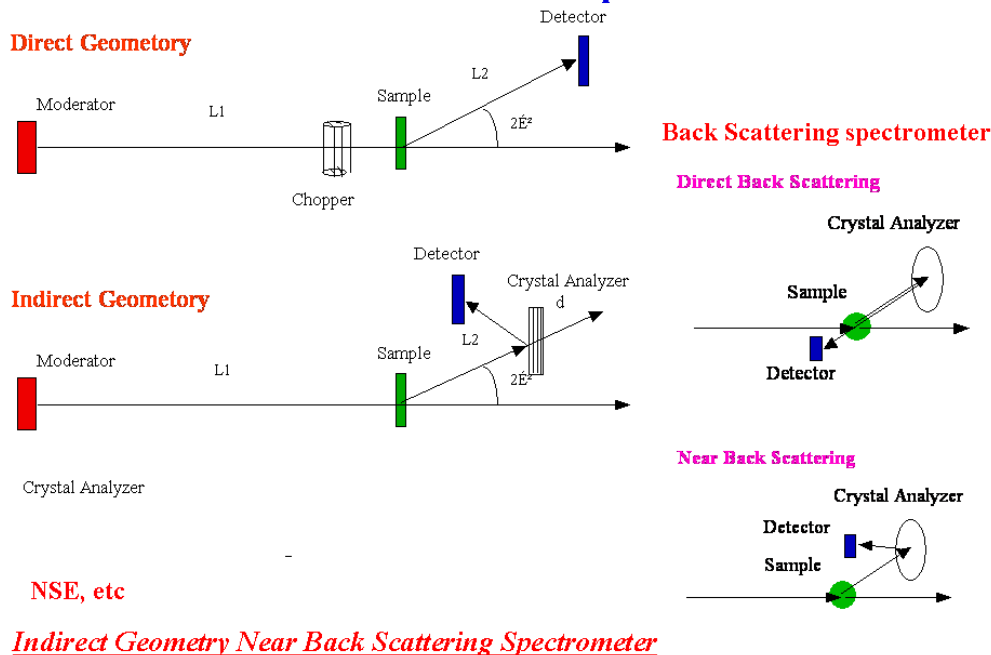


Science Target ➡ **Biomolecular Dynamics** (Protein, e.t.c.)
Complex Materials (Soft Matter, Chemistry)
Localizer Excitation (Tunnel, Phonon, Magnon)
Special Environments
 (High Temperature, High Pressure, e.t.c.,)

Required Specification for DNA

- Measurements for **Very Small Samples**; ~1mg and Low Background
 ➡ **High Efficiency and High Intensity Counting Rate at CM**
 Beam Flux at Sample Position: 1.6×10^9 [n/cm²/meV /sec] @2meV
 Int.[DNA@1MW] > $500 \times$ Int.[IRIS@160kw]
- Wide Energy Range at Around Several 10~100 μ eV
 ➡ **4 Analyzer Crystals: PG002**($\Delta E = 23 \mu$ eV), **Ge311**($\Delta E = 82 \mu$ eV)
Si111($\Delta E = 2.6 \mu$ eV), **Si311**($\Delta E = 10 \mu$ eV)
 Energy Range ; 3μ eV ~ 40 meV; more than 4 figures
- Wide Momentum Range: ➡ $Q = 0.05 \sim 3.8 \text{ \AA}^{-1}$
 Medium Momentum Resolution; ➡ $\Delta Q \sim 0.03 \text{ \AA}^{-1}$
- Separation between Incoherent and Coherent Scatterings. (Option)
 ➡ High Quantity Neutron Polarization Analyses; P~98%

Pulsed Neutron Inelastic Spectrometer



Energy Resolution Function for Crystal Analyzer Spectrometer

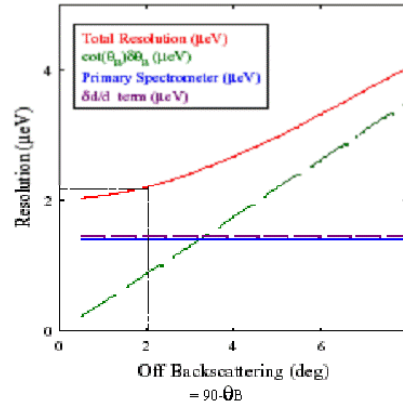
$$\delta\omega = \sqrt{\delta\omega_p^2 + \delta\omega_N^2}$$

$$\delta\omega_p = 2E_i \left[\left(\frac{\delta L_t}{L_t} \right)^2 + \left(\frac{\delta t_0}{t_i} \right)^2 \right]^{\frac{1}{2}}$$

$$\delta\omega_N = 2 \left[E_i^2 \left(\frac{\delta t_f}{t_i} \right)^2 + E_f^2 \left[(\cot(\theta_B) \delta\theta_B)^2 + \left(\frac{\delta d}{d} \right)^2 \right] \right]^{\frac{1}{2}}$$

Si(111) $\delta d/d = 1.86 \text{ \AA} \cdot 10^{-4}$
 PG(002) $\delta d/d = 4.5 \text{ \AA} \cdot 10^{-4}$

DBS Si(111) $\delta\omega_s = 0.56 \text{ \mu eV}$ $dE = 0.80 \text{ \mu eV}$
 NBS Si(111) $\delta\omega_s = 1.06 \text{ \mu eV}$ $dE = 1.50 \text{ \mu eV}$
 NBS PG(002) $\delta\omega_s = 9.0 \text{ \mu eV}$ $dE = 15.0 \text{ \mu eV}$



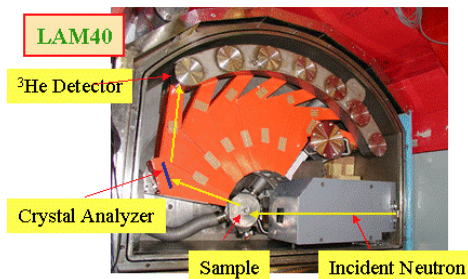
1. $\delta E \sim 23 \text{ \mu eV}$ at $L_1 \sim 39 \text{ m}$ by PG002 analyzer at $\theta_B \sim 80 \text{ deg}$.
 -> high efficiency
2. $\delta E \sim 82 \text{ \mu eV}$ at $L_1 \sim 39 \text{ m}$ by Ge311 analyzer at $\theta_B \sim 80 \text{ deg}$.
 -> wide Q range.
3. $\delta E \sim 3 \text{ \mu eV}$ at $L_1 \sim 43 \text{ m}$ by Si111 analyzer at $\theta_B \sim 87.5 \text{ deg}$, with a disk chopper
 -> high energy resolution

The indirect-geometry TOF crystal-analyzer spectrometer at KENS

LAM type spectrometer

Three indirect-geometry TOF crystal-analyzer spectrometer (KENS@KEK) (Prof. Inoue Gr since 1981)

- LAM-80ET mica analyzer DCsolid-CH₄
 mica002 (1.2 μeV), 004(5 μeV), 006(15 μeV)
- LAM-40 PG002 & Ge311 analyzer DCsolid-CH₄
 PG002(200 μeV ; -1.0~14.0meV)
 Ge311(900 μeV ; -17~30.0meV)
- LAM-D PG002 analyzer DC_liq.H₂O
 PG002(300 μeV ; -1.0~150.0meV)

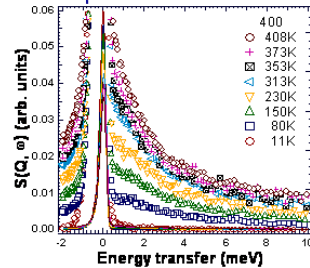


Wide Energy Range used 3 LAM Spectrometer
 (10 $\mu\text{eV} < E < 100\text{meV}$; Dynamic Range 10^4)

Example:

Low energy atomic dynamics in polymer thin films
 R.Inoue and T.Kanaya (ICR, Kyoto Univ.)

INS experimental results on LAM-40 in KENS



Thickness
 $\sim 400 \text{ \AA}$
 Mass
 $\sim 10 \text{ mg}$

Low Background

First observation of inelastic and quasielastic scattering spectrum for polymer thin films.
 Inoue, et al., PRL 95, 056102 (2005), PRE 74, 021801(2006)

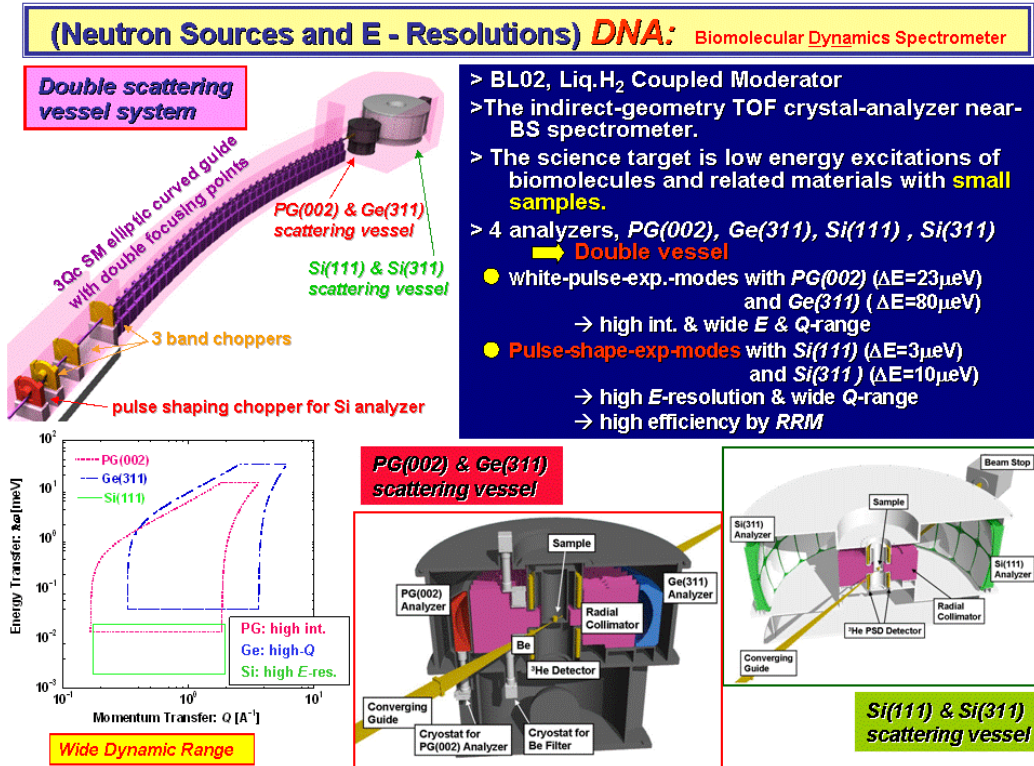
Present status

Necessity for very long measuring time
 (about 2 days / one measurement)
 Poor statistics data due to low neutron flux.

Limit of thickness $\sim 400 \text{ \AA}$
 Difficult measurements even on MARI in ISIS, now!!

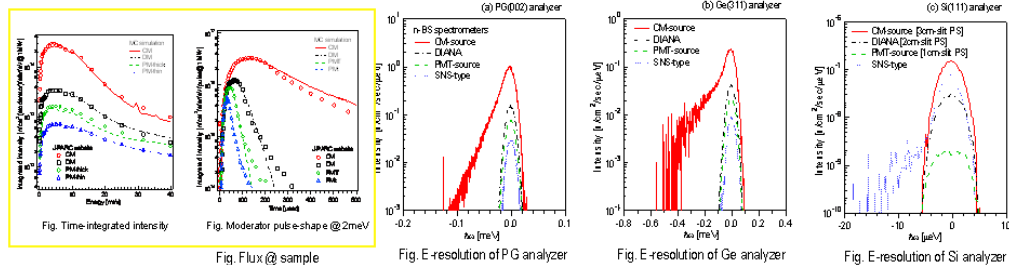
High Efficiency & Low Background LAM type Spectrometer:

LAM40@KENS(3kW) $\sim 1/5 \times$ MARI@ISIS(160kW) $\sim 1/10 \times$ IN6@ILL(60MW)



expected performance comparison, CM v.s. DM

Fig. E-resolution



→ **The long tail energy resolutions** → **MEM analysis**

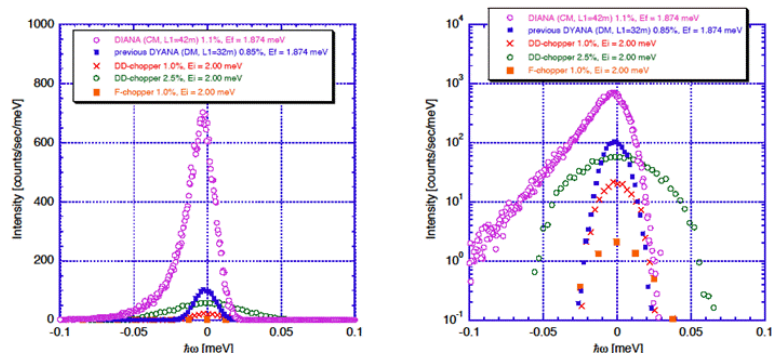
Table: performance comparisons

source (name of n-BS)	L_1 [m]	main guide section	analyzer	E_{el} [meV]	$\hbar\omega$ -range (one frame) [meV]	slit-width of PS [cm]	$\Delta\lambda$ [$\text{\AA}$]	$\Delta\hbar\omega$ [μeV]	sample-position intensity at E_{el} [$10^{14}\text{nvc}/\text{cm}^2/\mu\text{eV}/\text{sec}$]
★ CM (CM-source)	42	curved w60xh98 R2200m	PG(002)	1.87	$-0.3 < \hbar\omega < 4.3$	-	3.6	23	160
			Ge(311)	7.25	$-1.1 < \hbar\omega < E^*$	-	3.6	82	66
			Si(111)	2.09	± 0.04 [PS]	3	3.6	3.8	7.1
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

PS: pulse-shaping chopper

[Quantitative Comparison of Intensity and Energy Resolution by McStas]

- PG002 mode v.s. chopper Spectrometers



Type; $\Delta E/E$	ΔE [μeV]	Peak Intensity	Integrated Intensity.	Counting Efficiency	FOM
DNA ; 1.15%	23	702.	48.	72.	54.
Old Plan DNA ; 0.85%	17	102.	3.9	5.8	8.0
DD-chopper; 1%	20	21.	1.0	1.0	1.0
DD-chopper; 2.5%	50	58.	6.9	6.9	1.1
F-chopper; 1%	20	2.	0.10	0.10	0.1

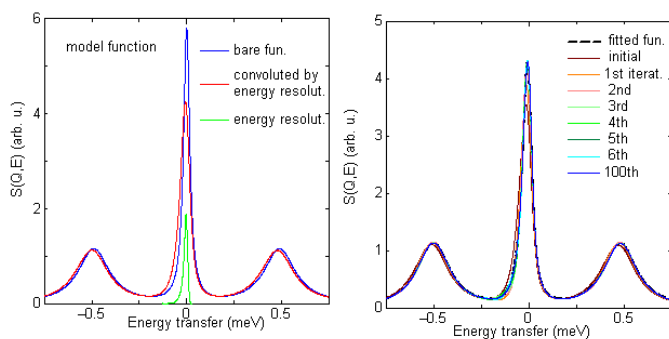
Table . Intensity Ratio (Based on DD-chopper(AMATERAS);1,0)
Using 20*20mm sample positions with same surface of Detector

A deconvolution of energy resolution function by MEM

→ Dr.Y.Kawakita

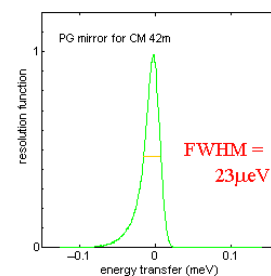
Model function

Center FWHM 20 μeV Relative Int. 0.5
Side band FWHM 100 μeV Relative Int. 0.5
Positions of peaks $\pm 500 \mu\text{eV}$

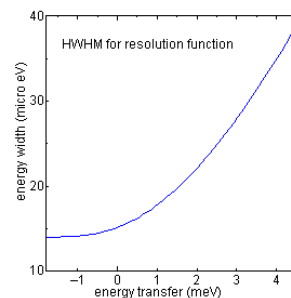


MEM results for PG mirror

We used a raw data for an initial fitting function.
It may be enough over the 100 times repetitions.



- Asymmetry of resolution function.



- Energy dependence of resolution function.

Frame overlap

Flight length was reconsidered to avoid a spike-like fast neutron background, so called T0-burst.

This means that high energy neutrons generated in every 40 ms may reach the detectors just after protons hit the target (the frequency of the pulsed neutron source is 25 Hz).

One should expect some undesired background of this type, even when installing T0-chopper and/or curved neutron guides.

1. $L < 24$ m (limitation from PG-analyzer)

2. $L < 47$ m (limitation from Ge-analyzer)

Then,

• **PMT-source type:** $L_1 = 21.5$ m

• **CM-source type:** $L_1 = 39$ & 43 m

• **SNS-type:** $L_1 = 84$ m

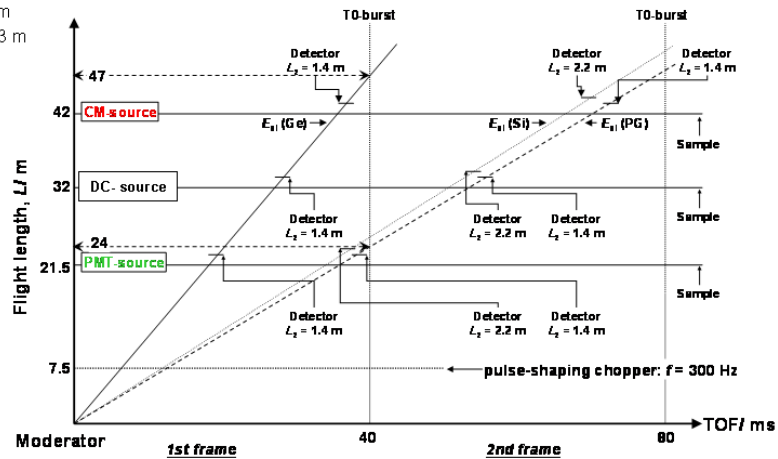
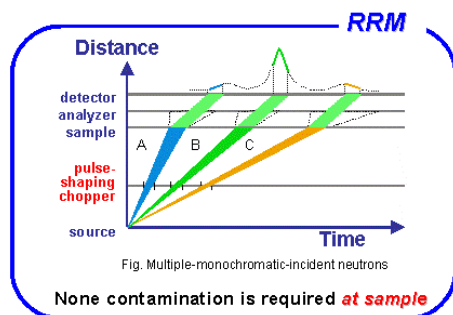
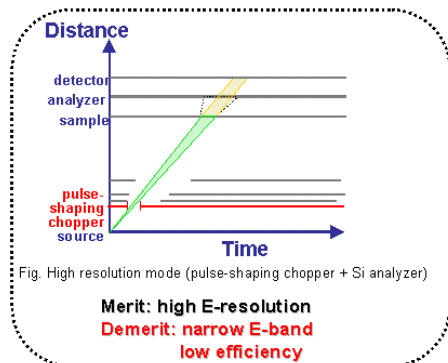
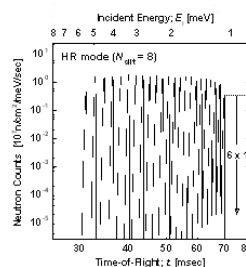
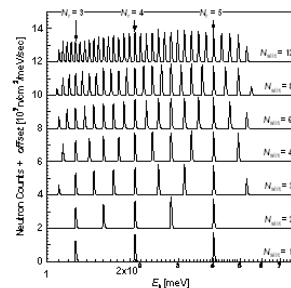
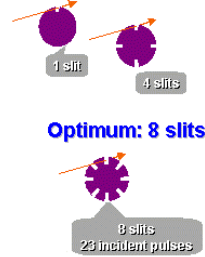


Fig. TOF diagram

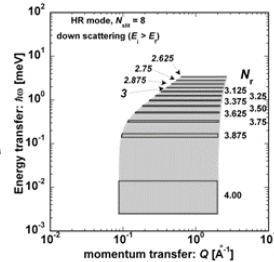
study of RRM capabilities (J. Neutron Res.)



Increasing the slits on the pulse-shaping chopper

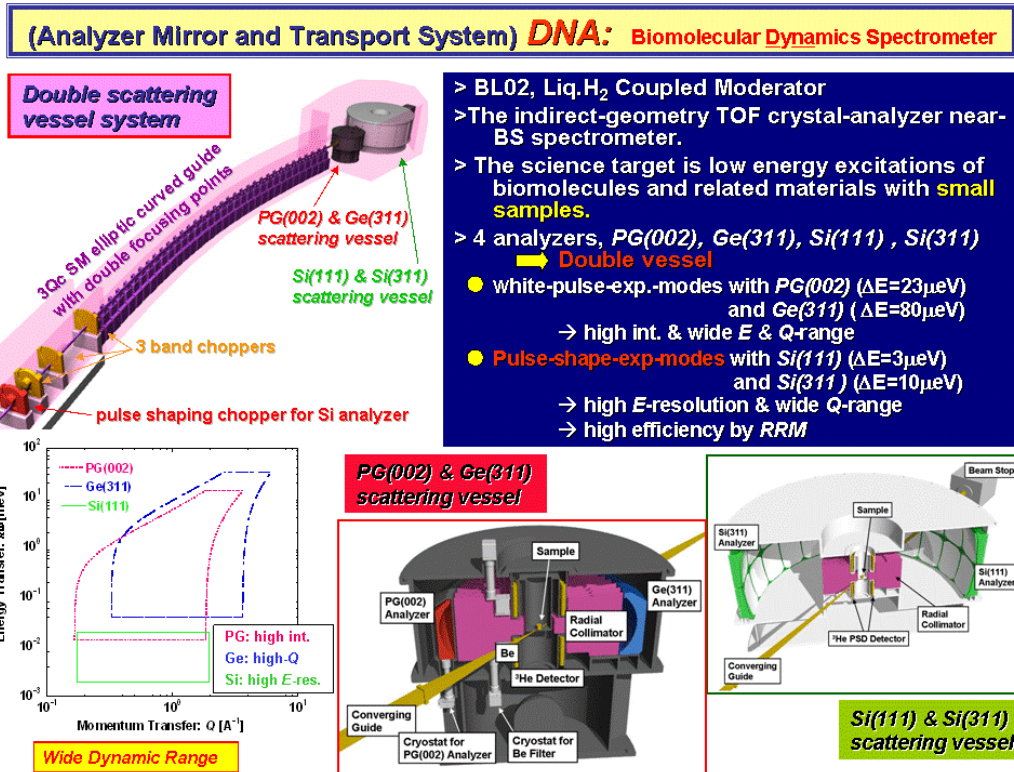


efficiency: $\times 23$



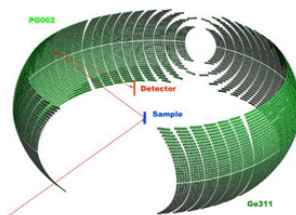
E-range: 0.02 meV in 1 scan

→ 4.4 meV in 10 scans



Upper stream part of DNA:
PG002&Ge311
Analyzer Crystals

Configuration of Crystal Analyzer



Principle of TOF focusing

The neutron beam which each crystal piece on the crystal analyzer reflected, is focused on the same point on a neutron detector at same of time.

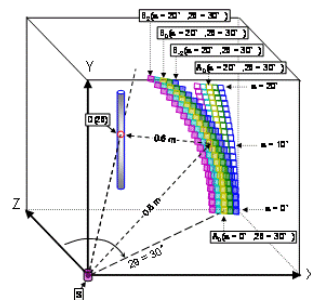


Fig: drawing of an analyzer-unit at $2\theta = 30^\circ$

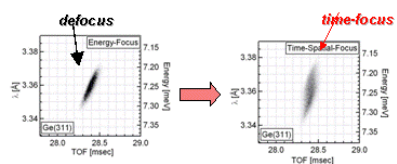
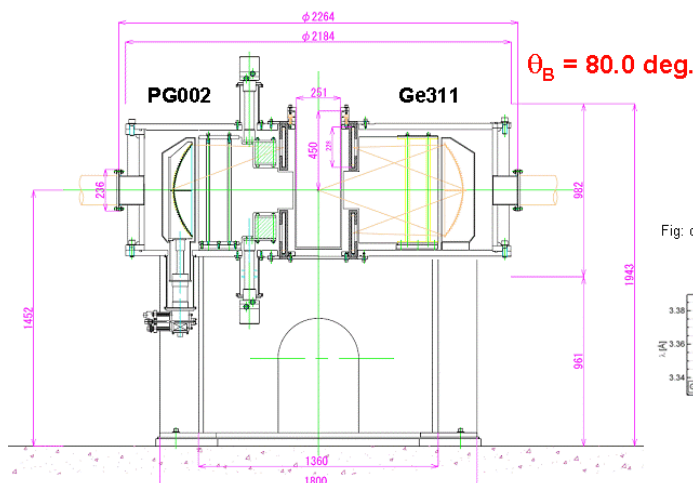


Fig: λ -TOF monitor @ detector-position

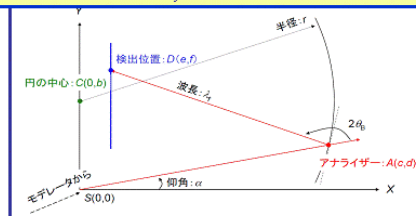
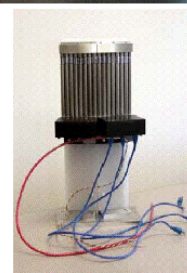
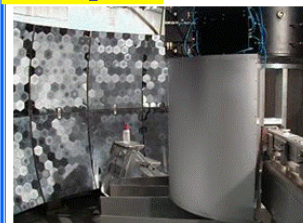
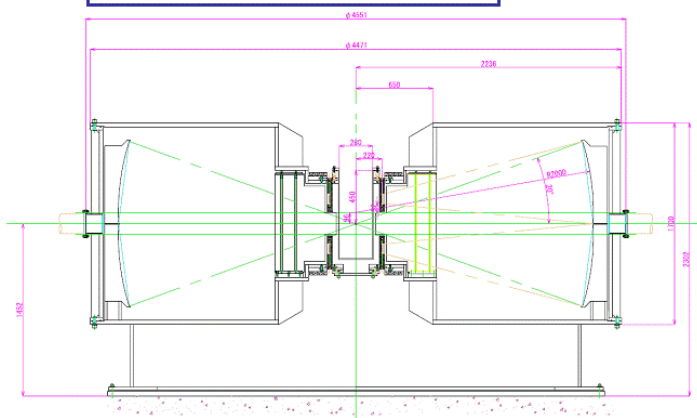


Downstream part of DNA: Si111&Si311 Analyzer Crystals

Principle of Si crystal analyzer

Si wafer is stacked on the

Spherical surface and analyzer neutron is detected on the each PSD position.


$$\theta_B = 87.5 \text{ deg.}$$


- DNA guide system : ellipsoid in vertical directions

Parameter of ellipsoid

 $a = 20.4 \text{ m}$
$$b = 0.0922 \text{ m}$$
$$l_{\text{SM}} = -1.2 \text{ m}$$
$$l_{\text{ge}} = 0,0 \text{ m}$$

19

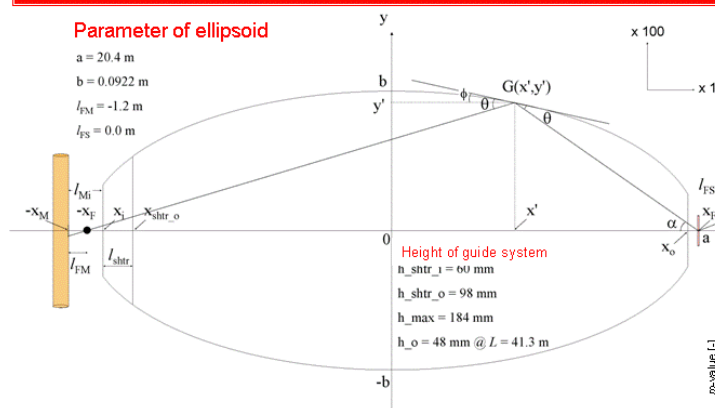


Fig.1:Optimized ellipsoid neutron guide system estimated by simulations (Y-axis/X-axis = $\times 100$)

Gain: 2.0~1.5

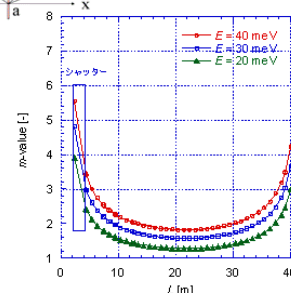
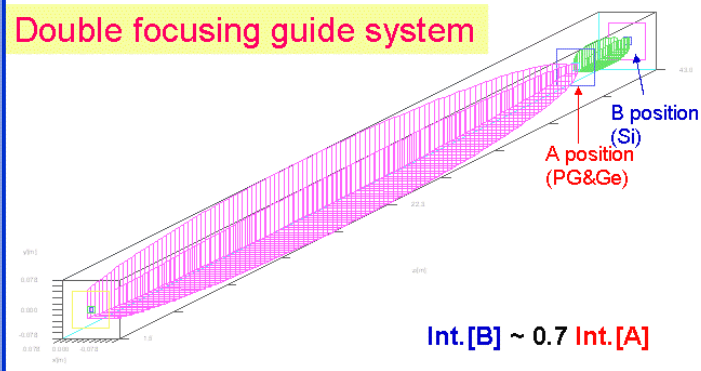
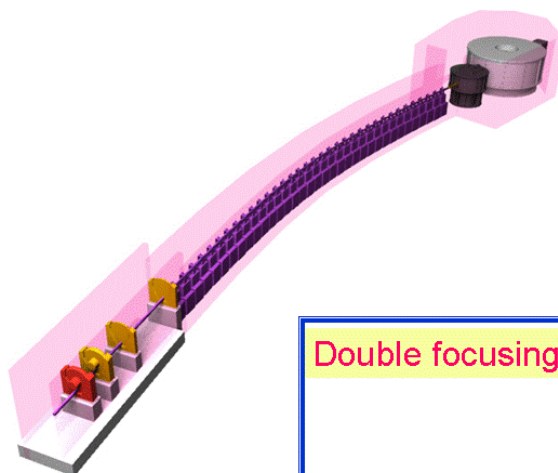


Fig2: Necessary SM m-value for specific neutron energies

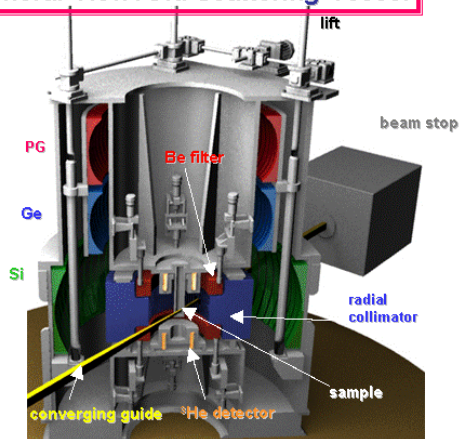
- DNA guide system : curved in horizontal directions

$E^* \sim 40$ meV ; $E_f = 7.25$ meV for Ge311 and $E_f = 65.25$ meV for Ge933

General view of DNA guide system



General View : Old Scattering Vessel



• High Cost Scattering Vessel
~38M.JPY

• Complex Structure to be
difficult the cooling PG mirror.

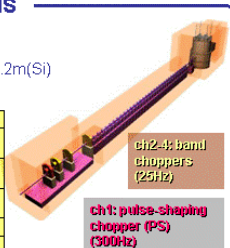


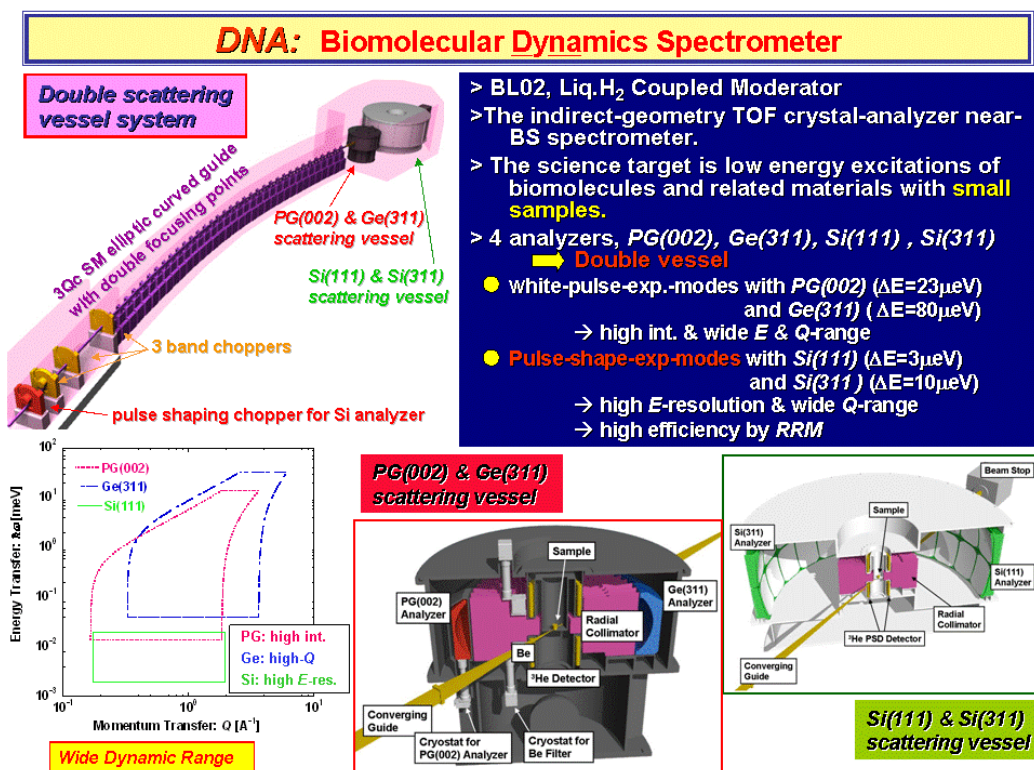
Separate Double Scattering
Vessel

SPECIFICATIONS

- Source: Coupled (25Hz)
- Flight length: L1=42m,
L2=1.4m(PG,Ge)/2.2m(Si)
- Scattering angle: 7.5° ~ 152.5°
- 3 analyzers: ΔQ=1.1 μstr

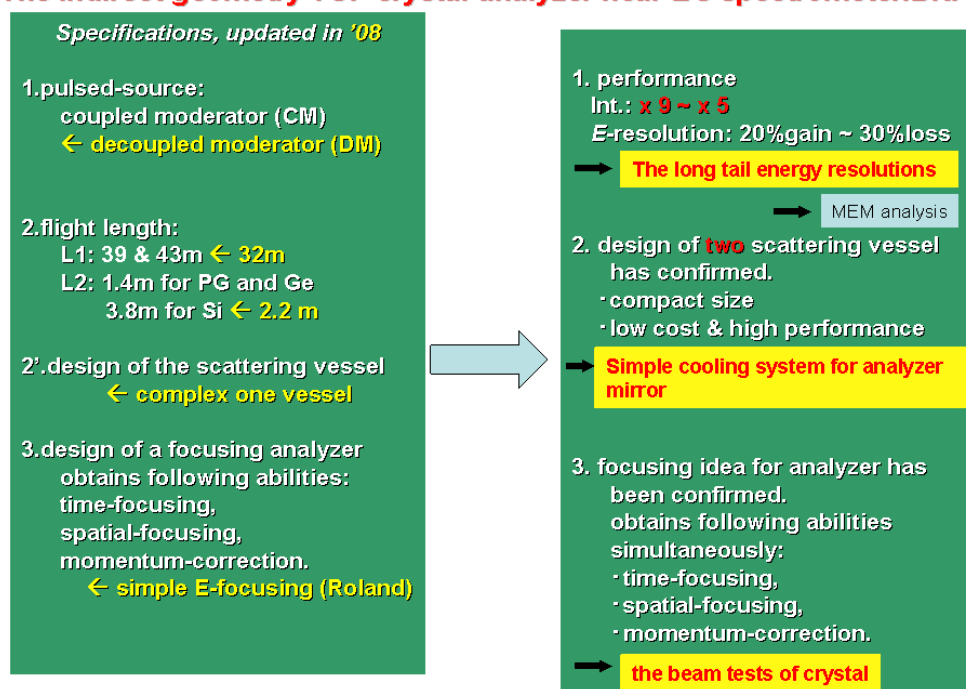
	ch1	ch2	ch3	ch4
applicati on	pulse- shaping	band-chopper		
disc	Double	Double	Singl e	Singl e
L [m]	7.5	8.5	10.05	12.75
f [Hz]	300	25	25	25
slit	30 mm	96"	113 "	144 "





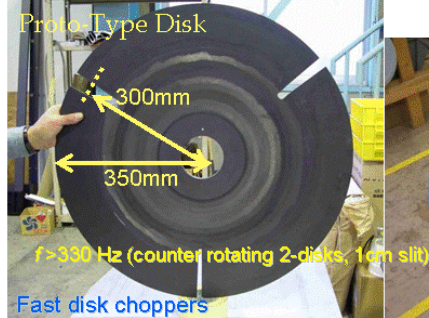
Conclusion: General Review of DNA

The indirect-geometry TOF crystal-analyzer near-BS spectrometer.DNA



Device Development ➡ Dr.K.Soyama

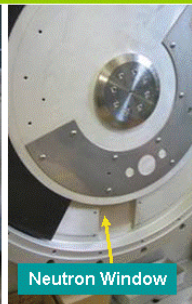
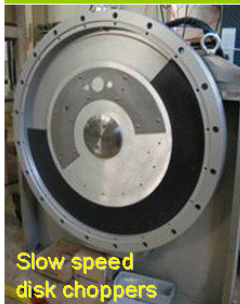
Development of Fast Disk-Chopper



R&D Record;
max. rev.:350Hz,
 without B4C resin
max. rev.:300Hz,
 with B4C resin

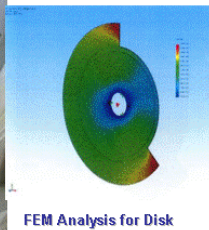
Disk Radius less than 350mm
 Accuracy <0.1 deg.
 $^{10}\text{B}_4\text{C}$: $T \sim 10^{-6}$ @100meV
 Easy Maintenance
 Etc.
 By Kobelco

Development of Band Disk Chopper



Rotation Speed: 25 Hz

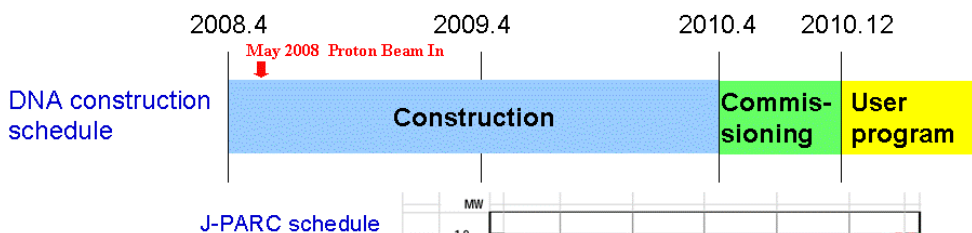
Slow speed disk chopper has been ready for manufacturing



Specification

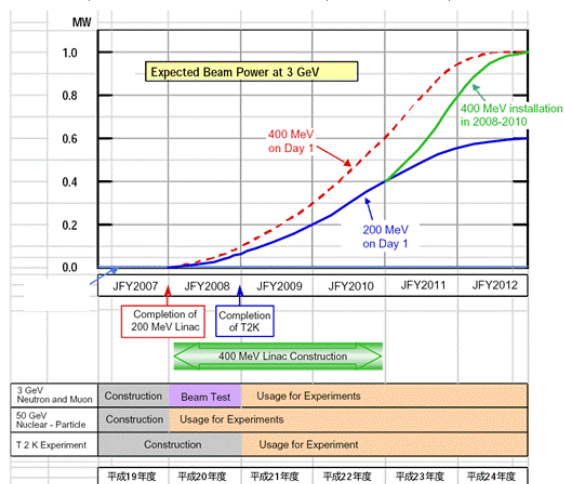
Speed: 25Hz
 Disk Radius less than 350mm
 Accuracy <0.1 deg.
 $^{10}\text{B}_4\text{C}$: $T \sim 10^{-6}$ @100meV
 Easy Maintenance
 Low Cost
 Etc.
 By Kobelco

Schedule



Cost

~100M.JPY



DNA Proposal Members

Construction & Research Group Construction K. Shibata (JAEA) N. Takahashi (JAEA) T. J. Sato (Univ. of Tokyo) S. Fujiwara (JAEA) I. Tsukushi (Chiba Inst. of Tech.) Y. Kawakita (Kyushu Univ.) Science Y. Jochi (Univ. of Tokyo) H. Nakagawa (JAEA) M. Nakasako (Keio Univ.) M. Kataoka (Nara Inst. Sci. Tech., JAEA) Adviser M. Arai (JAEA) T. Kanaya (ICR, Kyoto Univ.) A. Inaba (Osaka Univ.) S. Takeda (Hokkaido Univ.) F. Mezei (HMI, LANL)	Support Group Biology N. Go (JAEA) N. Niimura (Ibaraki Univ.) A. Kitao (Univ. of Tokyo) S. Ikura (Tokyo Ikashika Univ.) S. Saruwatari (Kitazato Univ.) K. Kuwata (Gifu Univ.) Y. Sugawara (Kitazato Univ.) K. Maenaka (Kyushu Univ.) K. Wakabayashi (Osaka Univ.) H. Urabe (Tokyo Kasei Univ.) Dieter Middendorf (Univ. of Oxford) A. Sokolov (Univ. of Akron) Physics D. Yamazaki (JAEA) Y. Takeda (JAEA) T. Matsumura (Tohoku Univ.) K. Iwasa (Tohoku Univ.)
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neutron source	coupled moderator, 100×100 mm ²		
moderator-sample distance: L ₁ [m]	39 & 43		
sample-detector distance: L ₂ [m]	1.4 (PG, Ge) / 3.8 (Si)		
neutron transportation	2.33m-4.32m, m=3 SM guide (shutter); w62h98 4.35m-39m, m=3 SM curved guide; w60h98, R2200m, cut-off-energy: 40meV 39m-41.85m, m=4,5,6 SM converging guide; w60h98 (entrance), w20h20 (exit)		
analyzer-bank	horizontal: $7.5^\circ \leq 2\theta \leq 155^\circ$, vertical: $-20^\circ \leq 2\theta \leq 20^\circ$, solid angle: 1.125 π sr.		
analyzer-crystal	PG(002)	Ge(311)	Si(111)
Bragg spacing [Å]	3.355	1.706	3.135
mosaicity [minutes]	42	30	-
Bragg angle [degree]	80.	80.	87.5
E _i [meV]	1.874	7.247	2.085
Q-range [Å ⁻¹]	0.17~1.8	0.33~3.6	0.18~2.0
ΔQ/Q [%]	1~40	1~40	1~40
wavelength-band: Δλ [Å]	3.6	3.6	3.6
ħω-range in 1 frame [meV]	-0.3~4.3	-1.1~40	-0.04~0.04
Δħω [meV]	23	82	3.8
Δħω/E _i [%]	1.2%	1.1%	0.18%
sample size	20×20 mm ² (up to 100×100 mm ²)		
detector-bank	$10^\circ \leq 2\theta \leq 152.5^\circ$		
diffraction detectors	$170^\circ \leq 2\theta \leq 175^\circ$		
detectors	ellipsoidal 3/4-inch-φ ³ He PSD (10atm), b=16 mm, a=20 mm		
higher-order-reflections filter	quenched-Be		
high-speed pulse-shaping chopper	50 - 300 Hz, R = 300 mm, L = 7.5 m, multi-slit to achieve RRM		
band chopper (double-disc) (single-disc)	25 Hz, R = 300 mm (L=8.5 m) 25 Hz, R = 300 mm (L=10.05 m, 12.75 m)		
polarizer	solar SM polarizer		

2.2 Neutron Sources and Energy Resolutions

Kaoru Shibata (JAEA)

1. Neutron Sources and Energy Resolutions

K. Shibata (J-PARC)

Outline

- 1.1 The neutron source at JSNS and geometry
- 1.2 Pulse shaping + Si Analyzer
- 1.3 Resolution function + MEM analysis
- 1.4 Frame overlap and RRM

Pulsed-source in MLF at J-PARC

MLF/J-PARC will have 4 kinds of pulsed neutron sources

Liq.H₂ Coupled Moderator ($\phi 15\text{ cm} \times 10^4\text{ cm}$) : CM

Liq.H₂ Decoupled Moderator ($13^w \times 12^h \times 6.2^t\text{ cm}^3$) : DM

Liq.H₂ Poisoned Decoupled Moderator thin side ($13^w \times 12^h \times 2.5(6.2)^t\text{ cm}^3$) : PM-thick

Liq.H₂ Poisoned Decoupled Moderator thick side ($13^w \times 12^h \times 3.7(6.2)^t\text{ cm}^3$) : PM-thin

The world n-BS spectrometers

IRIS, OSIRIS @ ISIS: source = DM, L1 = 36.4, 34 m

Si n-BS (BASIS) @ SNS:

source = poisoned moderator (PM), L1 = 84 m

Question:

Decoupled moderator is the best neutron Source for n-BS spectrometers ? or !

CM, L1 = 39 & 43 m → **CM-source n-BS**

DM, L1 = 32 m → **DNA Old Plan**

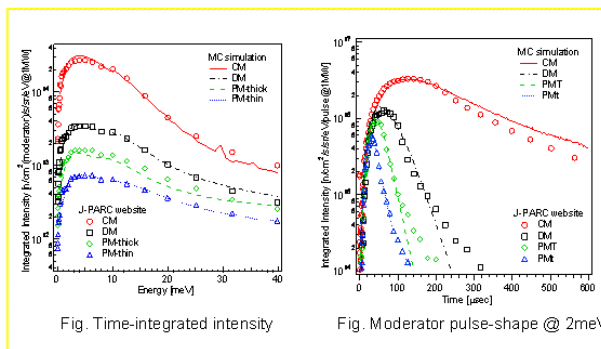
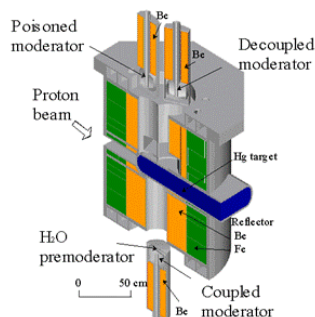
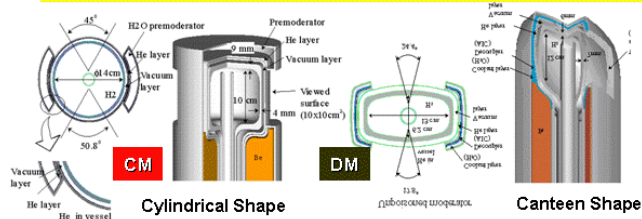


Fig. Time-integrated intensity

Fig. Moderator pulse-shape @ 2meV



Cylindrical Shape

Canteen Shape

MC simulations

MC simulations have performed by using **McStas** with the below model.

Vanadium sample has been used to obtain TOF spectra of incoherent elastic scattering.

1. Sample-position Intensities have been obtained.
2. Resolution functions have been estimated by the TOF spectra.

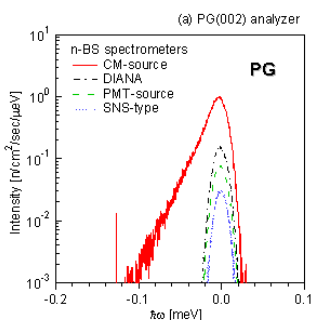
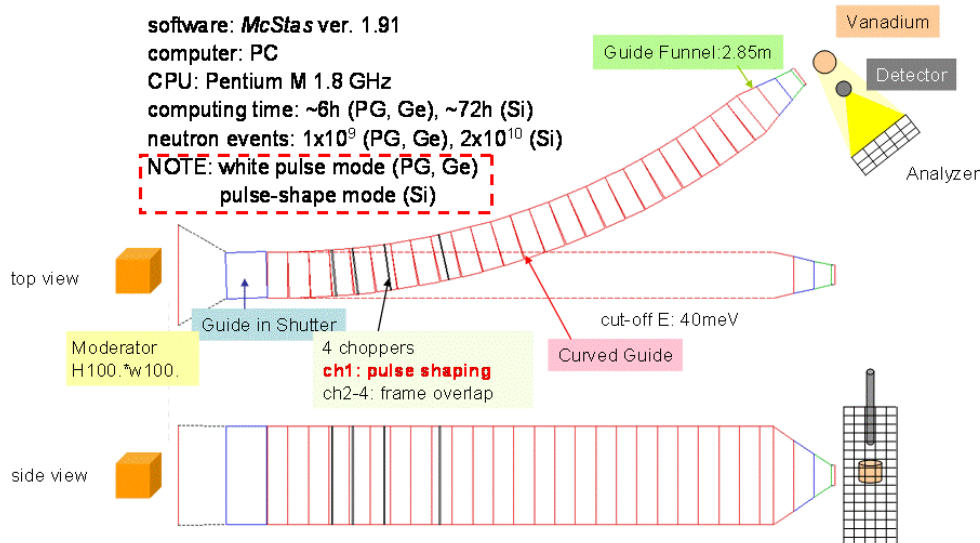


Fig. E-resolution of PG analyzer

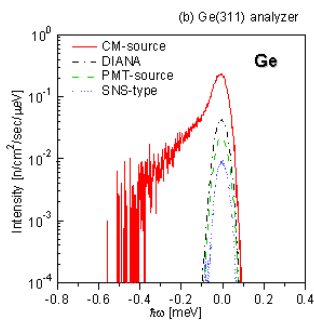


Fig. E-resolution of Ge analyzer

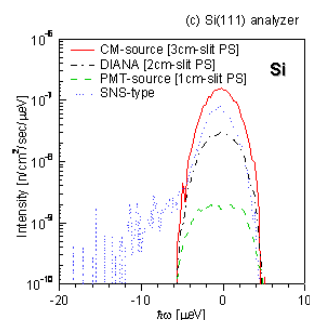


Fig. E-resolution of Si analyzer

source (name of n-BS)	L_1 [m]	main guide section	analyzer	E_{el} [meV]	$h\bar{k}l$ -range (one frame) [meV]	slit-width of PS [cm]	$\Delta\lambda$ [Å]	$\Delta h\bar{k}l$ [μeV]	sample-position intensity at E_{el} [10^4 n/cm²/sec/μeV]
★ CM (CM-source)	42	curved w60xw98 R2200m	PG(002)	1.87	-0.3 < $h\bar{k}l$ < 4.3	-	3.6	23	160
			Ge(311)	7.25	-1.1 < $h\bar{k}l$ < E^*	-	3.6	62	66
			Si(111)	2.09	± 0.04 [PS]	3	3.6	3.8	7.1
DM (DM-source)	32	curved w46xw98 R1650m	PG(002)	1.87	-1.0 < $h\bar{k}l$ < 1.8	-	4.7	17	1.7
			Ge(311)	7.25	-3.6 < $h\bar{k}l$ < 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 + TO- chopper w98xw98 0.5m-gap for TO-chopper	PG(002)	1.87	-0.2 < $h\bar{k}l$	-	6.9	17	8.6
			Ge(311)	7.25	-5.5 < $h\bar{k}l$	-	6.9	64	4.1
			Si(111)	2.09	± 0.014 [PS]	1	6.7	6.2	0.20
PMT (SNS-type)	84	curved w60xw98 R2200m	PG(002)	1.87	-0.4 < $h\bar{k}l$ < 0.8	-	1.9	15	3.2
			Ge(311)	7.25	-1.9 < $h\bar{k}l$ < 1.7	-	1.9	57	1.5
			Si(111)	2.09	-0.6 < $h\bar{k}l$ < 0.6	-	1.8	3.6	2.7

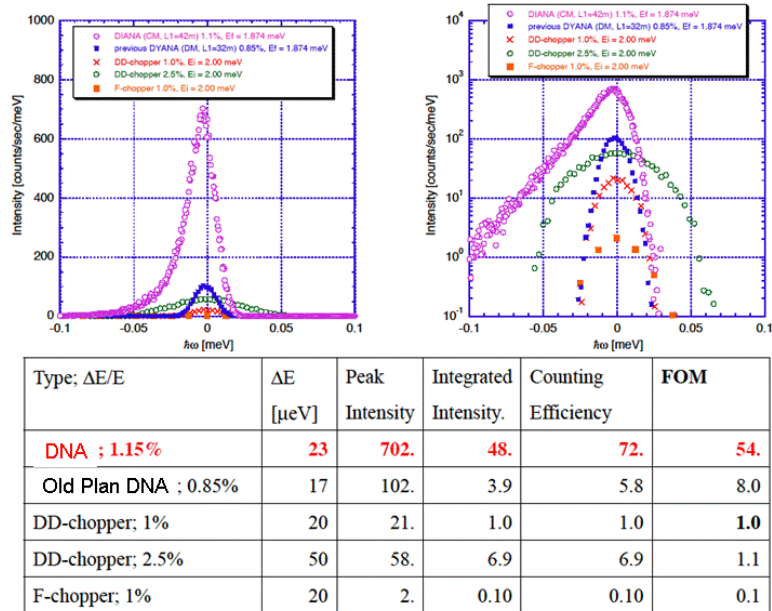
Curved guide: $E^* = 40$ meV

white-pulse-exp-mode (NO pulse-shape) give relatively high int. & wide $h\bar{k}l$ -range.

short L_1 gives wide $\Delta\lambda$

low int., caused by the moderators

[Quantitative Comparison of Intensity and Energy Resolution by McStas]
- PG002 mode v.s. chopper Spectrometers



Using 20*20mm sample positions with same surface of Detector

Table . Intensity Ratio (Based on AMATERAS;1,0)

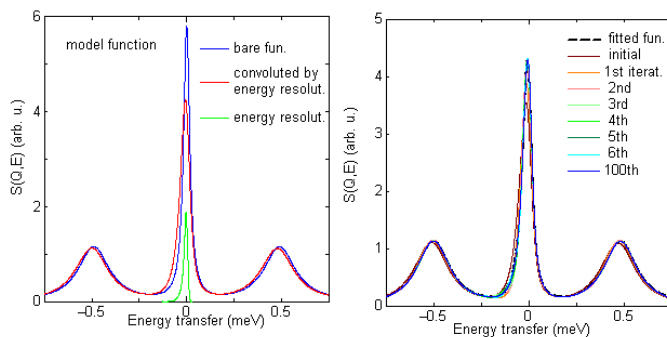
→ The long tail energy resolutions → MEM analysis

A deconvolution of energy resolution function by MEM

→ Dr.Y.Kawakita

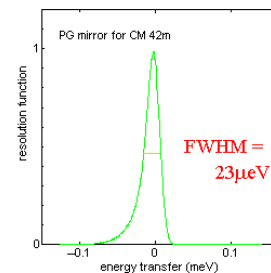
Model function

Center FWHM 20 μeV Relative Int. 0.5
 Side band FWHM 100 μeV Relative Int. 0.5
 Positions of peaks $\pm 500 \mu\text{eV}$

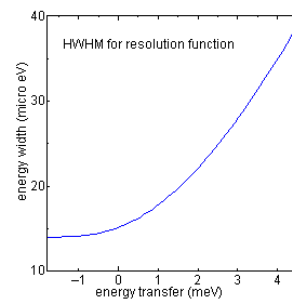


MEM results for PG mirror

We used a raw data for an initial fitting function.
 It may be enough over the 100 times repetitions.



• Asymmetry of resolution function.



• Energy dependence of resolution function.

Frame overlap

Flight length was reconsidered to avoid a spike-like fast neutron background, so called T0-burst.

This means that high energy neutrons generated in every 40 ms may reach the detectors just after protons hit the target (the frequency of the pulsed neutron source is 25 Hz).

One should expect some undesired background of this type, even when installing T0-chopper and/or curved neutron guides.

1. $L < 24$ m (limitation from PG-analyzer)

2. $L < 47$ m (limitation from Ge-analyzer)

Then,

• **PMT-source type:** $L_1 = 21.5$ m

• **CM-source type:** $L_1 = 39$ & 43 m

• **SNS-type:** $L_1 = 84$ m

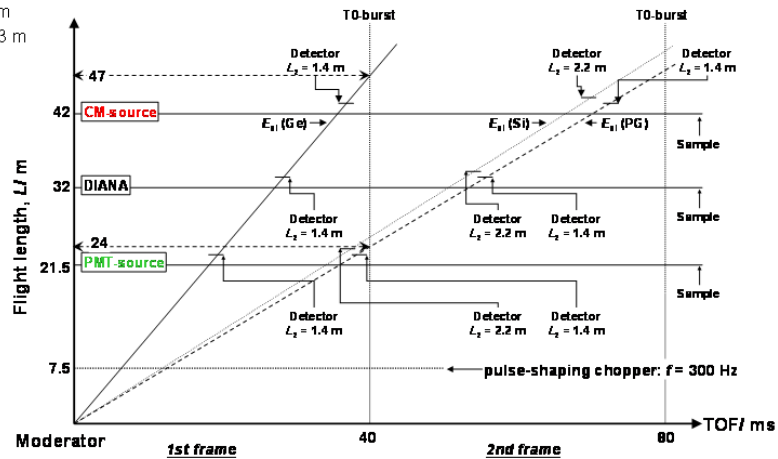
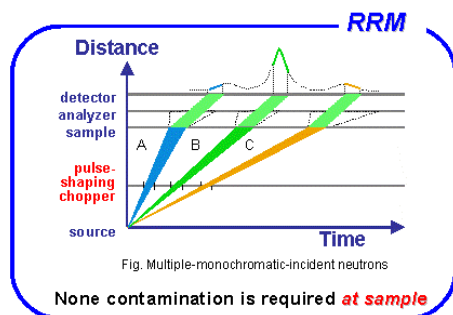
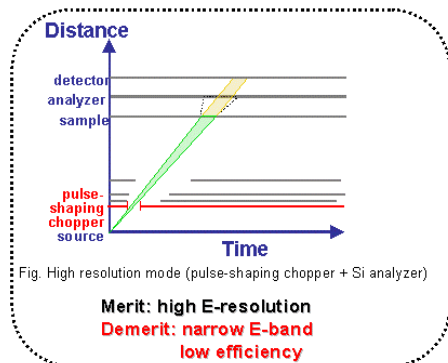
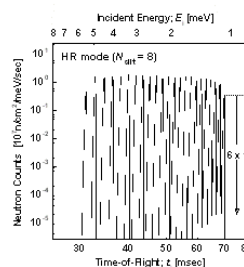
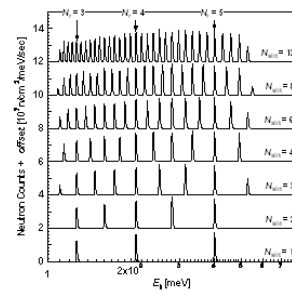
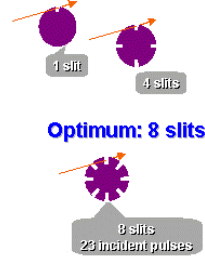


Fig. TOF diagram

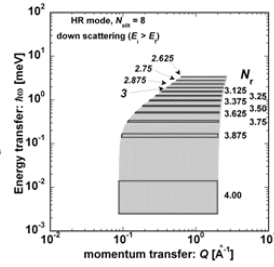
study of RRM capabilities (J. Neutron Res.)



Increasing the slits on the pulse-shaping chopper



efficiency: $\times 23$



E-range: 0.02 meV in 1 scan

→ 4.4 meV in 10 scans

Present Status of R&D for Fast Disk-Chopper (JAERI-Kobe Steel, Ltd.)

Short Burst Time ($\Delta t < 8 \mu\text{sec.}$) with High Precision Control

Disk Radius $< 350 \text{ mm} \rightarrow f > 330 \text{ Hz}$ (counter rotating 2-disks, 1cm slit)

Phase I: Study on Key Issues...

- CFRP+ $^{10}\text{B}_4\text{C}$ resin Disk, which can run @ 350Hz
- at the edge $\sim 780\text{m/sec.}$, $>170,000 \text{ G}$
- Phase Control Electronics & Technique

Status:

- 2005: Study on CFRP Material
 - ✓ FEM Analysis of Proto-Type Disks
 - ✓ Proto-Type Control Electronics
 - ✓ Proto-Type Disks

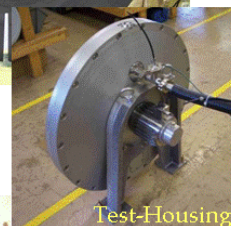
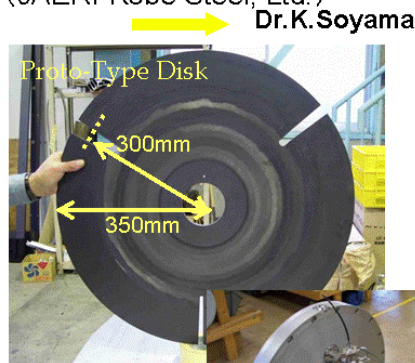
2006: Revolution Test is under going on a test-housing.

Product: 6 disks
Broken: 2 disks

Record; Max. Rev.: 350Hz, without B_4C resin
Rev.: 300Hz, with B_4C resin

2007:

- Magnetic Bearing
- counter rotating 2-disks



Conclusion: Neutron Sources and Energy Resolutions

> BL02, Liq. H_2 **Coupled Moderator CM**

> The indirect-geometry TOF crystal-analyzer near-BS spectrometer.

(c.f. MARS@PSI)

> 4 analyzers,

$\text{PG}(002)$, $\text{Ge}(311)$, $\text{Si}(111)$, $\text{Si}(311)$ $\rightarrow$ Double vessel A. & B.

A. White-pulse-exp.-modes with $\text{PG}(002)$ ($\Delta E = 23 \mu\text{eV}$) and $\text{Ge}(311)$ ($\Delta E = 80 \mu\text{eV}$)

$\rightarrow$ high int. & wide E & Q -range

- Beam Flux at Sample Position: $1.6 \times 10^9 [\text{n/cm}^2/\text{meV} / \text{sec}] @ 2 \text{ meV}$
- Int.[DNA@1MW] $> 500 \times$ Int.[IRIS@160kW]

$\rightarrow$ **The long tail energy resolutions**

$\rightarrow$ MEM analysis

B. Pulse-shape-exp.-modes with $\text{Si}(111)$ ($\Delta E = 3 \mu\text{eV}$) and $\text{Si}(311)$ ($\Delta E = 10 \mu\text{eV}$)

Fast Disk-Chopper: $L_{\text{ch}} = 7.5 \text{ m}$, $d = 30 \text{ mm}$, $r = 0.3 \text{ m}$, $f = 300 \text{ Hz}$

Pulse-shape (FWHM; $205 \mu\text{sec} \rightarrow 26.5 \mu\text{sec.}$)

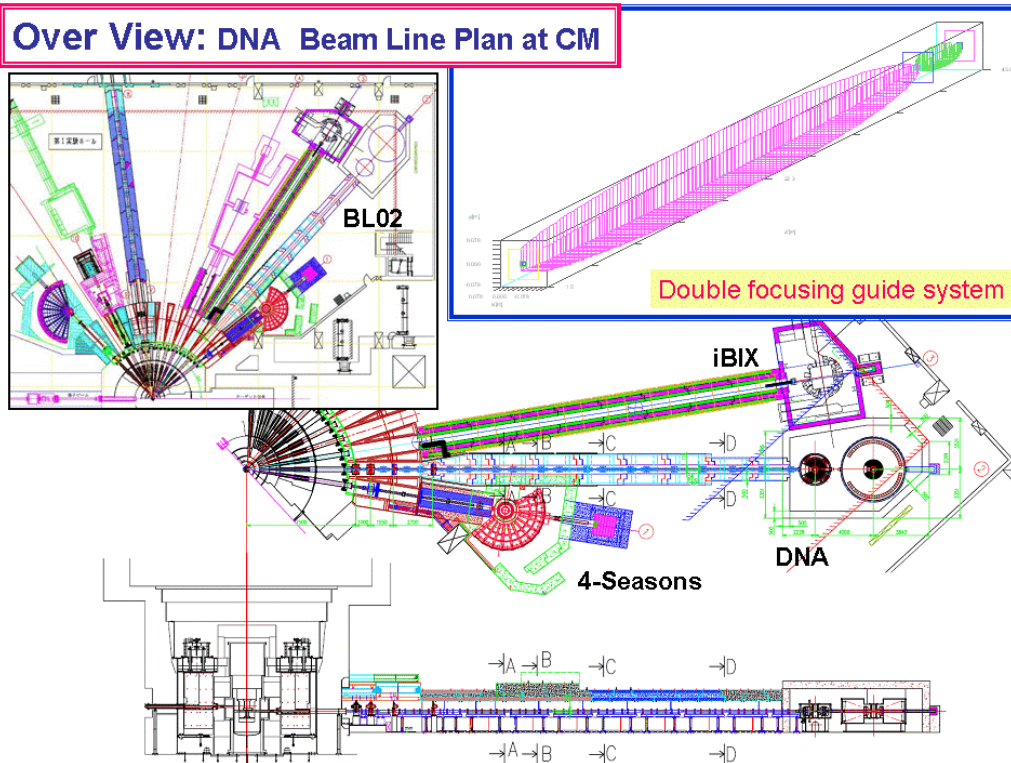
Energy Range ($-40 \mu\text{eV} < E < +40 \mu\text{eV}$)

$\rightarrow$ high E -resolution & wide Q -range

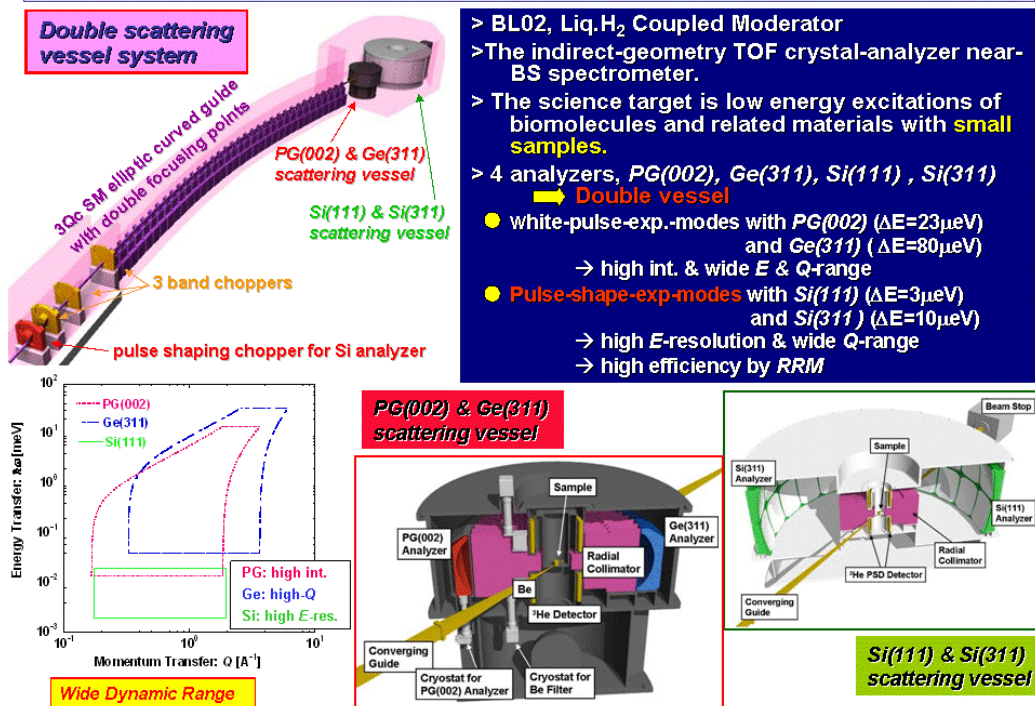
$\rightarrow$ high efficiency by RRM

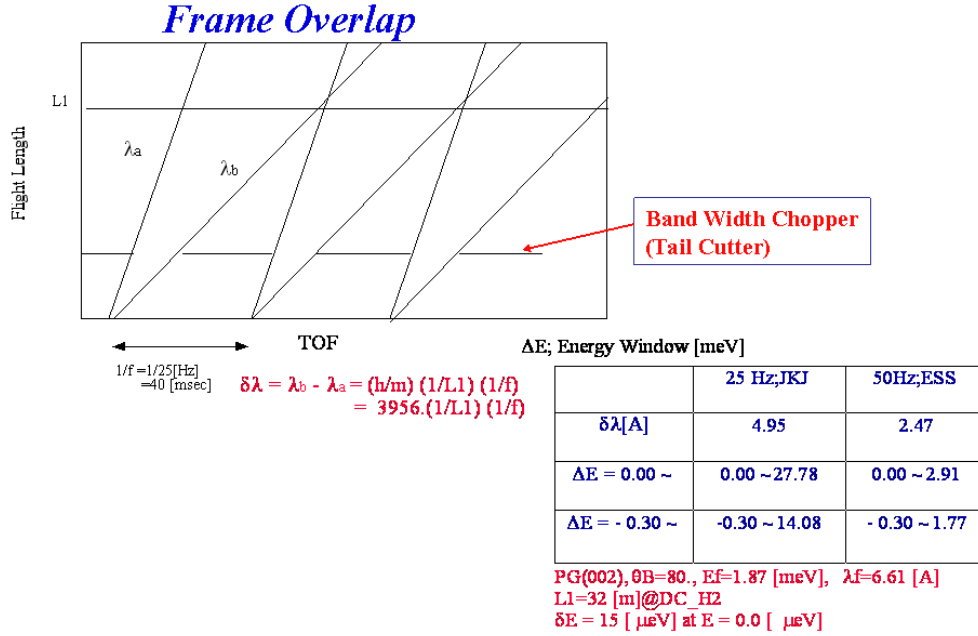
$\rightarrow$ **Development of Fast Disk-Chopper**

Over View: DNA Beam Line Plan at CM



DNA: Biomolecular Dynamics Spectrometer

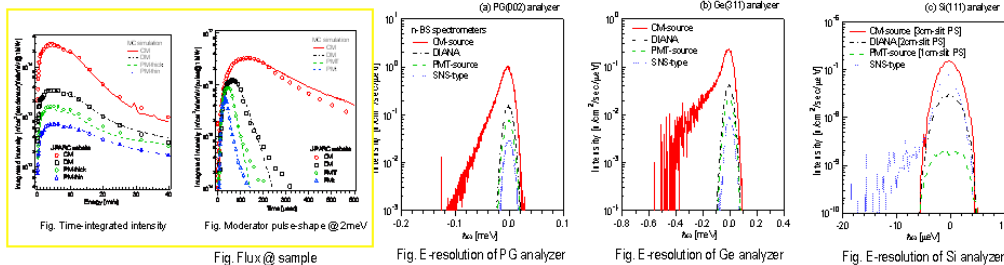




DNA: Unique Spectrometer @ 25 Hz

expected performance comparison, CM v.s. DM

Fig. E-resolution



The long tail energy resolutions

MEM analysis

Table: performance comparisons

source (name of n-BS)	L_1 [m]	main guide section	analyzer	E_{el} [meV]	$\hbar\omega$ -range (one frame) [meV]	slit-width of PS [cm]	$\Delta\lambda$ [Å]	$\Delta\hbar\omega$ [μeV]	sample-position intensity at E_{el} [$10^{14} \text{ nV cm}^{-2} / \mu\text{eV/sec}$]
★ CM (CM-source)	42	curved w60xh98 R2200m	PG(002)	1.87	$-0.3 < \hbar\omega < 4.3$	-	3.6	23	160
			Ge(311)	7.25	$-1.1 < \hbar\omega < E^*$	-	3.6	82	66
			Si(111)	2.09	$\pm 0.04 [\text{PS}]$	3	3.6	3.8	7.1
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	$\pm 0.014 [\text{PS}]$	2	4.6	4.8	1.4

PS: pulse-shaping chopper

2.3 Analyzer Mirror System

Nobuaki Takahashi (JAEA)

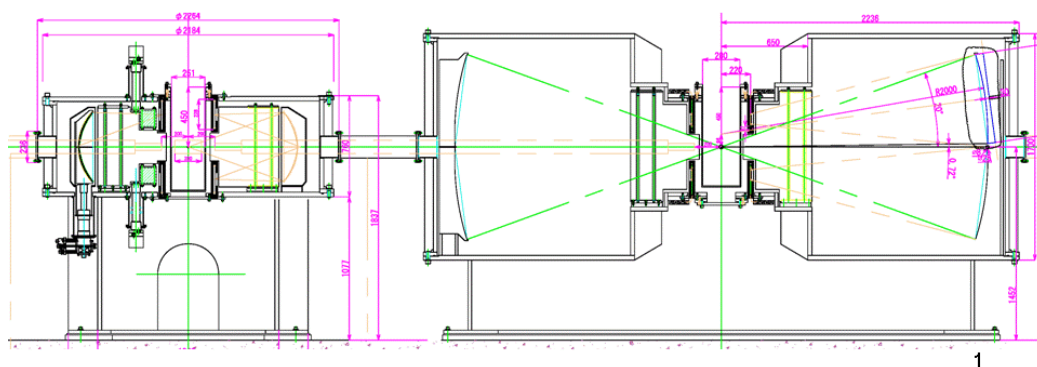
2. Analyzer Mirror System

N. Takahashi (J-PARC)

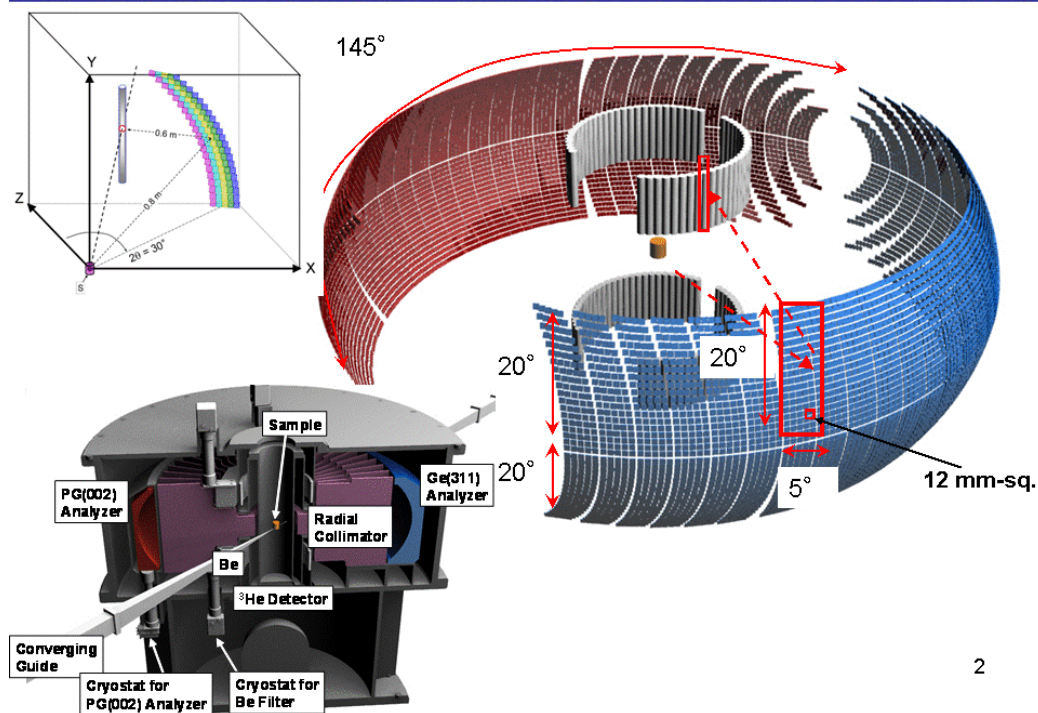


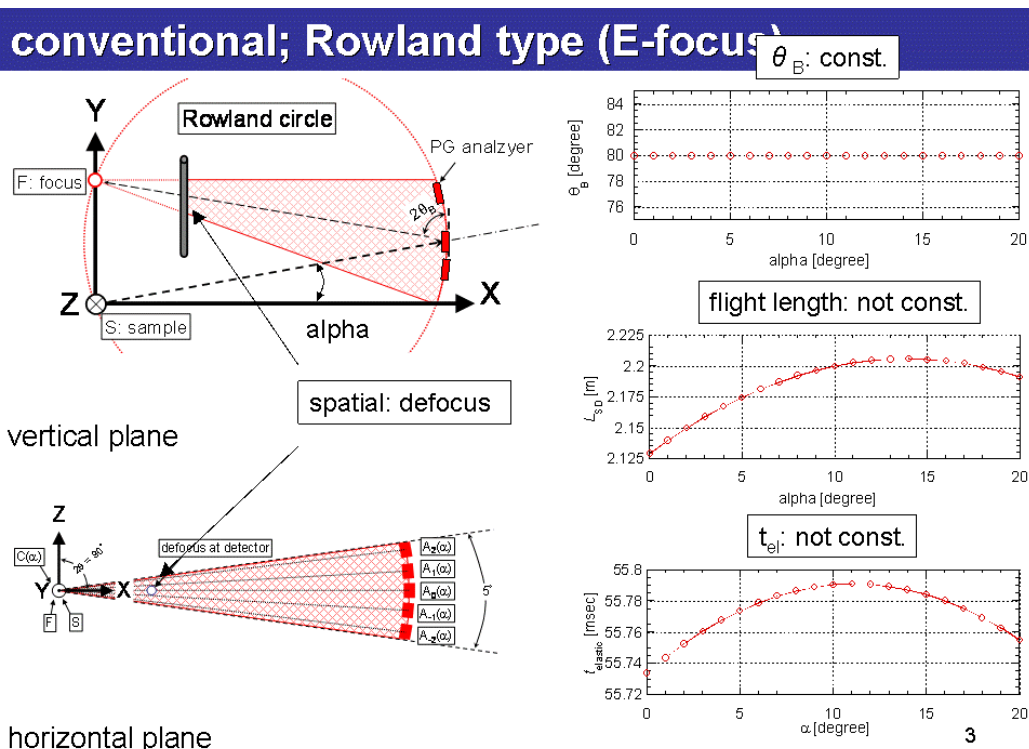
Overview

- 2.1. time-spatial-focusing analyzer mirror system for PG and Ge
- 2.2. Pixel correction system for Si mirror
- 2.3. Analyzer Crystal R&D



2.1. Analyzer bank design





Thermal Diffuse Scattering (TDS) B.T.M. Willis, Univ. Oxford ~20years

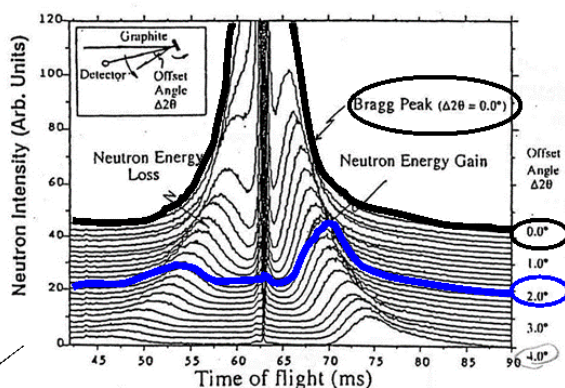
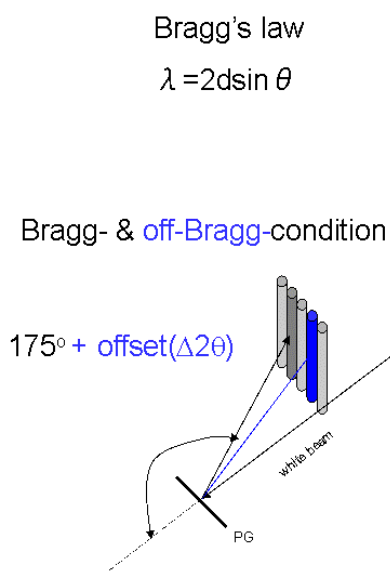
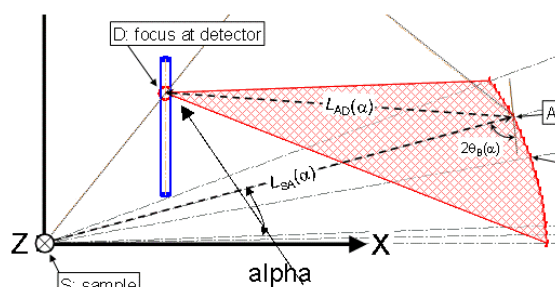


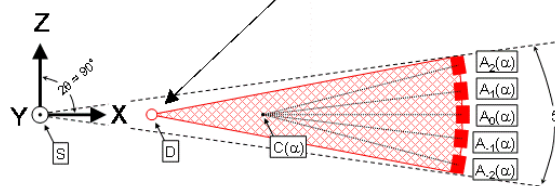
Fig. 2. The scattering patterns from a single crystal of pyrolytic graphite measured by time of flight white beam diffraction at a series of offset angles from the Bragg condition. Peaks due to phonon creation at shorter times and phonon annihilation at longer times are clear as the offset angle increases.

Design of the time-focusing analyzer

N. Takahashi et al.,
NIMA in press.

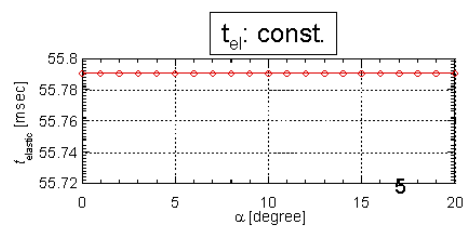
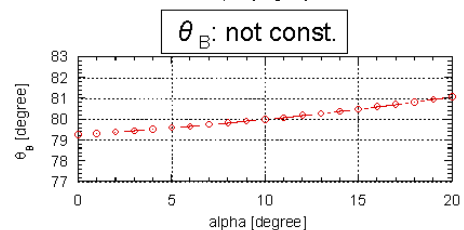
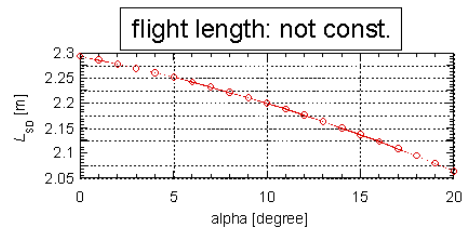


vertical plane



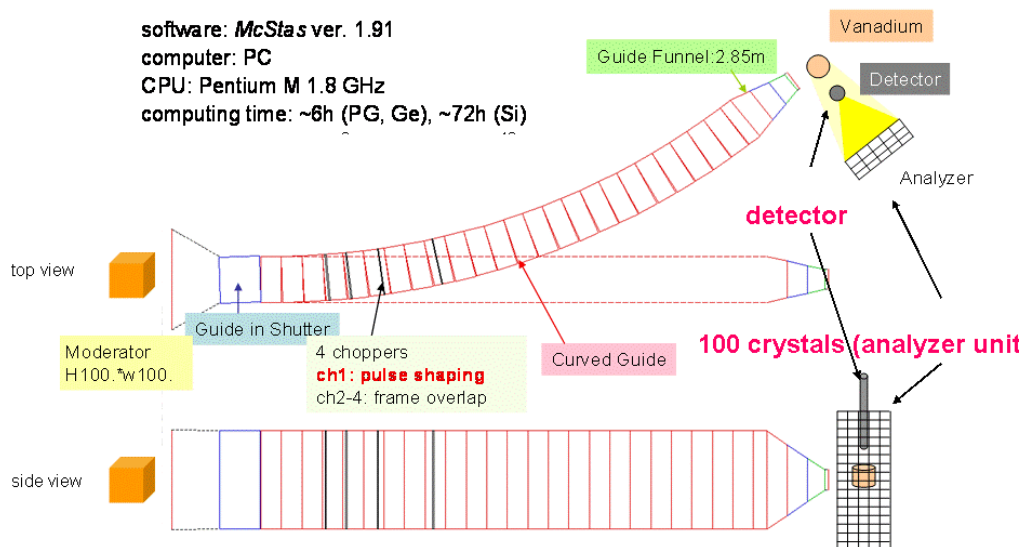
horizontal plane

spatial: focus



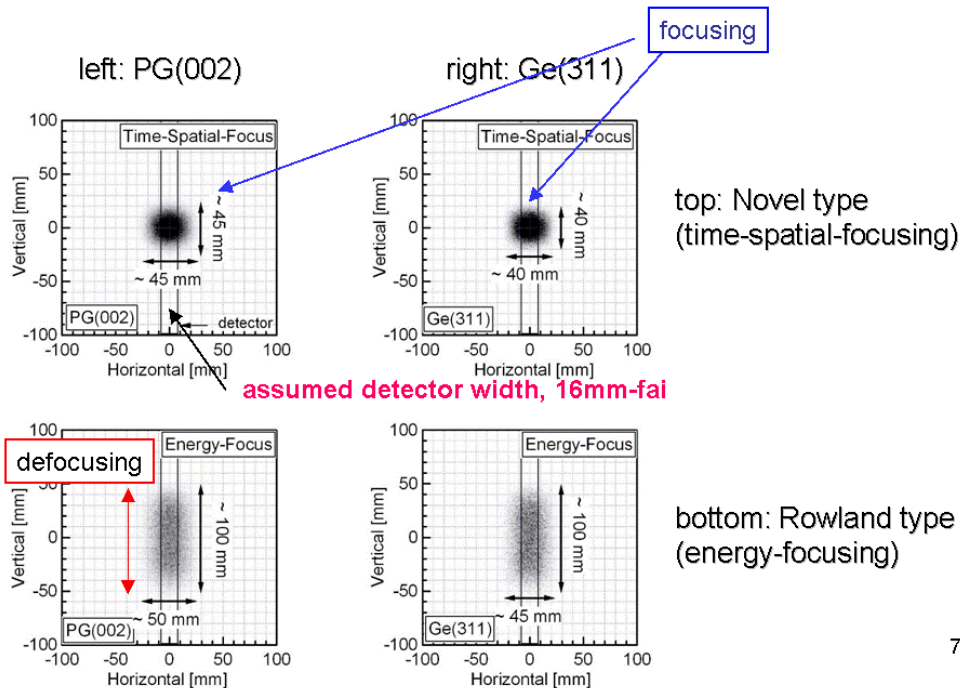
Monte-Carlo Simulation (McStas)

software: **McStas** ver. 1.91
computer: PC
CPU: Pentium M 1.8 GHz
computing time: ~6h (PG, Ge), ~72h (Si)

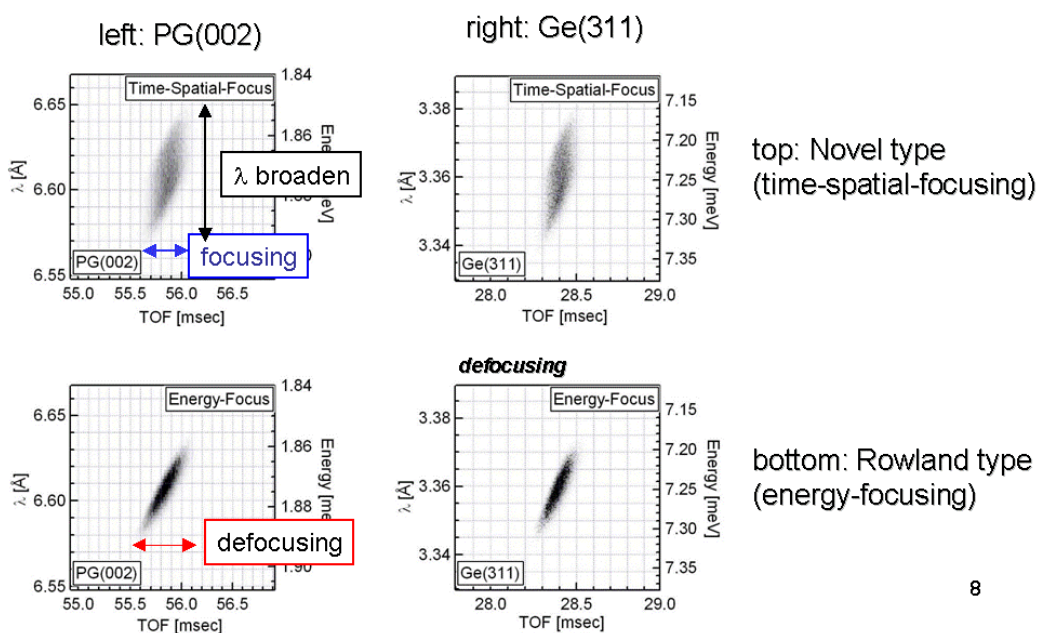


Spatial focusing performances

2D-PSD



Time focusing performances

 λ -TOF monitor

Scattering angle optimization

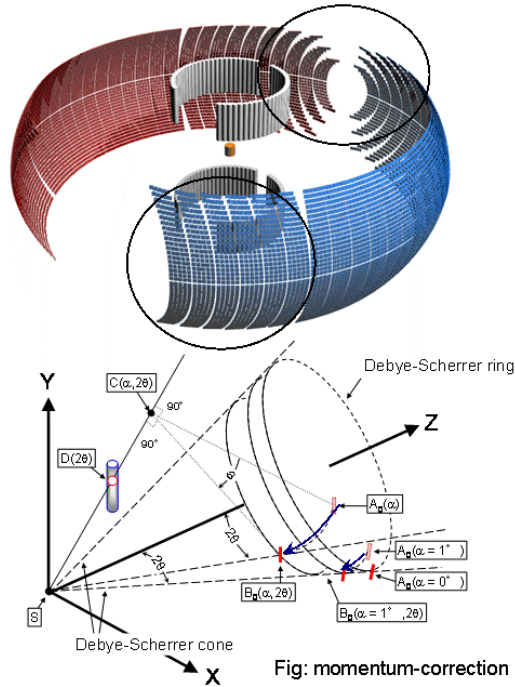


Fig: momentum-correction handling

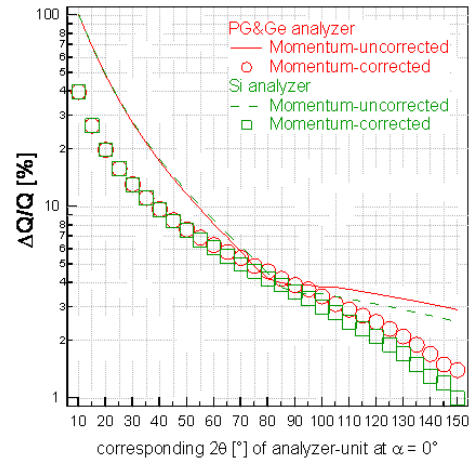


Fig: Q-resolution of momentum-corrected analyzer-units.

9

Appendix. Momentum-correction

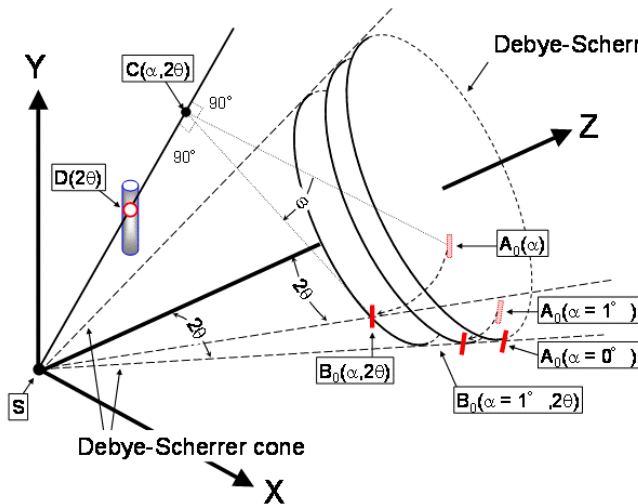
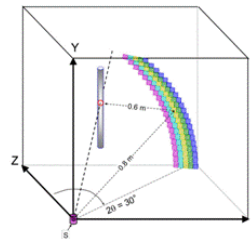


Fig: scattering angle correction of crystal-chips

$$\begin{aligned}\vec{CB}_0 \cdot \vec{CS} &= 0 \\ \vec{SB}_0 \cdot \vec{SZ} &= |\vec{SB}_0| \times |\vec{SZ}| \cos 2\theta \\ |\vec{CB}_0| &= |\vec{CA}_0| \\ \vec{CB}_0 \cdot \vec{CA}_0 &= |\vec{CB}_0| \times |\vec{CA}_0| \cos \omega\end{aligned}$$

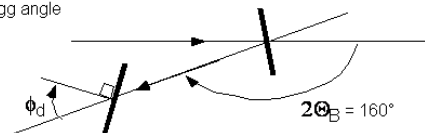


10

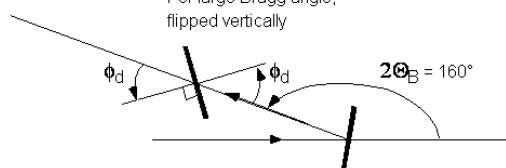
Appendix. detector focusing 1

as in Figs. 10 and 11 of PCP 2005, p1251.
The detector angle is to be measured
in the same sense as the Bragg angle,
and from the L_3 vector to the detector normal.

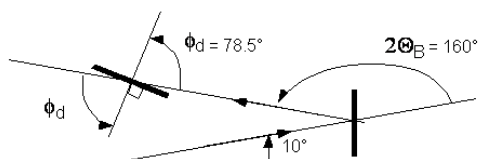
For large Bragg angle



For large Bragg angle,
flipped vertically



For Bragg angle 80° , flipped vertically,
rotated 10° , and for $\phi_d = 78.5^\circ$



11

Appendix. detector focusing 2

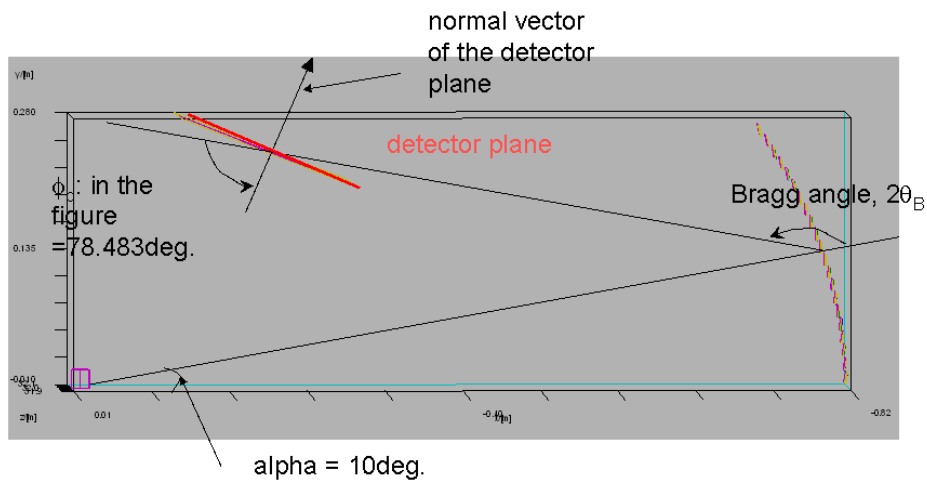
calculation of the theoretical detector
angle ϕ_d in JMC's theory

	mod2smp	smp2xtal	xtal2det	Bragg	JMC
	L1	L2	L3	theta_B	fai-d
	[mm]	[mm]	[mm]	[deg]	[deg]
PG	32000	800	600	80	78.48315
Si	32000	1200	989	87.5	37.05216
					43.97

12

Appendix. detector focusing 3

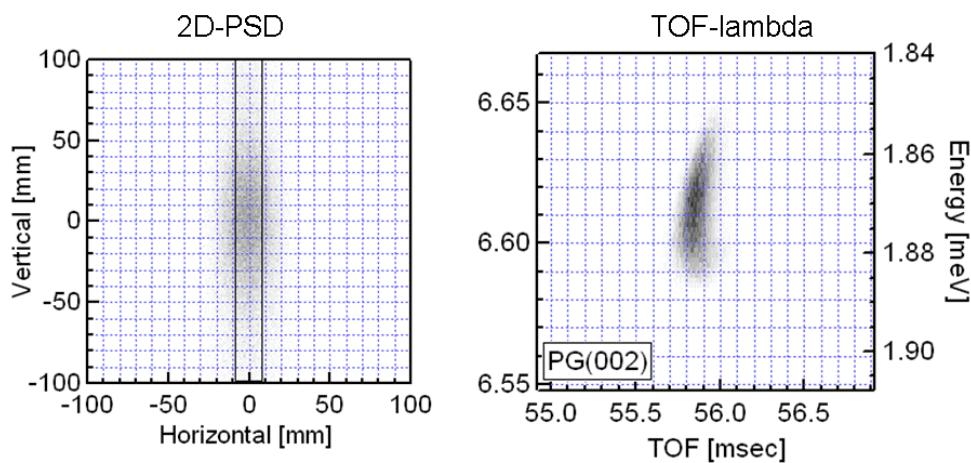
definition of the detector focusing angle, ϕ_d



13

Appendix. detector focusing 4

results $\phi_d = 78.483\text{deg.}$



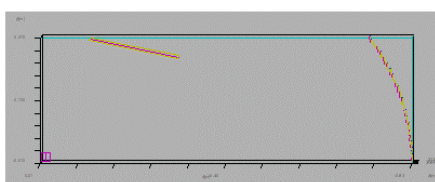
got worse compared to our result.

got better compared to our result.

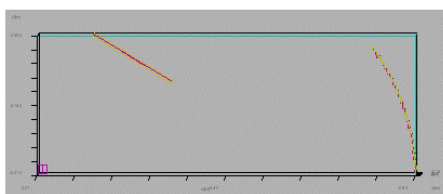
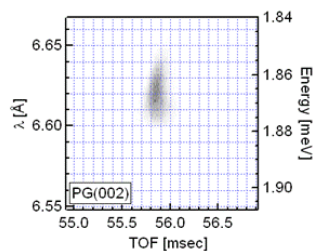
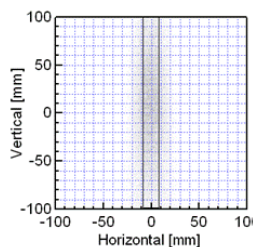
14

Appendix. detector focusing 5

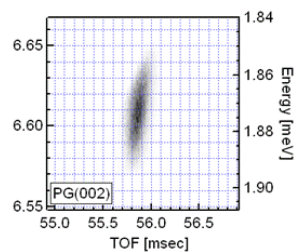
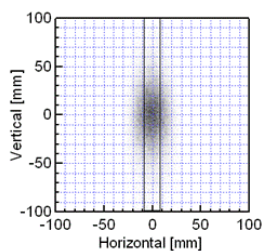
ϕ_d dependence 1



$88.483^\circ = \text{optimum} + 10^\circ$



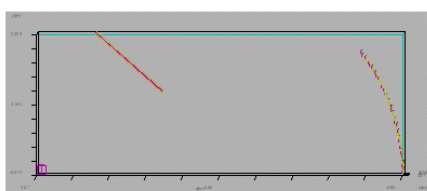
$68.483^\circ = \text{optimum} - 10^\circ$



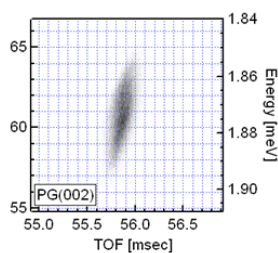
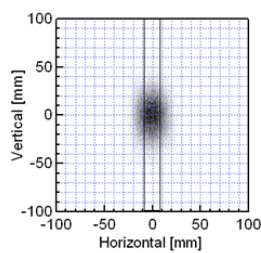
15

Appendix. detector focusing 6

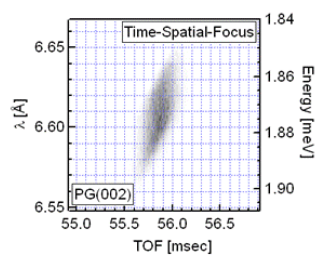
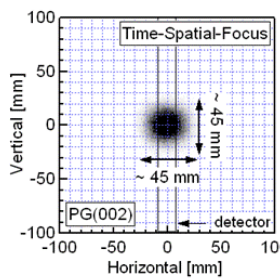
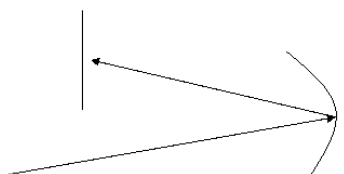
ϕ_d dependence 2



$58.483^\circ = \text{optimum} - 20^\circ$

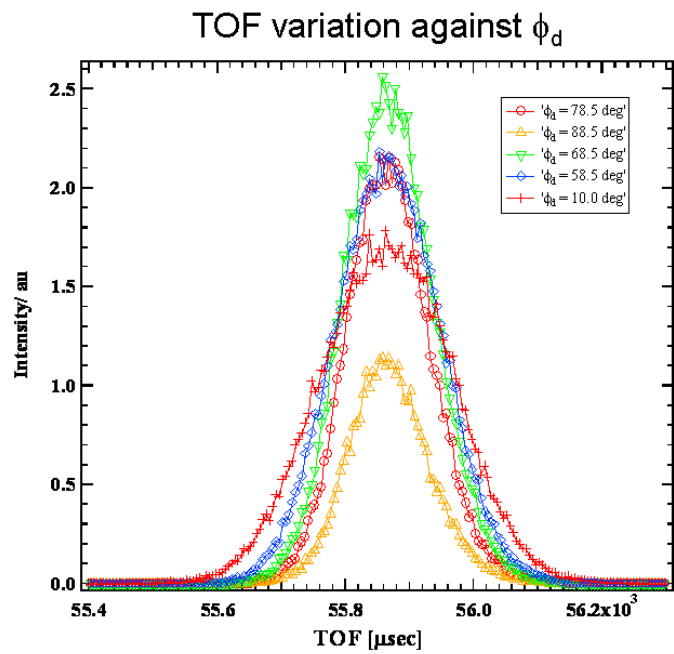


our case: $10^\circ = \text{optimum} - 68.483^\circ$



16

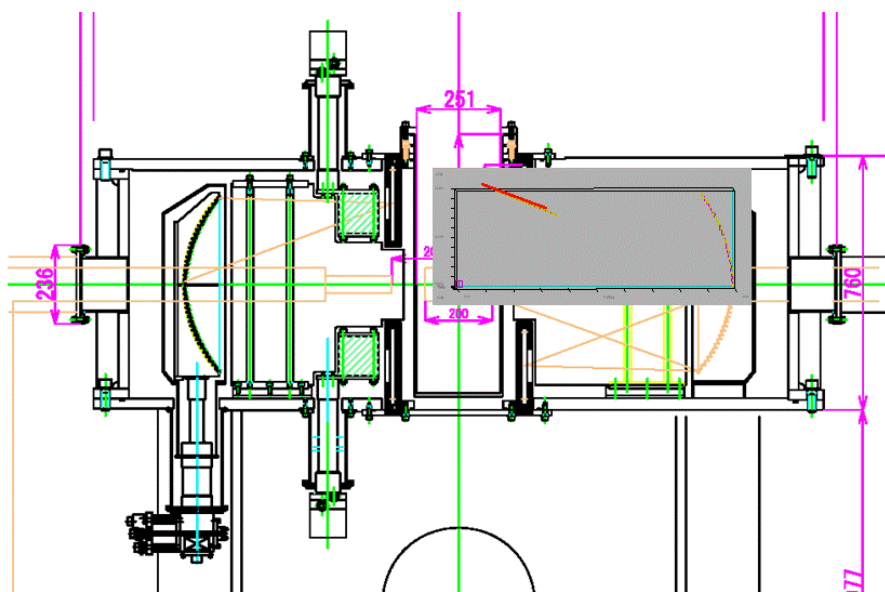
Appendix. detector focusing 7



17

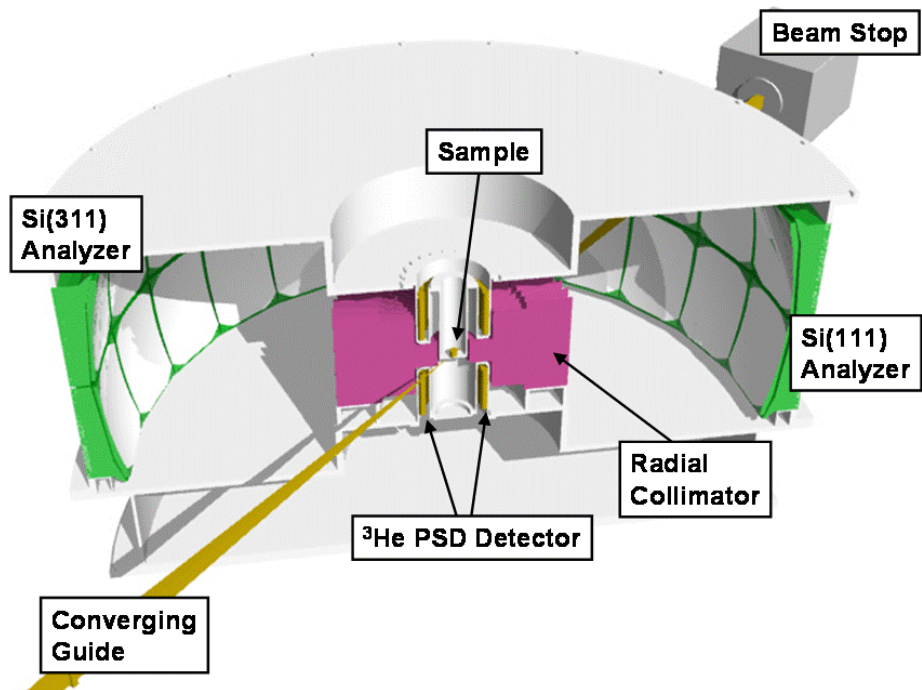
Appendix. detector focusing 8

Spatial bottleneck



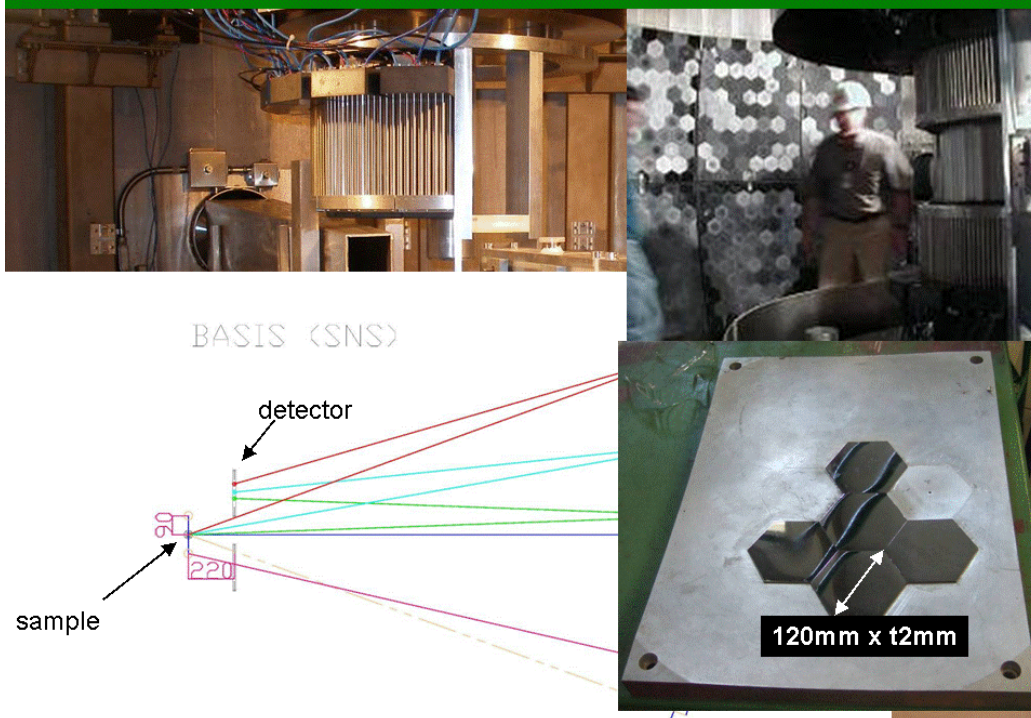
18

2.2. Pixel correction system for Si mirror

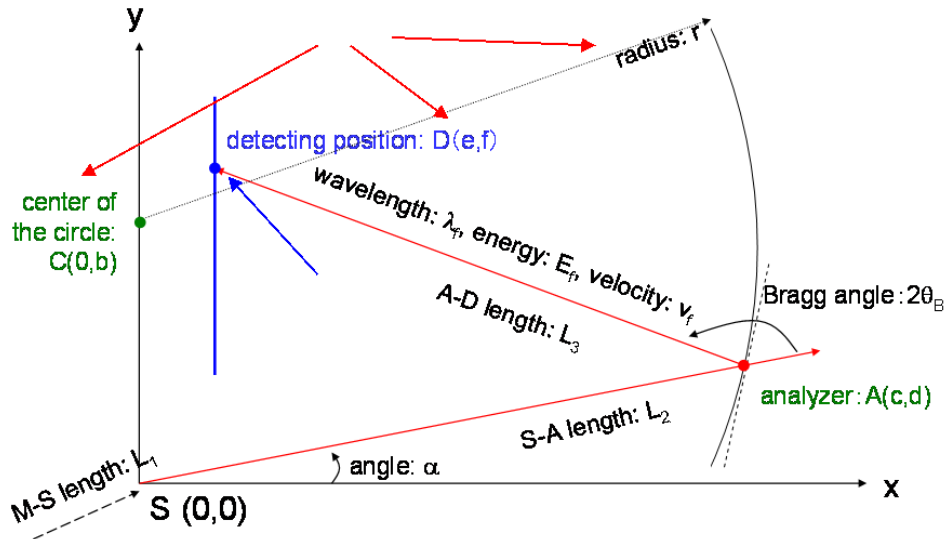


19

BASIS



Optimization of the design parameters



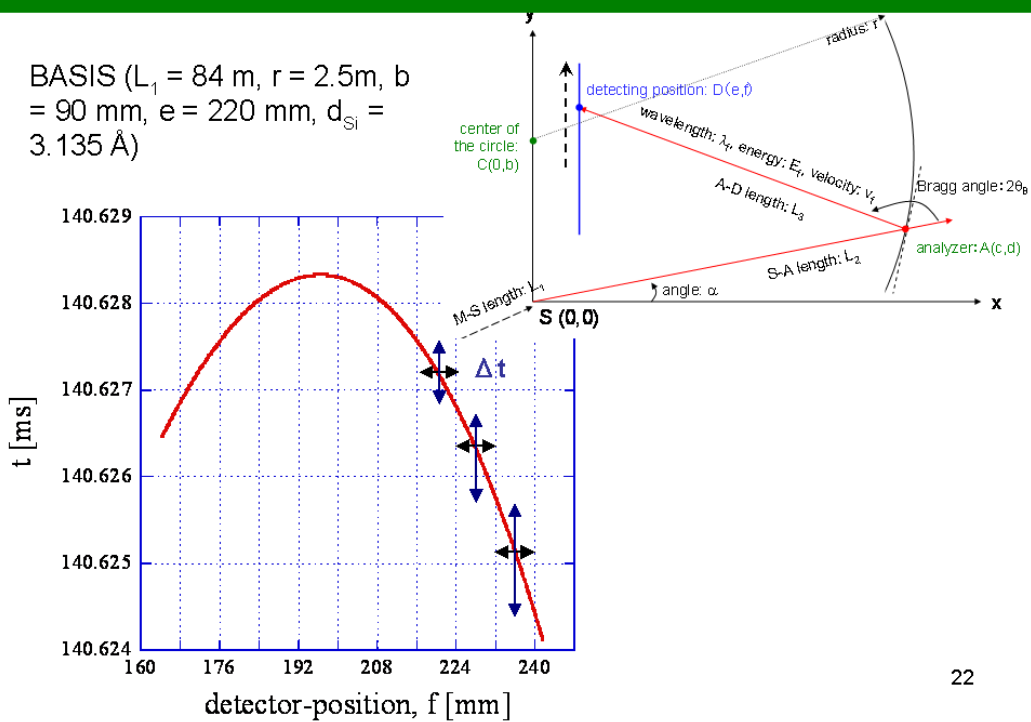
Arguments; C: center of the sphere, e: x-coordinate of detector, r: radius

Solutions: $t(f)$; f: y-coordinate of detectable position, t: TOF

21

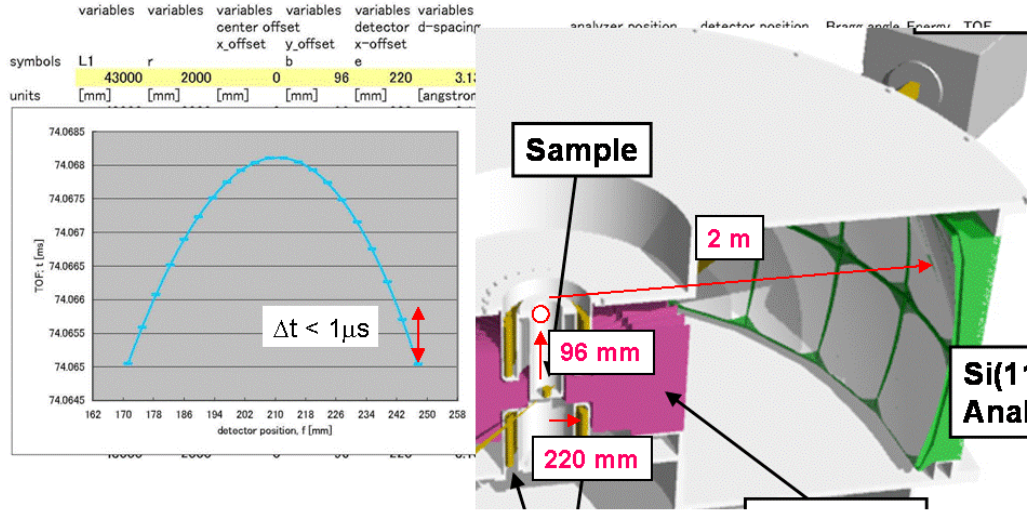
Result: BASIS

BASIS ($L_1 = 84$ m, $r = 2.5$ m, $b = 90$ mm, $e = 220$ mm, $d_{Si} = 3.135$ Å)



22

Result: DNA



23

contribution of delta-t on resolution

Total Resolution $\Delta\hbar\omega$

$$\Delta\hbar\omega = \sqrt{\delta\hbar\omega_p^2 + \delta\hbar\omega_s^2}$$

Primary (moderator-to-sample)

$$\delta\hbar\omega_p = 2E_i \left\{ \left(\frac{\delta x_1}{L_1} \right)^2 + \left(\frac{\Delta t_{ch}}{t_i} \right)^2 \right\}^{\frac{1}{2}}$$

In the DNA case, we use pulse-shape chopper. Then, Δt_{ch} is an opening time of the pulse-shaping chopper. When counter-rotating double-disc choppers ($f=300\text{Hz}$, $r=300\text{mm}$, $d=30\text{mm}$) are used, we can obtain $\Delta t_{ch} \sim 26 \mu\text{s}$.

$$\delta\hbar\omega_p \sim 1.97 \mu\text{eV}$$

Secondary (sample-to-analyzer)

$$\delta\hbar\omega_s = 2 \left\{ E_i^2 \left(\frac{\Delta x}{t_i} \right)^2 + E_f^2 \left[\cot(\theta_B) \delta\theta_B^2 + \left(\frac{\delta d_{Si}}{d_{Si}} \right)^2 \right] \right\}^{\frac{1}{2}}$$

When we choose parameters; $\delta\theta_B = 7.5 \text{ mrad}$, $\delta d_{Si}/d_{Si} = 3.5 \times 10^{-4}$. Then,

$$2E_f \cot(\theta_B) \delta\theta_B^2 \sim 1.48 \mu\text{eV}$$

$$2E_f \left(\frac{\delta d_{Si}}{d_{Si}} \right)^2 \sim 1.46 \mu\text{eV}$$

From the previous slide, $\Delta t < 1 \mu\text{s}$, then,

$$2E_i \left(\frac{\Delta t}{t_i} \right)^2 < 0.07 \mu\text{eV}$$

$$\delta\hbar\omega_s \sim 2.08 \mu\text{eV}$$

$$\Delta\hbar\omega \sim 2.86 \mu\text{eV}$$

Finally, the contribution of Δt on the total resolution is negligible.

24

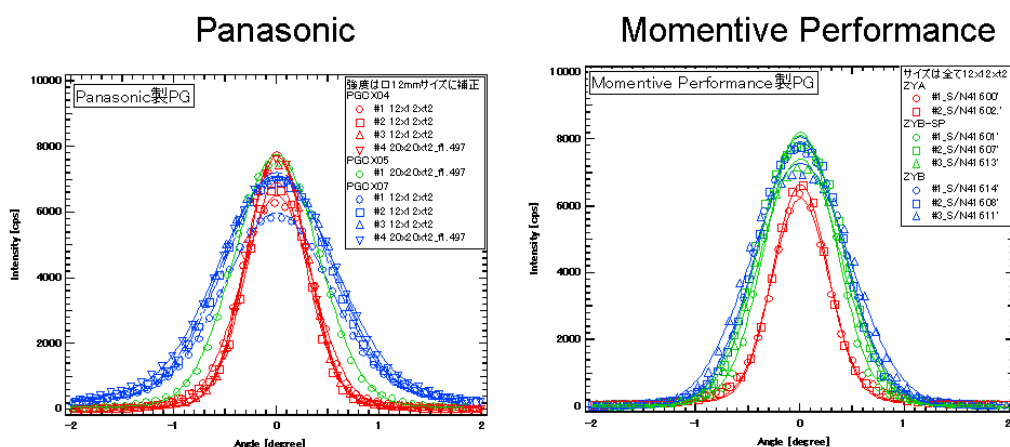


2.3. Analyzer Crystal R&D

2.3.1. PG(002), cost & performance

2.3.2. Ge(311), hot press

2.3.1. Neutron beam tests of PG(002)



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Summary of PG(002)

our target: 0.7 deg +/- 0.1 deg.

1\$=¥105

vender	model	mosaic spread (deg)*1	cast (\$)	note
Panasonic	PGCX04	X: 0.40~0.50 N: 0.62, 0.63, 0.64, 0.76, (0.61-0.82)		・size: 12.0±0.3mm t2.0±0.1mm
	PGCX05	X: 0.51~0.60 N: 0.91, 0.94, 0.99, 1.02, (0.69-0.78)		・recipe: stacking polyimide film and sintered at 3000°C at high pressure. (solid phase-solid phase method)
	PGCX07-SP	X: 0.6 ~0.8 N:	173	
	PGCX07	X: 0.61 ~1.00 N: 1.19, 1.20, 1.23, 1.28	173	
Momentive Performance	ZYA	X: 0.30~0.50 N: 0.55, 0.58, (0.55)		・size: 12.0±0.2mm t2.0±0.2mm
	ZYB-SP	X: 0.30~0.7 N: 0.72, 0.86, 0.88	162	・recipe: crystal growth of hydro carbon gas on a base material. (vapor- phase growth method)
	ZYB	X: 0.60~1.0 N: 0.89, 0.93, 1.09	113	
Optigraph	AGraph Z	X: 0.4 (catalog) →0.6 (exp) N: 1.8		28
	AGraph X	X: 0.8 N:		

2.3.2. Ge(311) stacking

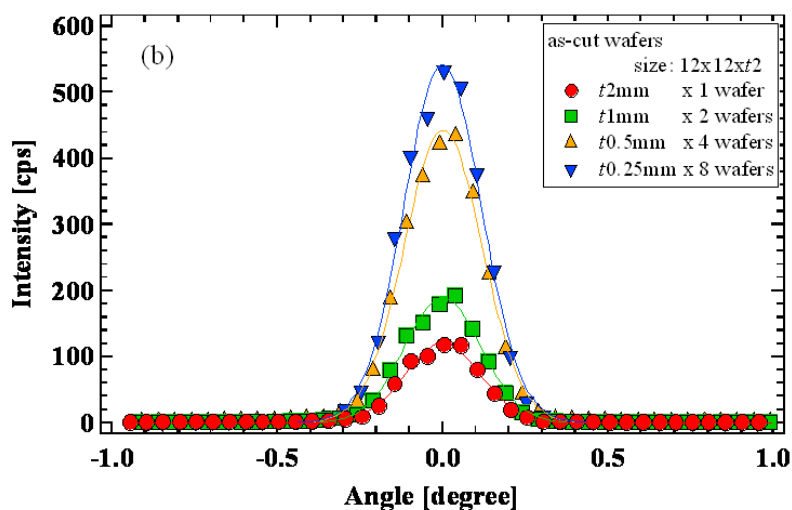


Fig. Rocking Curve of Ge(311) as-cut wafers. The total thicknesses are 2 mm.

Stacking thin wafers makes intensity gain. On the other hand, there is no bad influence on the width of the curve.

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hot press

$T = 888\text{ }^{\circ}\text{C}$, $P = 50 \sim 300\text{ kgf/cm}^2$

our target mosaic: 0.5 deg.

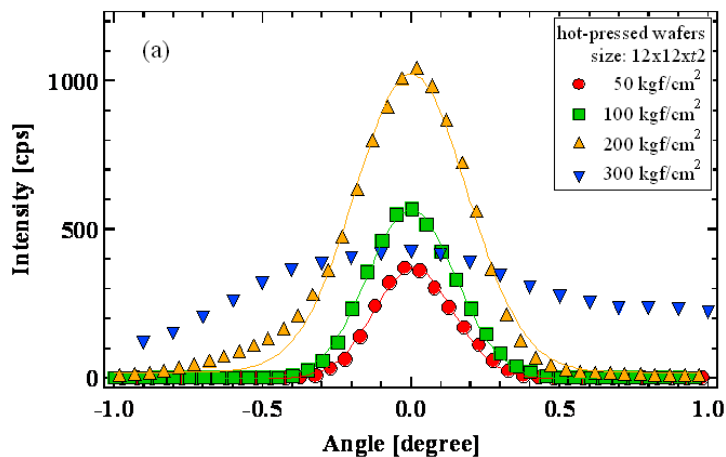


Fig. rocking curves of hot pressed Ge(311) crystals.

/ Hot press treatment is much better than stacking as-cut wafers.

/ Optimum pressure is 200 kgf/cm².

mosaic: av. $0.35^{\circ} \pm 0.15^{\circ} < 0.5^{\circ}$

30

Appendix. comparison with LAM-40 at KENS

Table: hot pressed Ge(311) crystals used in LAM-40 at KENS

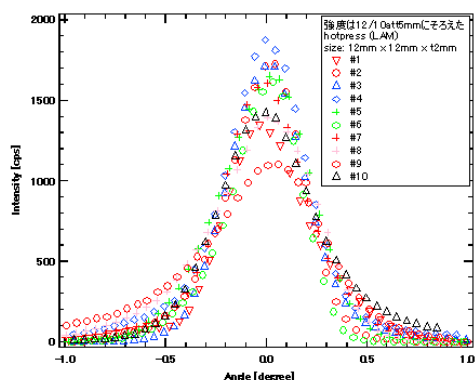
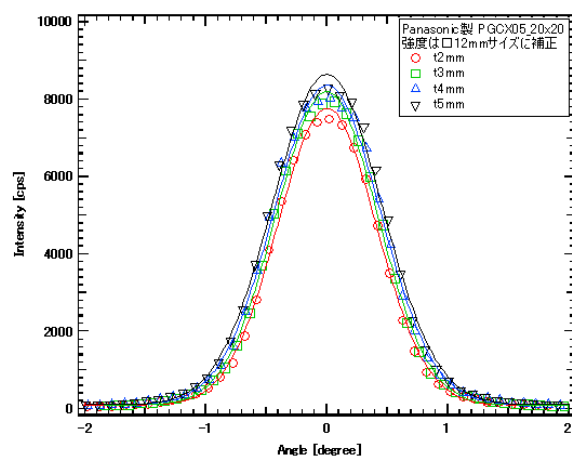


Fig. rocking curves of hot pressed Ge(311) wafers used in LAM-40.
size: 12 x 12 x t2

	mosaic η [degree]	integrated intensity I [-]	note
#1	0.32	461	
#2	0.33	611	
#3	0.40	720	
#4	0.35	692	
#5	0.44	767	
#6	0.29	494	
#7	0.38	655	
#8	0.50	747	
#9	0.56	658	
#10	0.47	706	
LAM-40	0.40	651	average
JAEA	0.33	352	P=200kgf/cm²

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Appendix. Neutron beam tests of PG(002) thickness



PGCX05

thickness t [mm]	mosaic η [度]	integrated intensity I [-]	FOM * I/ η^2 [-]
2	0.910	1.00	1.00
3	0.938	1.09	1.03
4	0.986	1.17	1.00
5	1.016	1.25	1.00

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Appendix. data spread

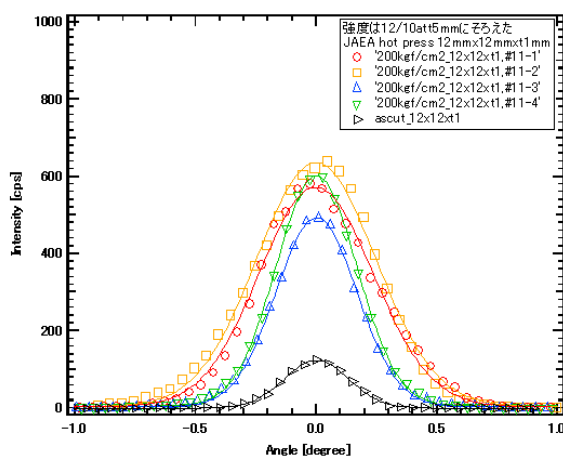


Fig. Ge(311) hot pressed at $P = 200 \text{ kgf/cm}^2$

Table: data spread of Ge(311) hot pressed at $P = 200 \text{ kgf/cm}^2$

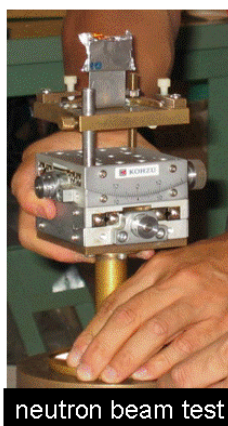
	mosaic η [degree]	integrated intensity I [-]	note
#1	0.46	277	t=1mm
#2	0.49	326	t=1mm
#3	0.24	125	t=1mm
#4	0.23	148	t=1mm
av.	0.35	219	t=1mm

data spread: av. $0.35 \pm 0.15 < 0.5$

33

Appendix. measurement conditions

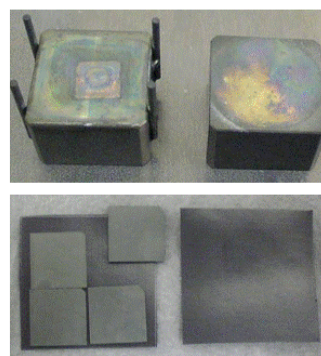
- 3axis (MUSASI@JRR3 guide hall)
- $E_i = 13.5 \text{ meV}$
- collimator: [Mon. PG002]-[20']-[sample]-[40']-[Det.]
- attenuator: acrylic board, t5mm



neutron beam test



hot press instrument



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2.4 Neutron Transportation System

Nobuaki Takahashi (JAEA)

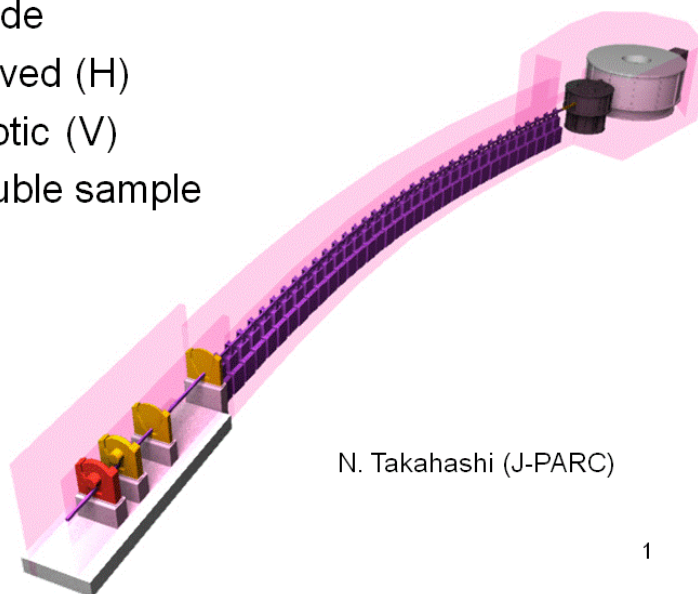
3. Neutron Transportation System



Outline

3.1. neutron guide

- 3.1.1. curved (H)
- 3.1.2. elliptic (V)
- 3.1.3. double sample



N. Takahashi (J-PARC)

1

3.1. neutron guide

Required Performance

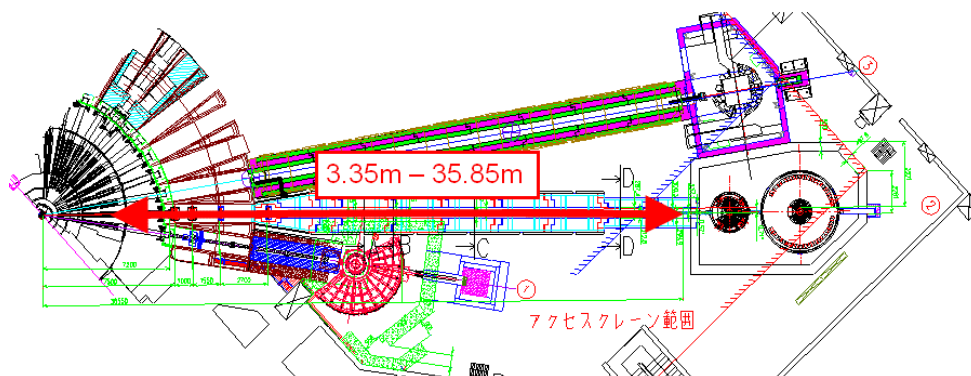
- High Intensity
 - taking advantage of high int. at low-E (~2meV)
- spatial, angular distribution at sample
 - not necessary very fine ones
- $E < 40\text{meV}$ is sufficient
 - $E_{f_Ge311} = 7.2\text{meV}$, $E_{f_Ge933} = 65\text{meV}$

2

3.1.1. curved (H)

Table. design parameters of curved guides

	m [-]	w [mm]	R [m]	L* [m]	curved section [m]	L1[m]	E* [meV]
DNA	3	60	2200	32.5	32.5 (3.35~35.85)	39	40
IRIS	-	43	2350	28.4	31.3	36.41	13



3

3.1.2. elliptic (V)

N. Takahashi et al., Proc. ICANS-XVIII

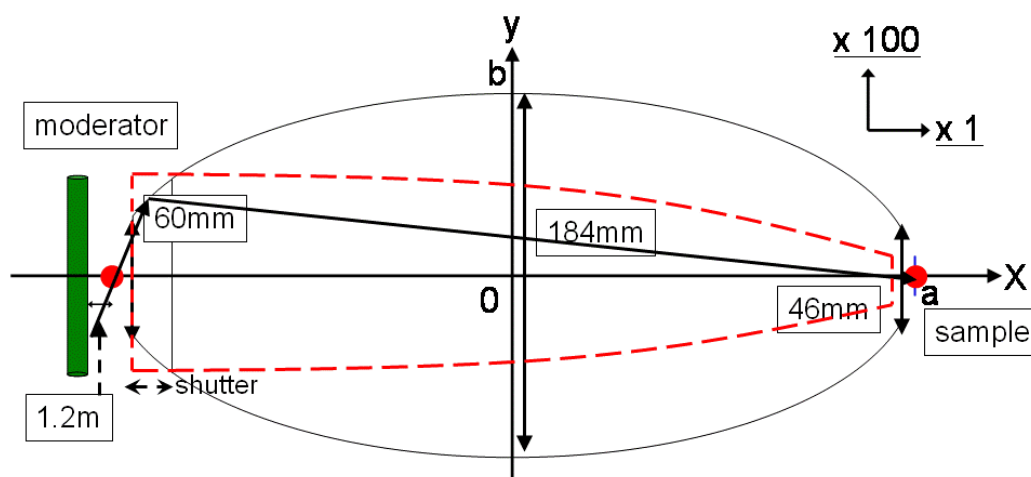
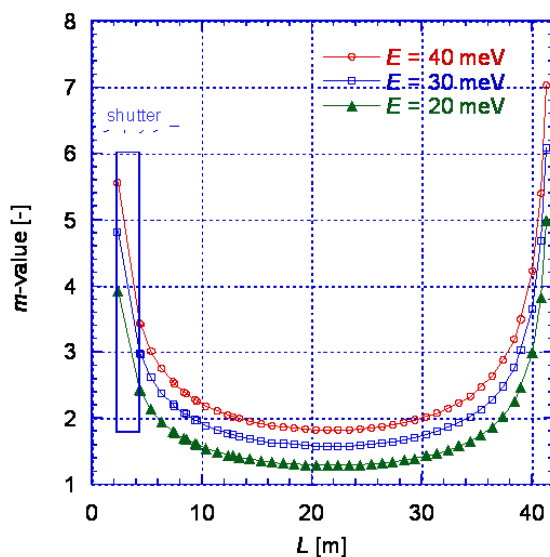


Fig. elliptic guide

4

mirror index optimization

Fig. L-dependence of m -value

5

Summary of neutron guide1: geometry

shutter
 L: 2.3m → 4.3 m
 w: 60mm (straight)
 h: 60mm → 98mm (elliptical)
 m: 3

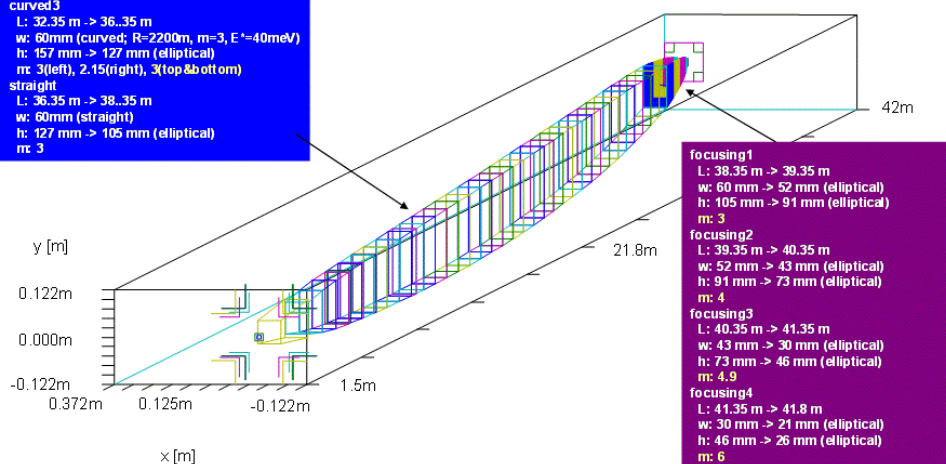
curved1
 L: 4.35 m → 12.35 m
 w: 60mm (curved; R=2200m, m=3, E'=40meV)
 h: 98 mm → 164 mm (elliptical)
 m: 3(left), 2.15(right), 3(top&bottom)

curved2
 L: 12.35 m → 32.35 m
 w: 60mm (curved; R=2200m, m=3, E'=40meV)
 h: 164 mm → 184 mm → 157 mm (elliptical)
 m: 3(left), 2.15(right), 2.15(top&bottom)

curved3
 L: 32.35 m → 36.35 m
 w: 60mm (curved; R=2200m, m=3, E'=40meV)
 h: 157 mm → 127 mm (elliptical)
 m: 3(left), 2.15(right), 3(top&bottom)

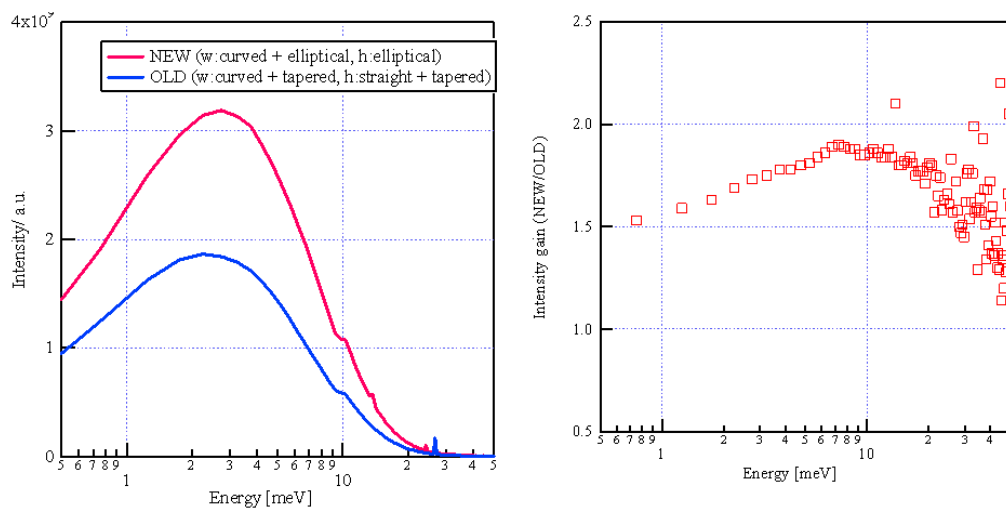
straight
 L: 36.35 m → 38.35 m
 w: 60mm (straight)
 h: 127 mm → 105 mm (elliptical)
 m: 3

the guide geometry of DNA spectrometer



6

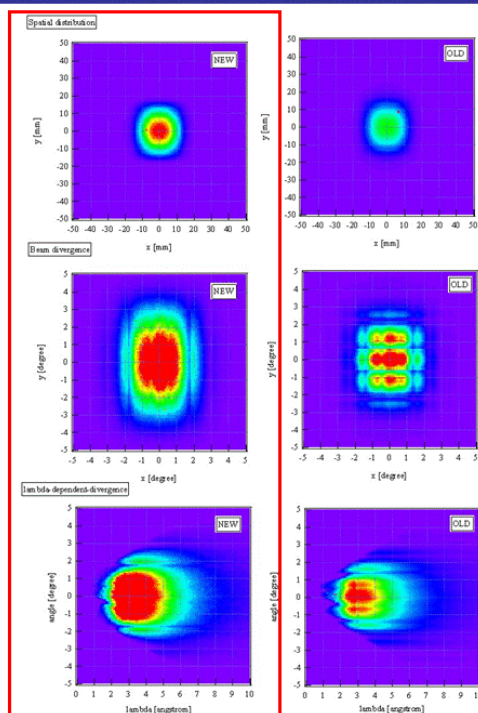
Summary of neutron guide2: performance



7

Spatial distribution & Beam divergence

New model



spatial distribution

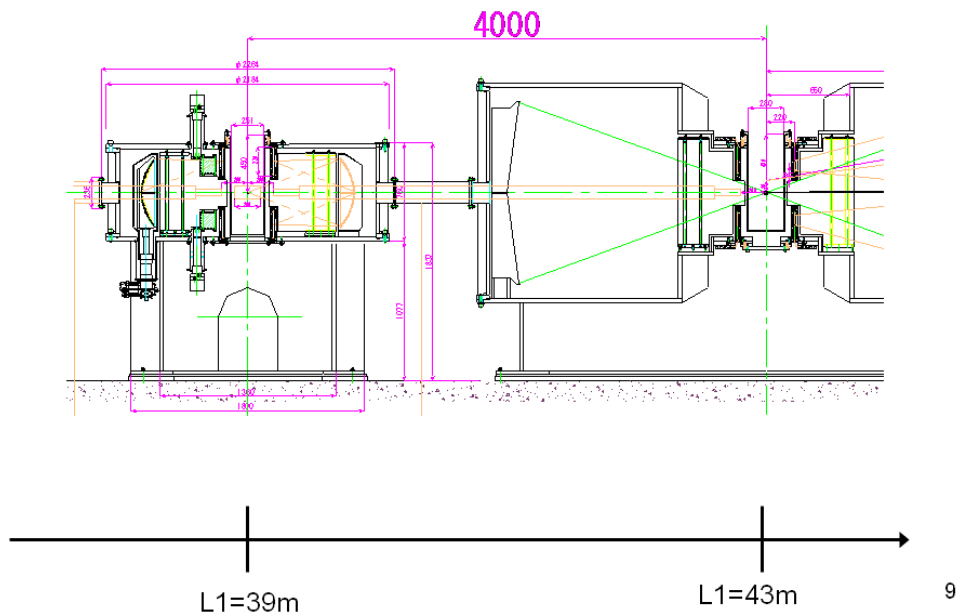
beam divergence

divergence v.s.
wavelength

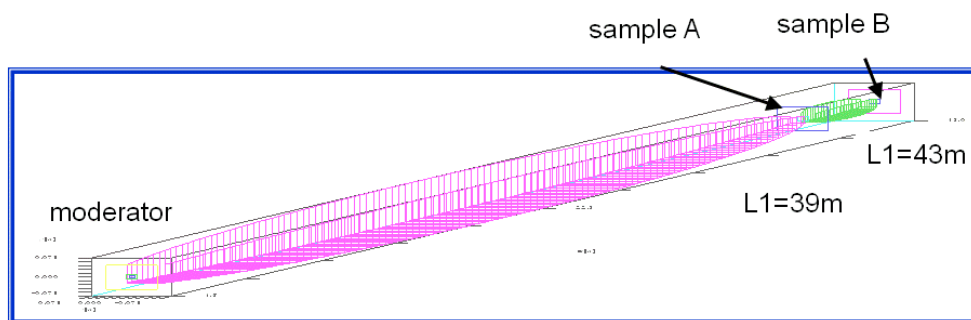
8

3.1.3. double sample system

- Introducing neutrons effectively toward a sample in the vessel at downstream



double focusing guide system (elliptic)



The first neutron guide. (red)

- V&H: elliptic. Focal points are moderator & sample.
- cross section of exit at $L=38.8\text{m}$; 27 mm-sq.

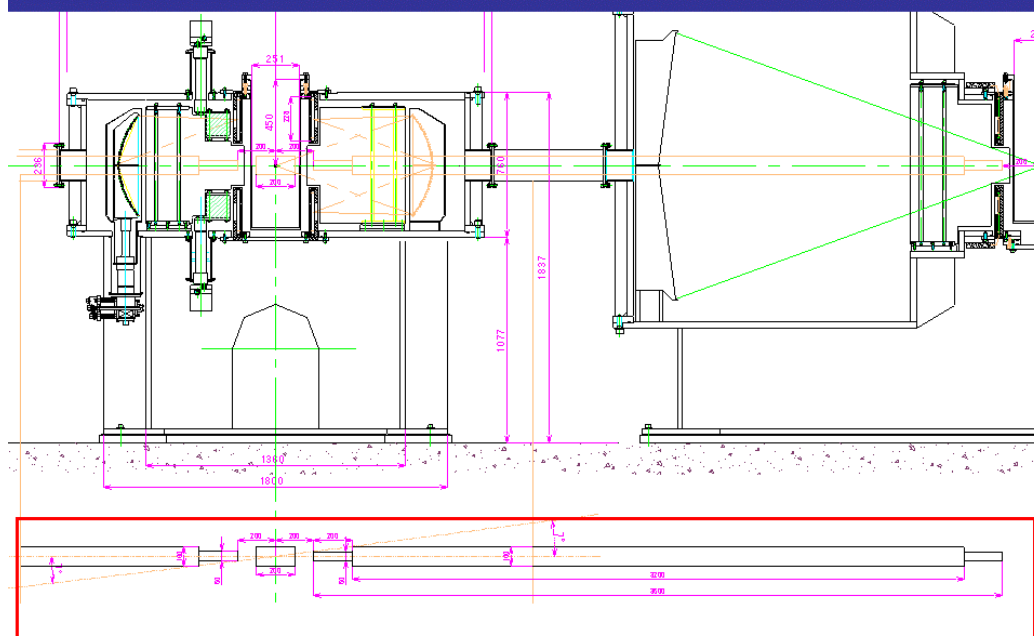
The second neutron guide. (green)

- L : 39.2 m $\rightarrow$ 42.8 m
- V&H: elliptic. focal points are both samples.
- cross section of entrance at $L=39.2\text{ m}$ & exit at $L=42.8\text{m}$; 27 mm-sq.
- 6 Qc supermirror

Intensity ratio, sample-B / sample-A 60% ~ 70%

10

discussion..



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2.5 Spectrometer Packaging

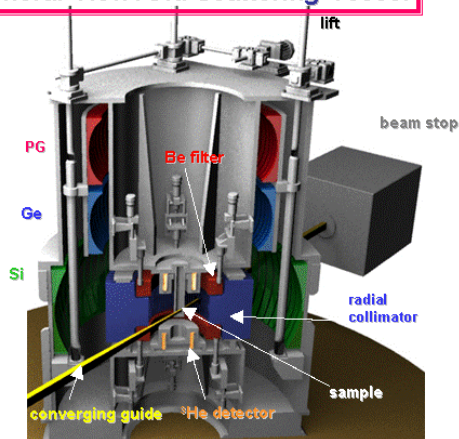
Kaoru Shibata (JAEA)

4. Spectrometer Packaging

Outline

/ vacuum chamber
 / mirror cooling
 / Be filter
 / solar collimator
 / U-tube PSD
 / diffraction detectors
 / sample environment

General View : Old Scattering Vessel



• High Cost Scattering Vessel
 ~ 38M.JPY

• Complex Structure to be
 difficult the cooling PG mirror.



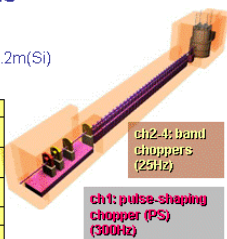
Separate Double Scattering
 Vessel

> 10M.JPY

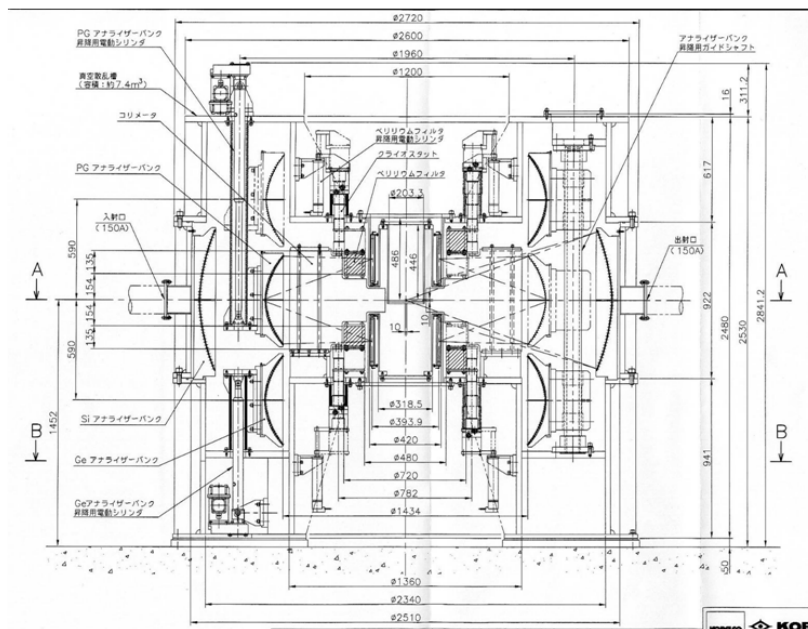
SPECIFICATIONS

- Source: Coupled (25Hz)
- Flight length: L1=42m,
L2=1.4m(PG,Ge)/2.2m(Si)
- Scattering angle: 7.5° ~ 152.5°
- 3 analyzers: ΔQ=1.1μ str

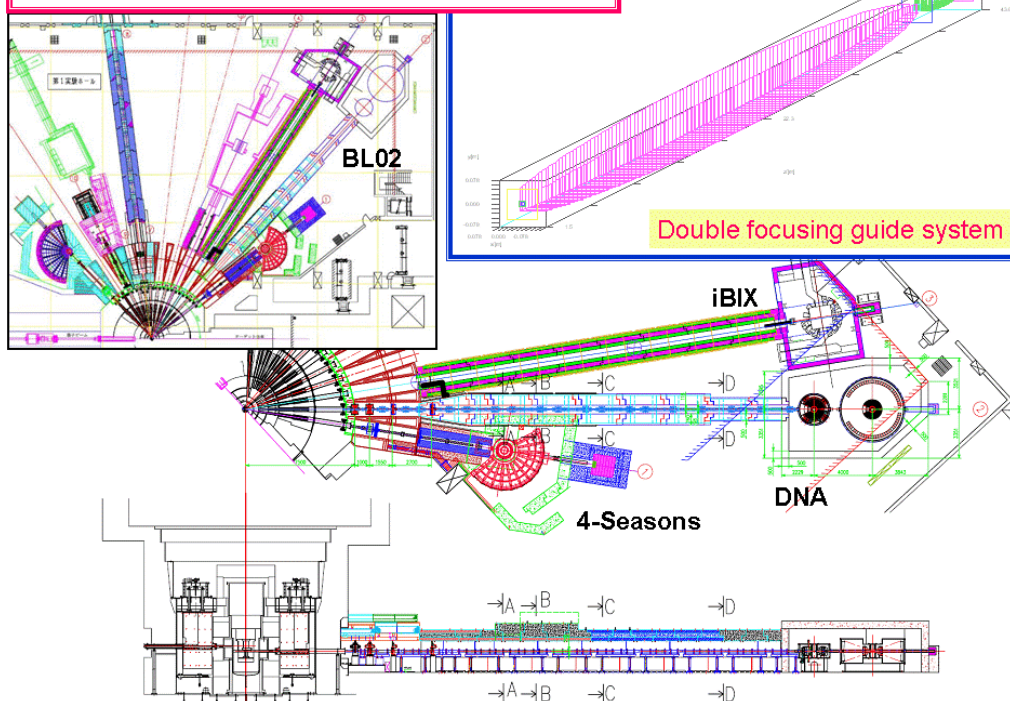
	ch1	ch2	ch3	ch4
application	pulse-shaping	band-chopper		
disc	Double	Double	Single	Single
L [m]	7.5	8.5	10.05	12.75
f [Hz]	300	25	25	25
slit	30 mm	96"	113"	144"



Old Plan of Scattering Vessel

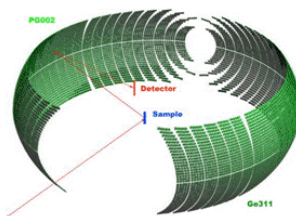


Over View: DNA Beam Line Plan at CM



Upper stream part of
DNA:
PG002&Ge311
Analyzer Crystals

Configuration of Crystal Analyzer



Principle of TOF focusing

The neutron beam which each crystal piece on the crystal analyzer reflected, is focused on the same point on a neutron detector at same tof time.

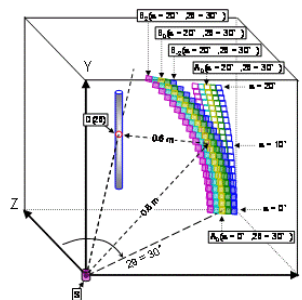


Fig: drawing of an analyzer-unit at $2\theta = 30^\circ$

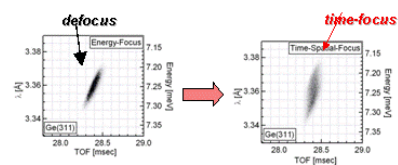
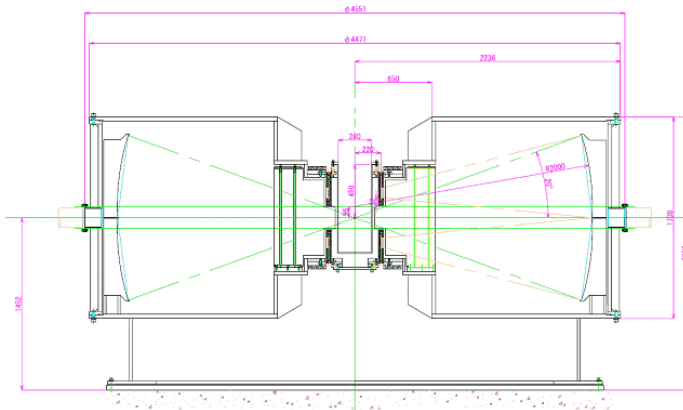
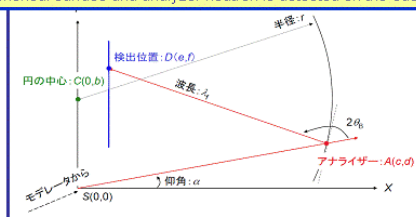


Fig: λ -TOF monitor @ detector-position

Downstream part of DNA: Si111&Si311 Analyzer Crystals

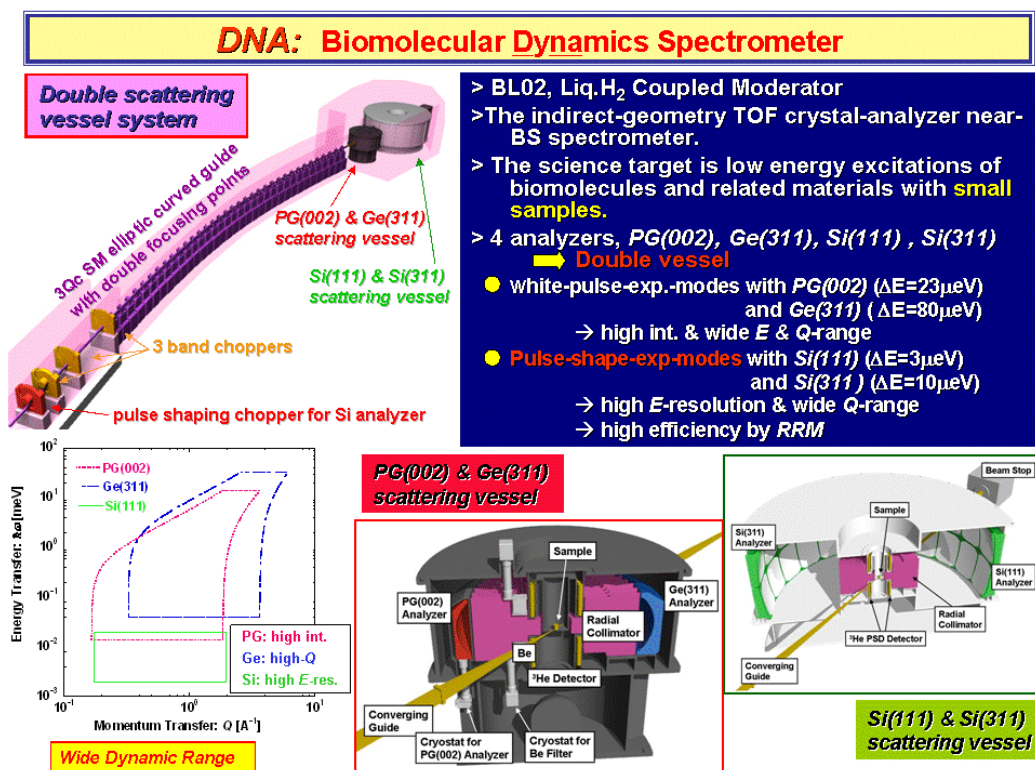
Principle of Si crystal analyzer

Si wafer is stacked on the
Spherical surface and analyzer neutron is detected on the each PSD position.



BASIS@SNS



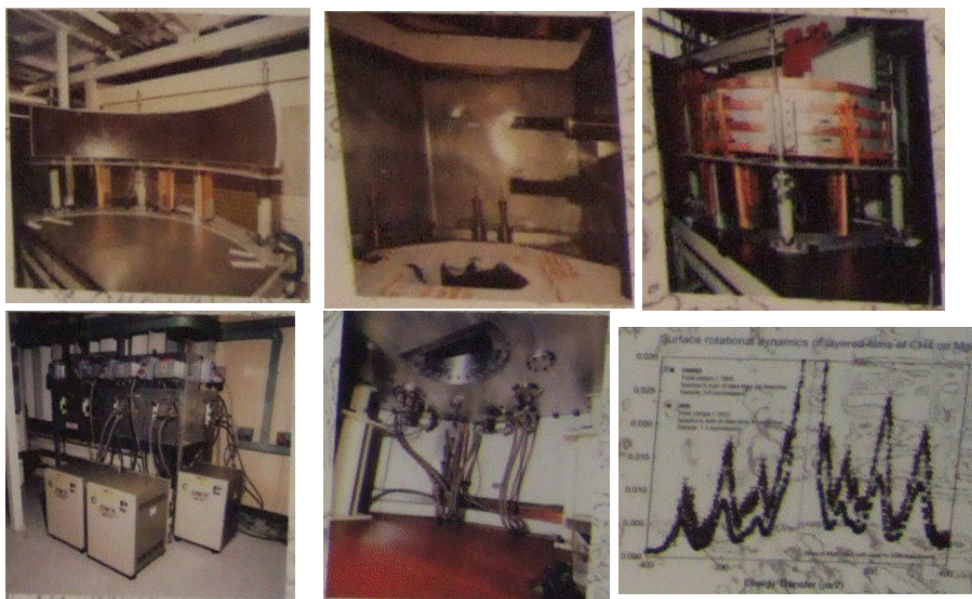


4. Spectrometer Packaging

- / vacuum chamber
- / **mirror cooling**
- / Be filter
- / solar collimator
- / U-tube PSD
- / diffraction detectors
- / sample environment

Cooling of the OSIRIS Graphite Analyser

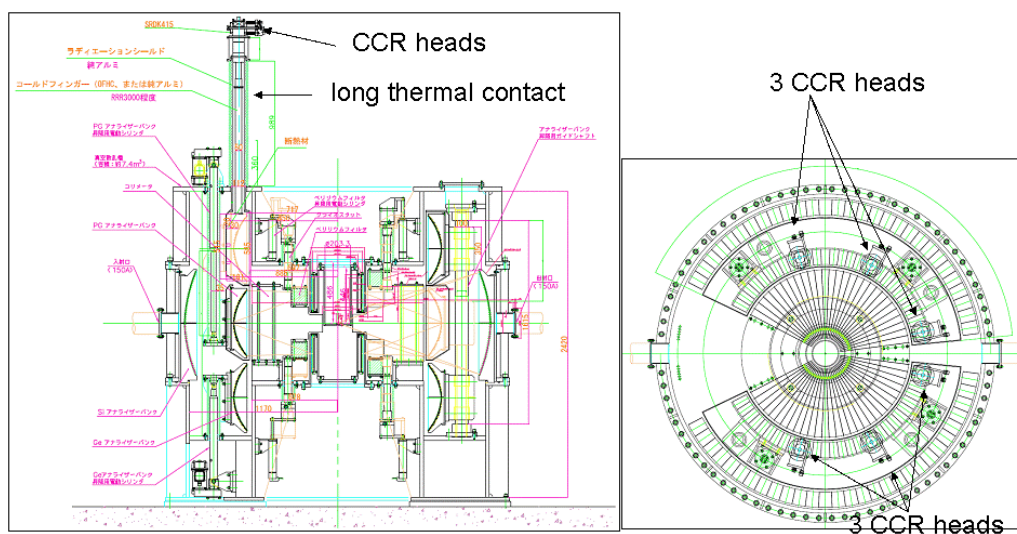
- Reduce the TDS.
- installation of three 4K Sumitomo CCR heads. Machining of the three holes entailed
- the cooldown to a steady temperature $\sim 4.0\text{K}$ in just 48 hours.

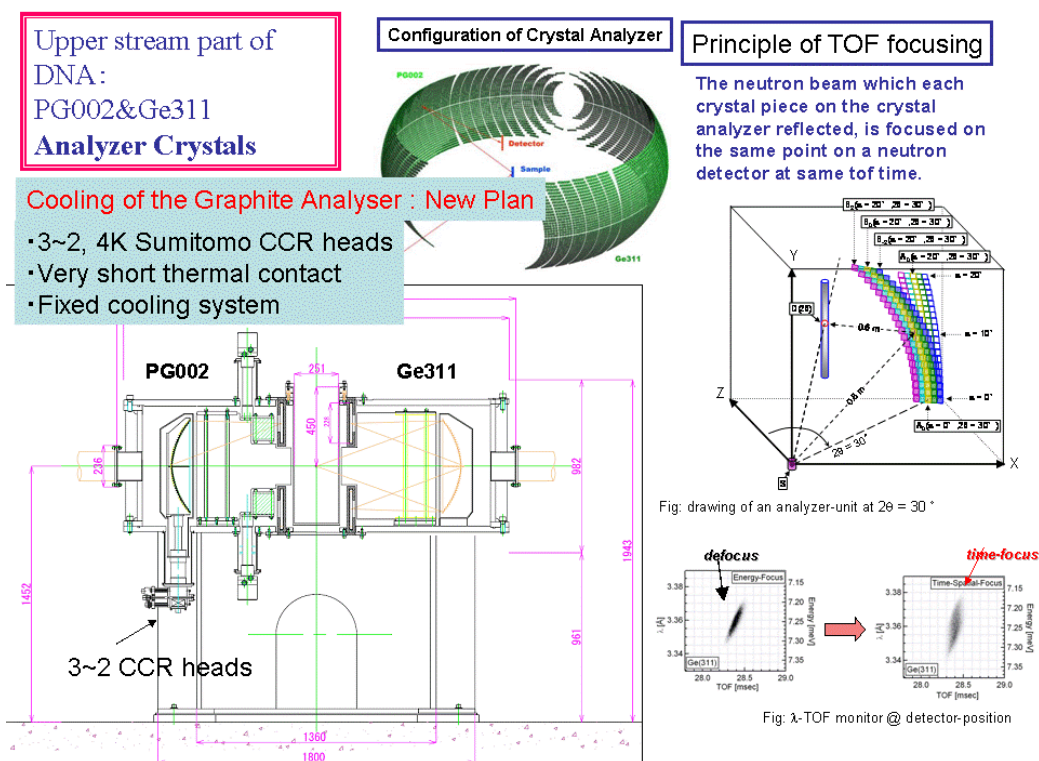


Cooling of the Graphite Analyzer : Old Plan

- 3 × 2, 4K Sumitomo CCR heads
- Very long thermal contact ~ 1.2 m
- Moving cooling system

Difficult to construct cooling system



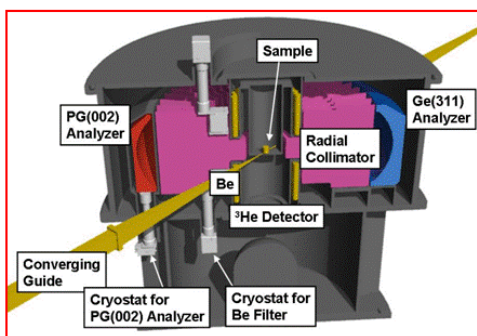


4. Spectrometer Packaging

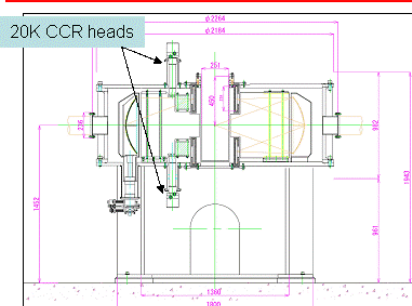
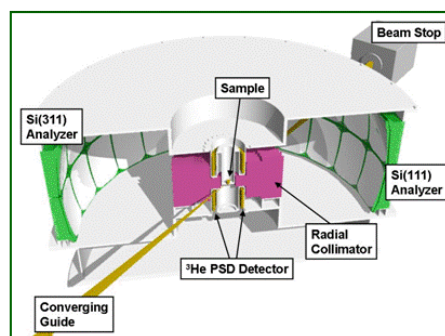
- / vacuum chamber
- / mirror cooling
- / **Be filter**
- / **solar collimator**
- / U-tube PSD
- / diffraction detectors
- / sample environment

DNA: Be filter cooling system & solar collimator

PG(002) & Ge(311) scattering vessel



Si(111) & Si(311) scattering vessel

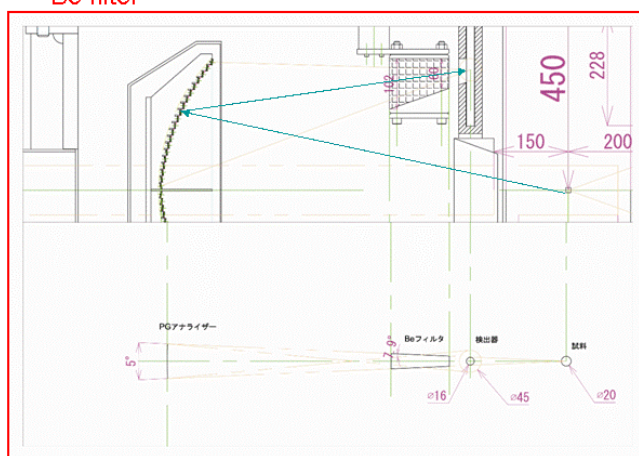


- two, 20K Sumitomo CCR heads
- Very short thermal contact
- Fixed cooling system
- Be fan shape:
 - thickness~120mm,
 - 5deg. open angle

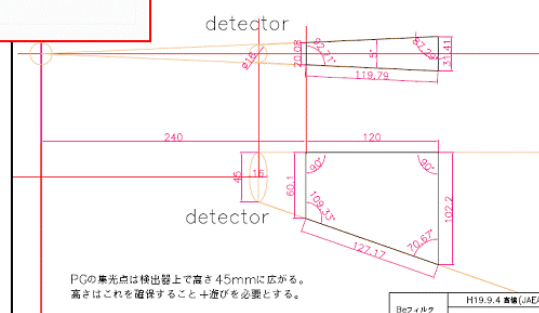
solar collimator

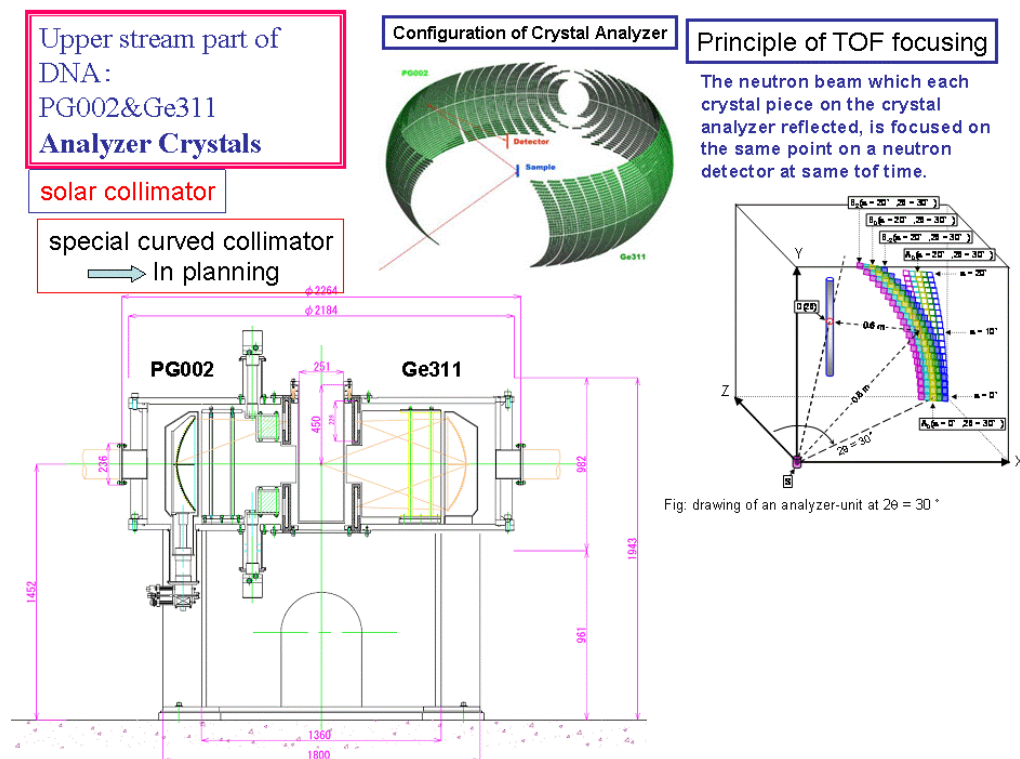
- Si second scattering vessel: **Vertical collimator**
- PG, Ge first scattering vessel:  **special curved collimator**

Be filter



直径φ16mmである。(角度では5度に収まるよう設計している)
を確保すること+Iのスペーサーを考慮に入れること。(この図では遊びは考慮外)





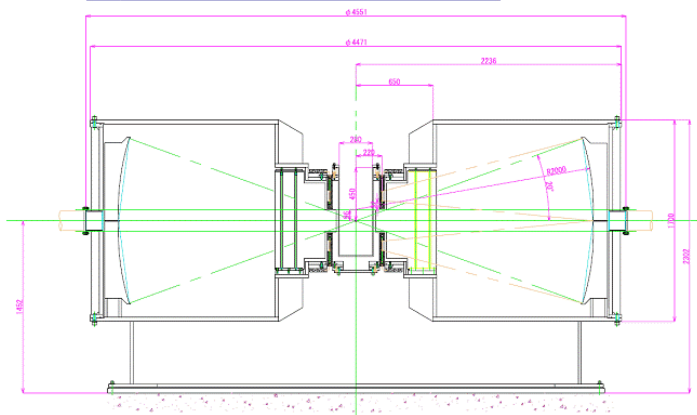
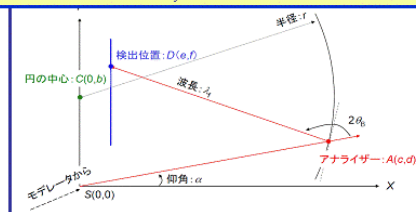
4. Spectrometer Packaging

- / vacuum chamber
- / mirror cooling
- / Be filter
- / solar collimator
- / **U-tube PSD**
- / diffraction detectors
- / sample environment

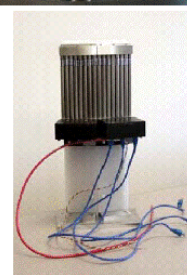
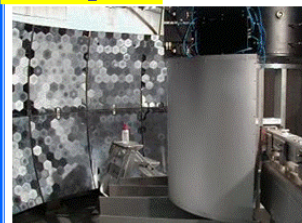
Downstream part of DNA: Si111&Si311 Analyzer Crystals

Principle of Si crystal analyzer

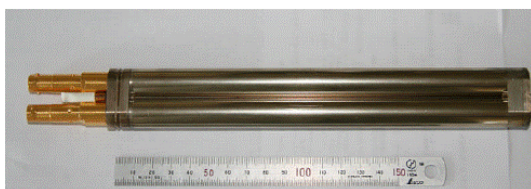
Si wafer is stacked on the
Spherical surface and analyzer neutron is detected on the each PSD position.



BASIS@SNS

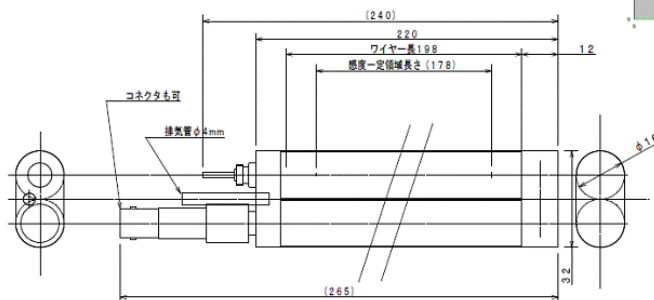
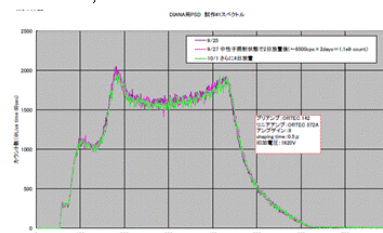
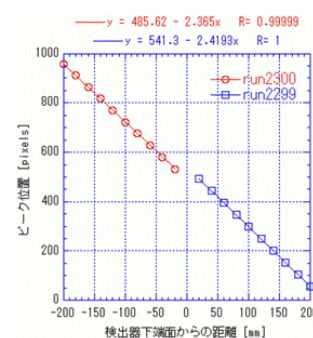


TOSHIBA; U-tube 3He PSD

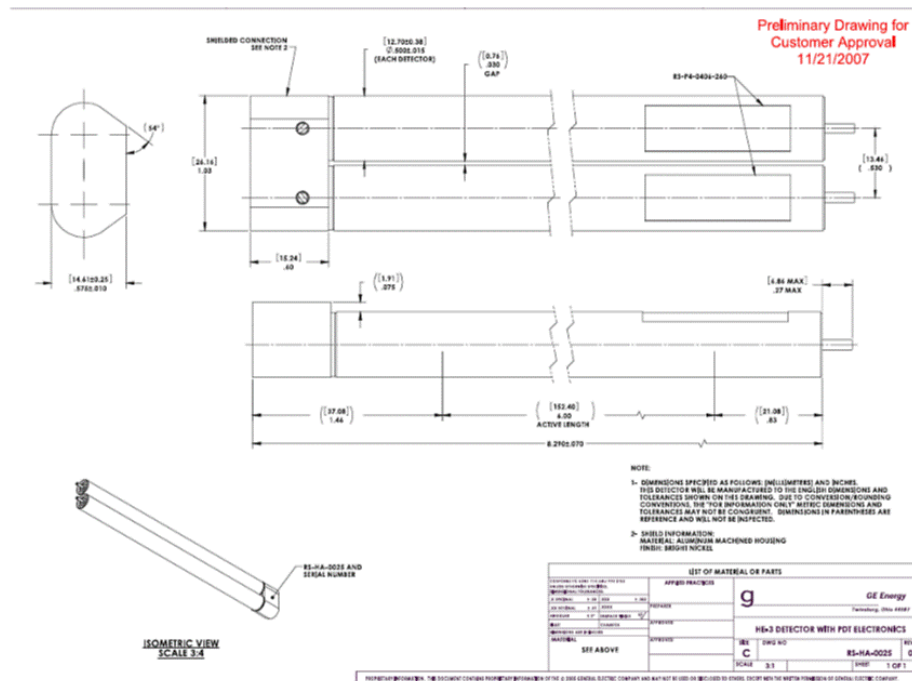


Prototype U-tube PSD

1. Max Voltage; 2.6kV
2. Insulating Resistance; 1.0E+13 ohm@500V
3. 3He gas leak; <0.1e-10 Pa·m³/s
4. Test Voltage; 1640 V
5. Resistance; 4.07 k ohm


$$\text{gas} : 3\text{He} \quad 10\text{atm} (@0^\circ\text{C}) + \text{CF}_4$$


GE U-tube PSD



GE U-type PSD

Document Number: SS-P4-0406-260

Original date: 11/21/2007

Page: 4 of 4

Rev level and date: 0

Performance SpecificationsElectrical Performance Specifications

Resistance: 1.00E+12 ohms
 Capacitance: (±20%) 8 pF
 Test Voltage: 1440 volts Charge output: 2000 fem to-C
 Group Match: 5 %
 Plateau Length: 200 volts
 Plateau Slope: 2 %/100 v
 Resolution %: .. (PuBe)< 13 %
 Operating Voltage Range: 900 to 1500 volts

Nuclear Performance Specifications

Thermal Neutron Sensitivity: (± 20 %) 8.99 cps/hr
 Neutron Flux range: 1.49E+00 to 6.38E+03 nv
 Gamma Sensitivity: cps/R/hr
 Gamma Flux range: to R/hr
 Internal Alpha Background: 0 to 0.00039 cps
 Lifetime:

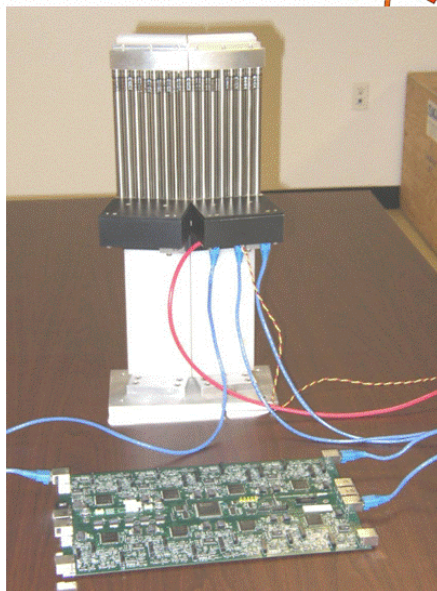
Environmental Specifications

Maximum Voltage: 2000 volts
 Maximum Temperature: 100 °C
 Minimum Temperature: -25 °C
 Maximum Humidity: 60 %
 Maximum count rate change is 2 % from 25 °C to 100 °C
 Constant Temperature Drift: ± 1 %
 Maximum neutron flux: 1.28E+04 nv
 Maximum gamma flux: R/hr
 Shock/Vibration: N/A
 Dimensional Tolerance: N/A
 Customer Specs: N/A

Backscattering Instrument



- 15cm x 1.3cm Reuter Stokes LPSDs
- 8 Atm. ^3He
- Sausage configuration



Experimental Facilities Division

Oak Ridge National Laboratory

Backscattering Array



May, 2008

Experimental Facilities Division

Oak Ridge National Laboratory

4. Spectrometer Packaging

- / vacuum chamber
- / mirror cooling
- / Be filter
- / solar collimator
- / U-tube PSD
- / **diffraction detectors**
- / sample environment

Diffraction Detector

Purpose

- Monitoring of sample status
- Incident neutron spectrum at sample position by V measurement.
- Long-d diffraction measurements

At PG(002) & Ge(311) scattering vessel

- TOF measurement
- Back scattering (main) & 90 deg. scattering (option)
- Configuration :planning

At Si(111) & Si(311) scattering vessel

- Angler dispersive measurement
 <- narrow incident spectrum band $[-40\mu\text{eV} < E_i < +40\mu\text{eV}]$
- Wide angle detector bank
- Configuration :planning

4. Spectrometer Packaging

- / vacuum chamber
- / mirror cooling
- / Be filter
- / solar collimator
- / U-tube PSD
- / diffraction detectors
- / **sample environment**

sample environment

Special Environments

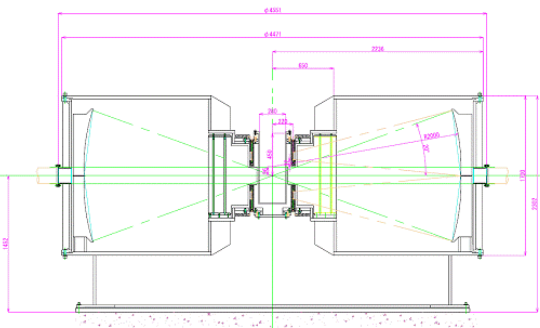
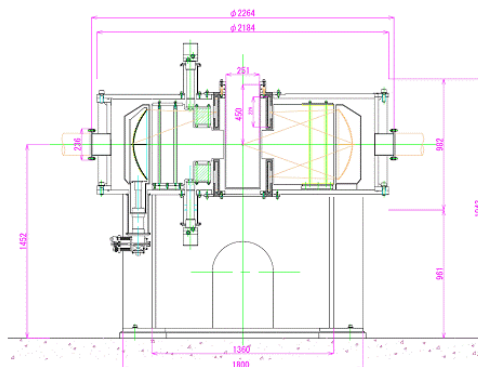
- Top loading cryo.
- High Temperature
- High Pressure, e.t.c.,

sample environments
for high temperature

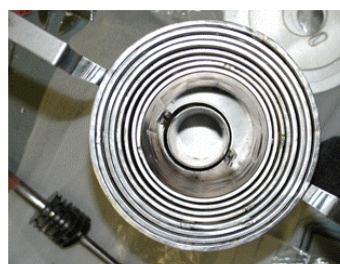
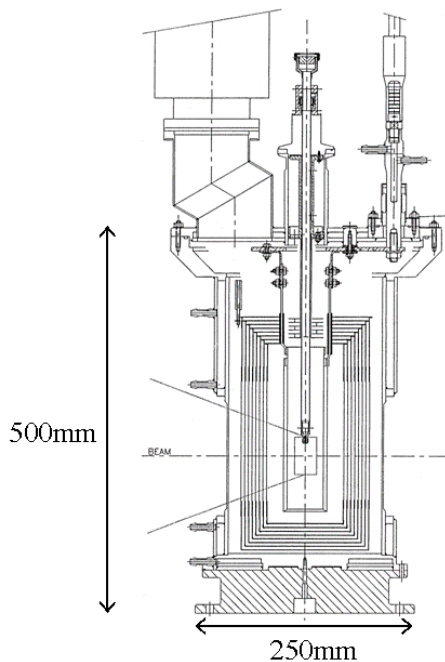
furnace: radiation heater:
foil heater or IR heater
less than **251mm Φ**

laser : excitation
(visible laser)
& high temperature
(CO₂ laser)
from **the top or the bottom**
of instrumental vessel

refrigerator



Example
ILL 1800C furnace AS Scientific product



2.6 Data Analysis

Yukinobu Kawakita (Kyushu Univ.)

5. Data analysis

De-convolution of resolution function for BS-TOF spectrometer
by using MEM (Maximum Entropy Method)

1. Outline of data analysis
2. Example for MEM application in IXS
model independent analysis (scientific reason)
3. Outline of MEM
4. De-convolution of resolution function for BS-TOF
correction of asymmetrical & E-dependent resolution fun.
(technical reason)
general tendency of MEM procedure
5. MEM de-convolution for PG mirror set in DNA
6. Summary

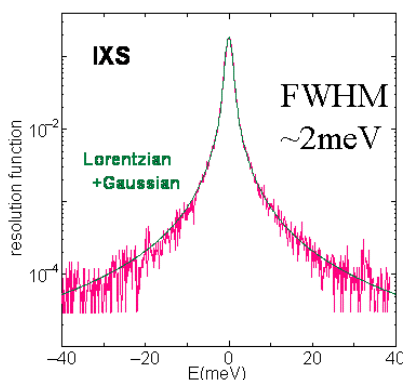
Outline of data analysis

0. software framework
 - measurement software
(highly depend on what research we want to perform)
 - data analysis software
 - DAQ -> TOF data
 - DAQ group (Dr. Nakatani)
 - DNA group (Dr. Nakagawa & Kawakita)
 - TOF -> I(Q,E) -> S(Q,E)

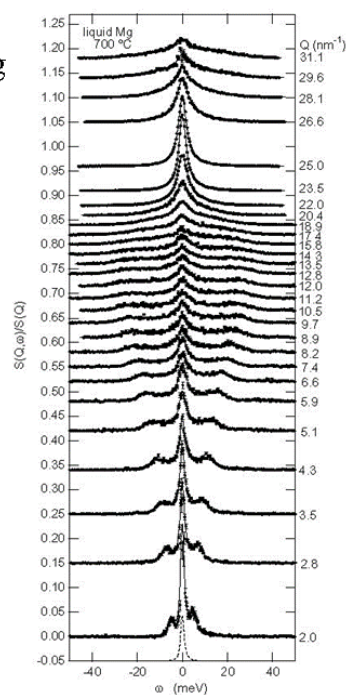
Outline of data analysis

1. TOF $\rightarrow$ I(Q,E)
 - time step $\rightarrow$ energy step (binning)
 - scattering angle $\rightarrow$ momentum transfer
2. subtraction of background counts from each spectrum
3. subtraction of scattering contribution of a container
 - taking into account absorption
4. correction of detailed valance factor
5. de-convolution of resolution function (MEM)
6. surface interpolation onto the lattice points in Q-E space
7. subtraction of multiple scattering process (qMC)
8. analysis for scientific interpretation
 - EISF, width of QENS, v-DOS
 - Fourier transformation
 - deducing intermediate scattering function
 - van-Hove $G(r,t)$
 - memory function etc.

$S(Q,E)$ of liquid Mg at 700°C
obtained by inelastic X-ray scattering
resolution function



incident X-ray energy 21.8keV
for Si(11 11 11) analyzer
 $dE/E \sim 10^{-7}$
constant $2\theta \sim$ constant Q
Energy resolution is unique.



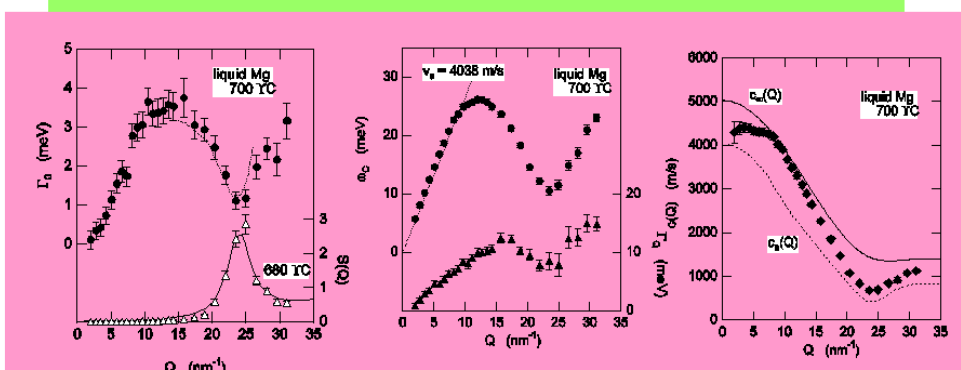
Analysis using dynamical model

Damped Harmonic Oscillator (DHO) model

$$S(Q, \omega) = \left[\frac{\hbar \omega / k_B T}{1 - \exp(-\hbar \omega / k_B T)} \right] \frac{A_0}{\pi} \frac{\Gamma_0}{\Gamma_0^2 + \omega^2} \quad \text{the central peak}$$

$$+ \left[\frac{1}{1 - \exp(-\hbar \omega / k_B T)} \right] \frac{A_Q}{\pi} \frac{4\omega \Omega_Q \Gamma_Q}{(\omega^2 - \Omega_Q^2)^2 + 4\Gamma_Q^2 \omega^2} \quad \text{side bands}$$

$$\Omega_Q = \sqrt{\omega_Q^2 - \Gamma_Q^2}$$

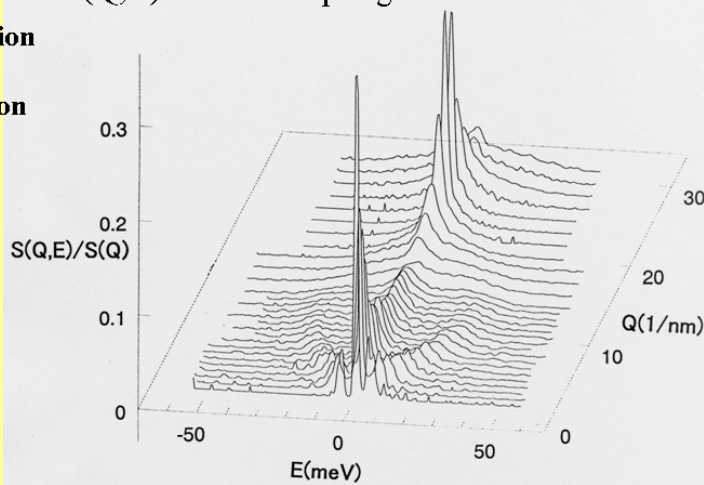


properties of
resolution fun. in IXS

**Symmetrical resolution
identical in any
energy-transfer region**

$S(Q, E)$ after decoupling of the resolution function by
maximum entropy methods

$S(Q, E)$ after decoupling of the resolution fun.

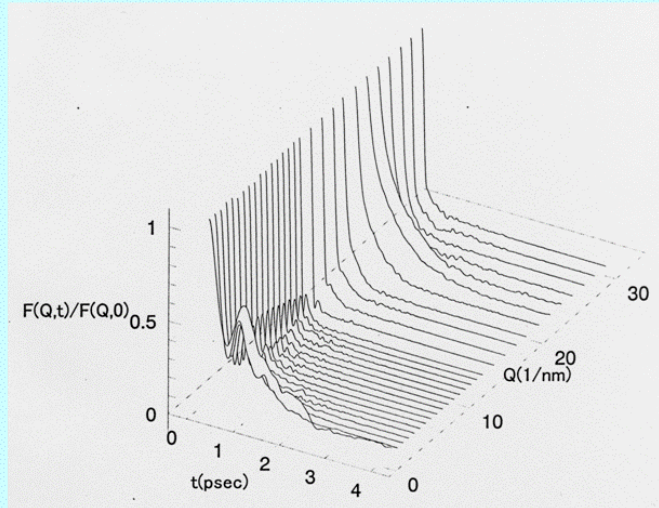


Intermediate scattering function $F(Q,t) \leftarrow S^*(Q,E)$

$$S^*(Q,E) = S(Q,E) \exp(-E/2k_B T)$$

$$F(Q,t) = \int_{-\infty}^{+\infty} S(Q,E) \exp(iEt/\hbar) dE$$

$$\psi(Q,t) = F(Q,t)/F(Q,0) = \langle \rho_Q(t) \rho_{-Q}(0) \rangle / \langle |\rho_Q(t)|^2 \rangle$$



Langevin equation

$$\frac{d\psi(Q,t)}{dt} = -\int_0^t M_1(Q,t-t') \psi(Q,t') dt'$$

$$\frac{dM_1(Q,t)}{dt} = -\int_0^t M_2(Q,t-t') M_1(Q,t') dt'$$

where $M_i(Q,t)$ is i-th order memory function.

$$\frac{d^2\psi(Q,t)}{dt^2} + \omega_0^2(Q) \psi(t) + \int_0^t dt' M_2(t-t') \frac{d\psi(Q,t')}{dt'} = 0$$

$$\omega_0^2(Q) = \frac{k_B T Q^2}{m S(Q)} = c_0^2(Q) Q^2$$

model function with two exponential decays

$$M_2(Q,t) = (\gamma - 1) \omega_0^2(Q) \exp(-D_T Q^2 t) + \Delta^2(Q) [A(Q) \exp(-t/\tau_\alpha(Q)) + (1 - A(Q)) \exp(-t/\tau_\mu(Q))]$$

How good ? What meaning ?

experimental memory function

Outline of MEM

de-coupling of resolution function by the Maximum Entropy Method (MEM)

$$\tilde{S}_i = \tilde{S}_{cal}(Q, E_i) / S(Q) = \int_{-\infty}^{+\infty} S(Q, E) R(E - E_i) dE / S(Q)$$

a priory Structure factor $S^{(0)}(Q, E)$

Information Entropy

$$\chi = - \sum_{i=1}^N \tilde{S}_i \log[\tilde{S}_i / \tilde{S}_i^{(0)}]$$

Constraints given by statistical errors $e(Q, E)$ in $\tilde{S}_{obs}(Q, E)$

$$C = 1/N \sum_{i=1}^n \left| \tilde{S}_{cal}(Q, E_i) - \tilde{S}_{obs}(Q, E_i) \right|^2 / e(Q, E_i)^2$$

Lagrange's method of undetermined multipliers

$Q(E) = \chi - \frac{1}{2} \lambda C$ where λ is Lagrange multiplier.

$$\frac{\partial Q(E)}{\partial \tilde{S}_i} \left(= \frac{\partial \chi}{\partial \tilde{S}_i} \right) = 0 \rightarrow S^{(1)}(Q, E_i) \approx S^{(0)}(Q, E_i) (1 + \Delta(E_i) \lambda)$$

$$C = 0 \rightarrow \lambda$$

$S^{(1)}$ is an approximate solution satisfying entropy maximum, $\frac{\partial \chi}{\partial \tilde{S}_i} = 0$,

under the constraint, $C = 0$.

When C is calculated strictly with $S^{(1)}$ and larger than 1,

$S^{(2)}$ will be created using $S^{(1)}$ instead of $S^{(0)}$

These procedures will be iterated until $C < 1$.

III. moderator possibilities; 1. Motivation (J. Chem. Phys. Sol.)

Motivation: Is decoupled moderator the best neutron source for near-backscattering (n-BS) spectrometers?

The world n-BS spectrometers

DIANA @ J-PARC: source = decoupled moderator (DM), $L_1 = 32$ m

IRIS, OSIRIS @ ISIS: source = DM, $L_1 = 36.4, 34$ m

Si n-BS @ SNS: source = poisoned moderator (PM), $L_1 = 84$ m

J-PARC will have 4 moderators for neutron sources → Simulation study of 4 virtual n-BS to compare expected performances

coupled moderator (CM) with $L_1 = 42$ m → **CM-source n-BS**

decoupled moderator (DM) with $L_1 = 32$ m → **DIANA**

poisoned (thick) moderator (PMT) with $L_1 = 21.5$ m → **PMT-source n-BS**

poisoned (thin) moderator (PMT) with $L_1 = 84$ m → **SNS-type n-BS**

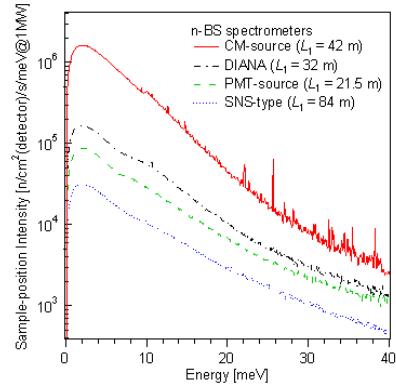
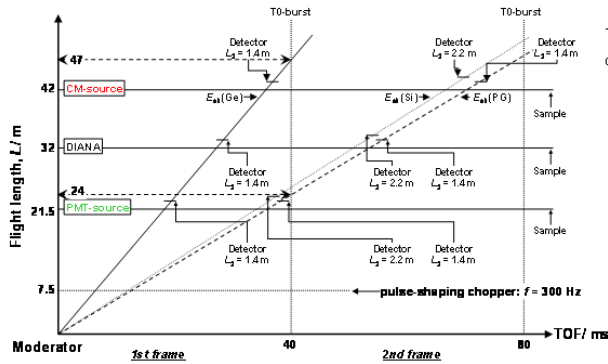


Fig. Flux @ sample

To avoid T0-burst BG,
1. $L_{\text{PM}} < 24$ m (limitation from PG-analyzer)
2. $L_{\text{PM}} < 47$ m (limitation from Ge-analyzer)
Then,
• **PMT-source type:** $L_1 = 21.5$ m
• **CM-source type:** $L_1 = 42$ m
• **SNS-type:** $L_1 = 84$ m (same as SNS)

from N. Takahashi

III. moderator possibilities; 2. expected performances

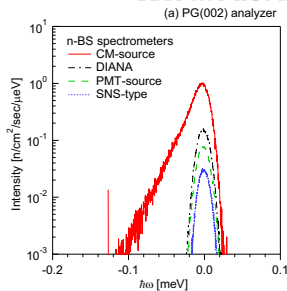


Fig. E-resolution of PG analyzer

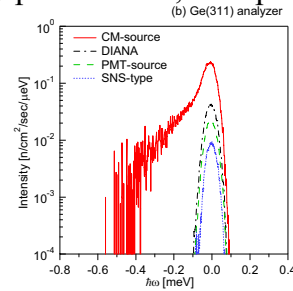


Fig. E-resolution of Ge analyzer

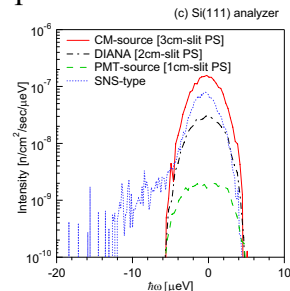


Fig. E-resolution of Si analyzer

Table: performance comparisons

source (name of n-BS)	L_1 [m]	main guide section	analyzer	E_M [meV]	$h\omega$ -range (one frame) [meV]	slit-width of PS [cm]	$\Delta\lambda$ [Å]	$\Delta h\omega$ [meV]	sample-position intensity at E_M [10^{10} n/cm²/(sec)/eV]	merit	demerit
★ CM (CM-source)	42	curved w60x98 R2200m	PG(002)	1.87	$-0.3 < h\omega < 4.3$	-	3.6	23	160	$\times 5 \sim 9$ intensity (PG, Ge, Si [PS])	$30 \sim 35\%$ worse resolution (PG, Ge)
			Ge(311)	7.25	$-1.1 < h\omega < E^*$	-	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	$\times 3$ wider band (Si [PS])	
DM (DIANA)	32	curved w60x98 R1650m	PG(002)	1.87	$-1.0 < h\omega < 1.8$	-	4.7	17	17		
			Ge(311)	7.25	$-3.6 < h\omega < E^*$	-	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 w60x98 0.5m-gap for T0-chopper	PG(002)	1.87	$-0.2 < h\omega$	-	6.9	17	8.6	wide band (PG, Ge)	$\times 1/2$ intensity (PG, Ge)
			Ge(311)	7.25	$-5.5 < h\omega$	-	6.9	64	4.1		$\times 1/7$ intensity (Si [PS])
			Si(111)	2.09	± 0.014 [PS]	1	6.7	6.2	0.20		
PMT (SNS-type)	84	curved w60x98 R2200m	PG(002)	1.87	$-0.4 < h\omega < 0.8$	-	1.9	15	3.2	10 ~ 12 % better resolution (PG, Ge)	$\times 1/5$ intensity (PG, Ge)
			Ge(311)	7.25	$-1.3 < h\omega < 17$	-	1.9	57	1.5	$\times 2$ intensity (Si)	narrow band (PG, Ge)
			Si(111)	2.09	$-0.6 < h\omega < 0.6$	-	1.8	3.6	2.7	$\times 43$ wider band (Si)	

Curved guide: $E^* = 40$ meV

First trial:
an asymmetric resolution
with E dependency proportional to E

Model function

Center Lorentzian 0.4meV FWHM

Excitations DHO 0.8meV FWHM

Model resolution 0.2meV FWHM

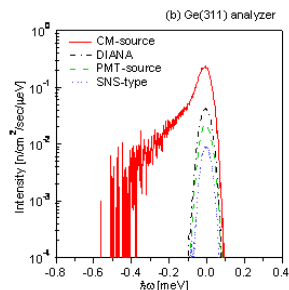
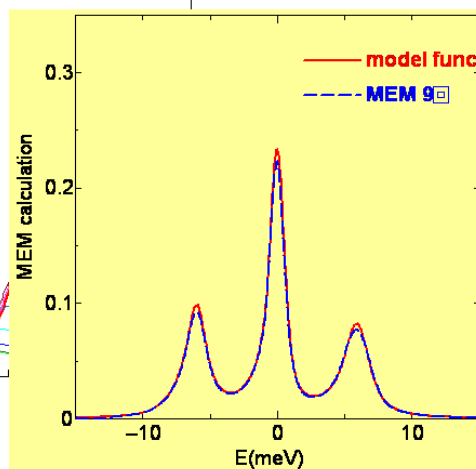
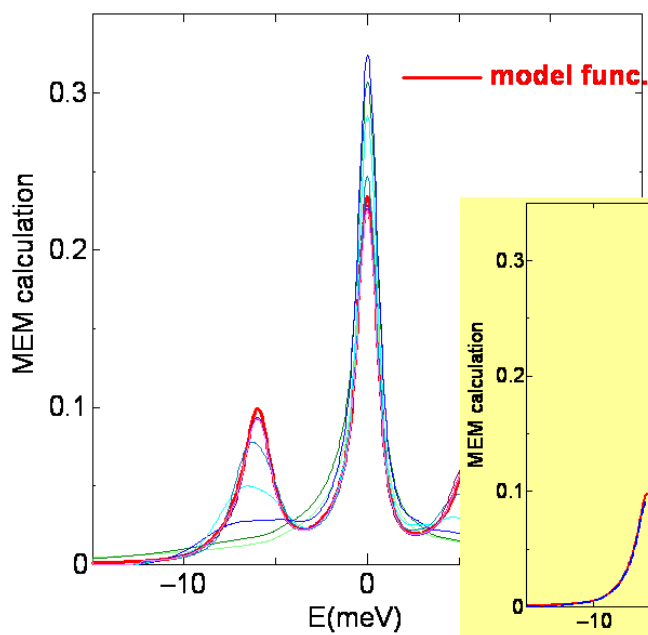
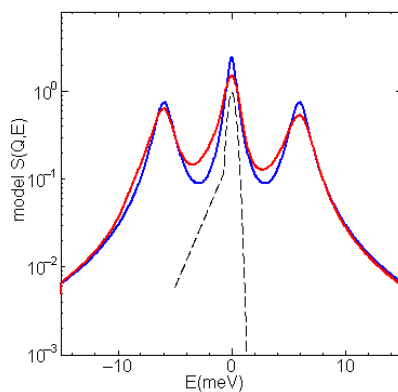
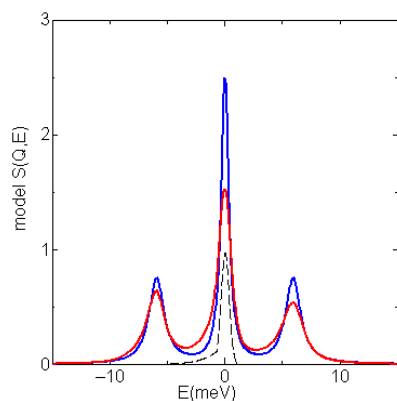
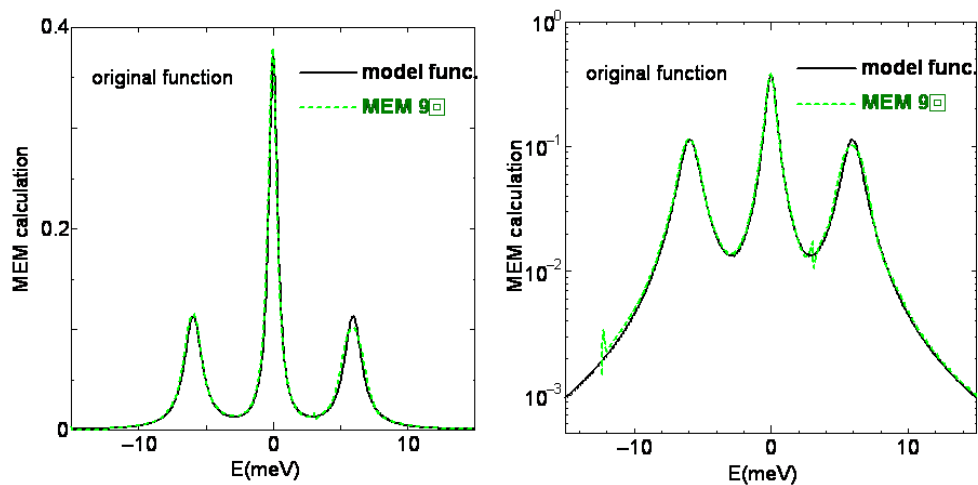


Fig. E-resolution of Ge analyzer

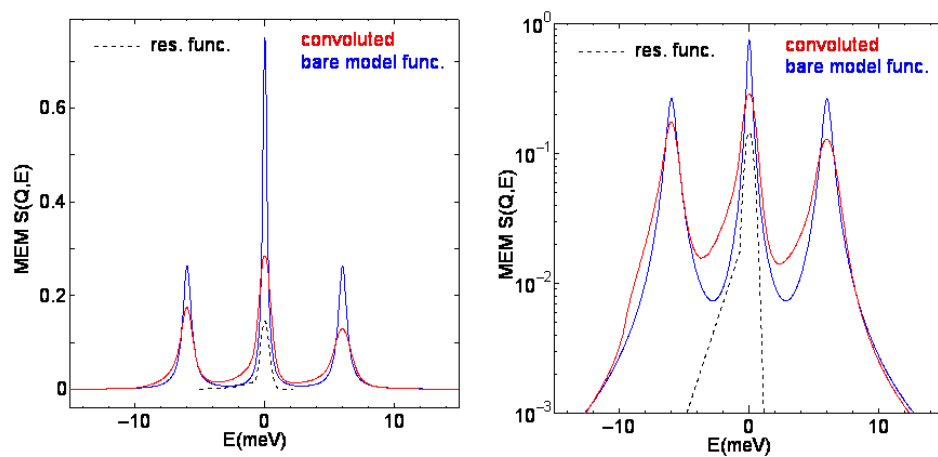


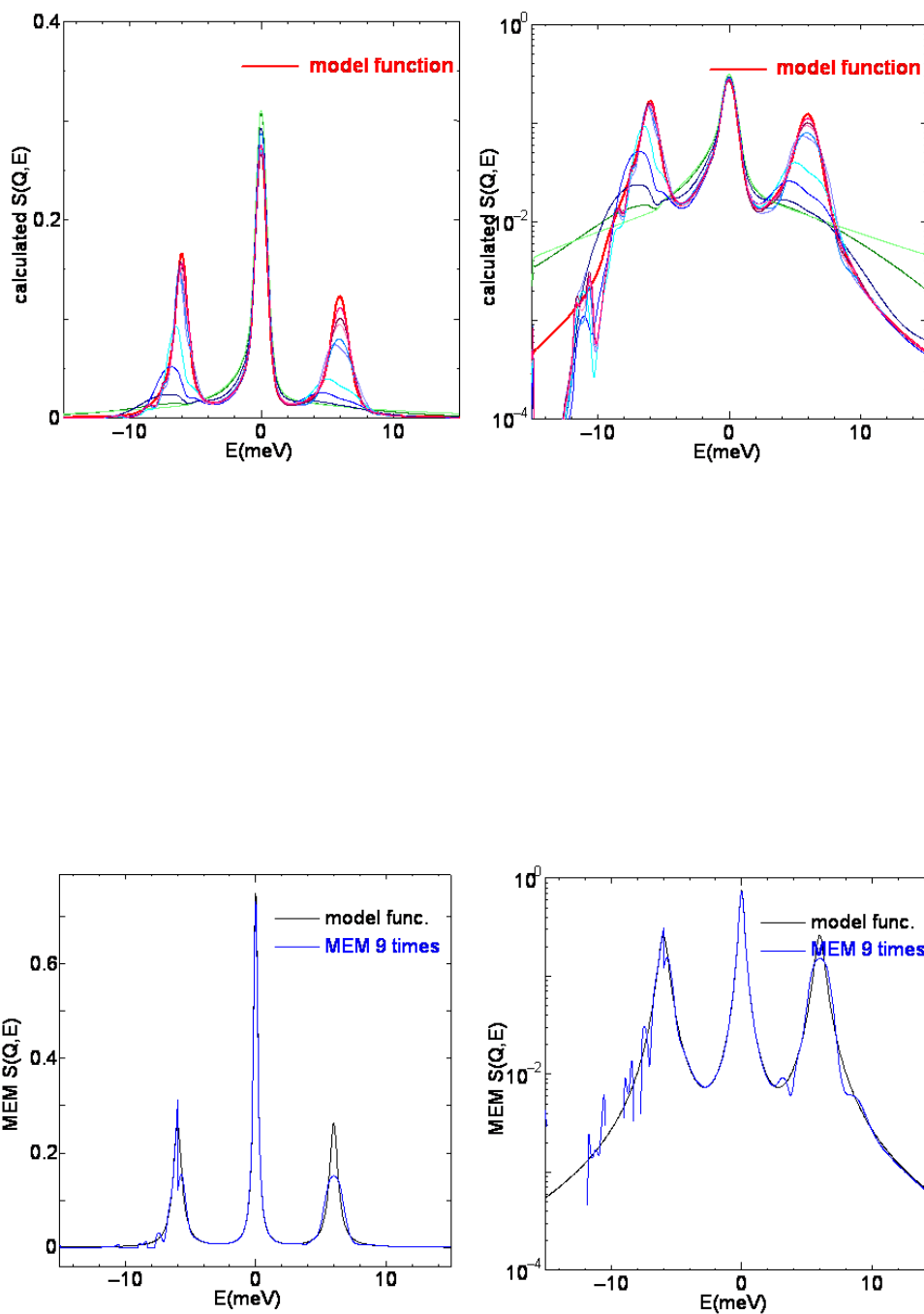


severe case

center Lorentzian 0.2meV FWHM

excitation DHO 0.4meV FWHM



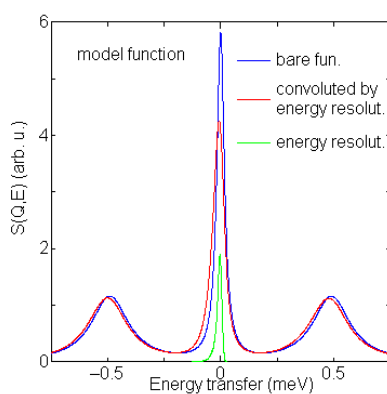
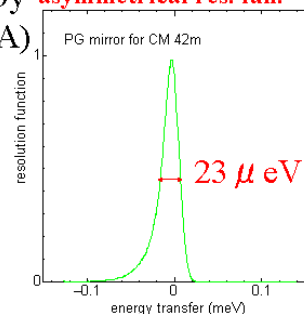


MEM has no stochastic process
 given res. fun. & initial fun. $\rightarrow$ unique solution
 We must use a good initial function.

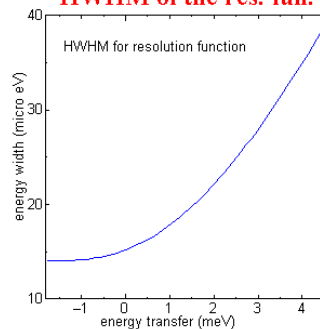
De-convolution of energy resolution function by **asymmetrical res. fun.** Maximum entropy method (PG mirror for DNA)

Model function

center FWHM $20 \mu\text{eV}$ relative intensity 0.5
excitation FWHM $100 \mu\text{eV}$ relative intensity 0.5
excitation energy $\pm 500 \mu\text{eV}$



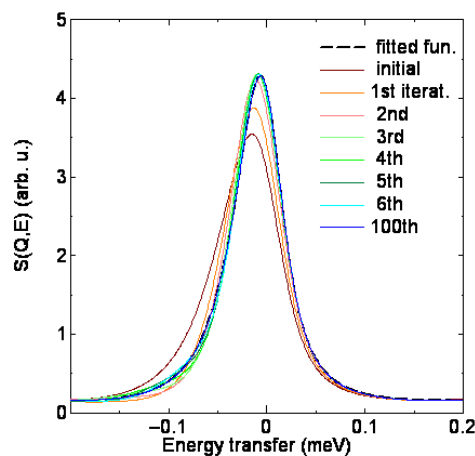
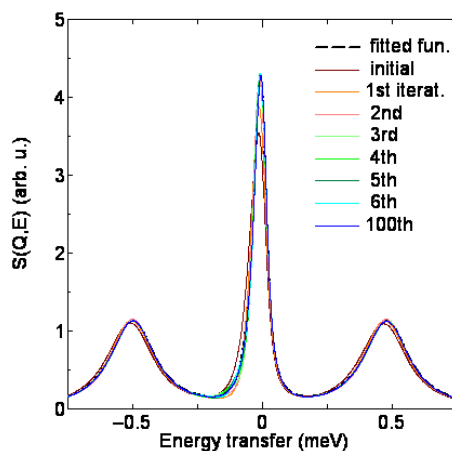
Energy dependence of HWHM of the res. fun.



MEM results for PG mirror

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

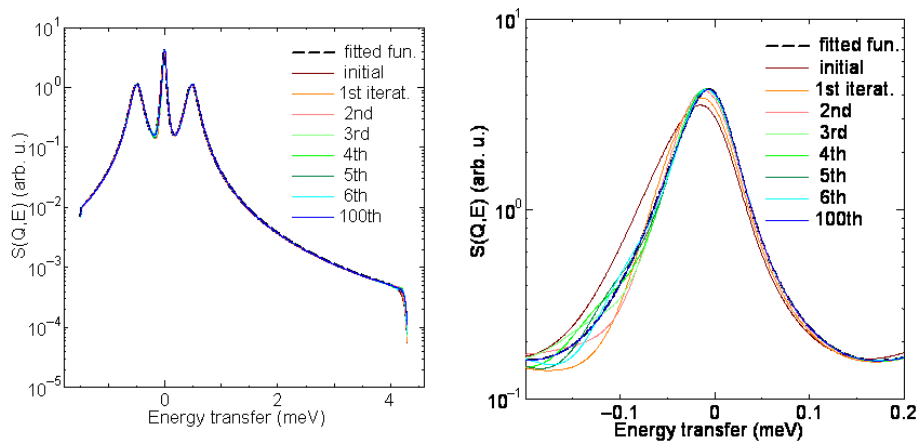
Initial fun. = observed data $\otimes$ resolution fun.



almost complete reproduction by 100 times iteration of MEM

MEM results for PG mirror

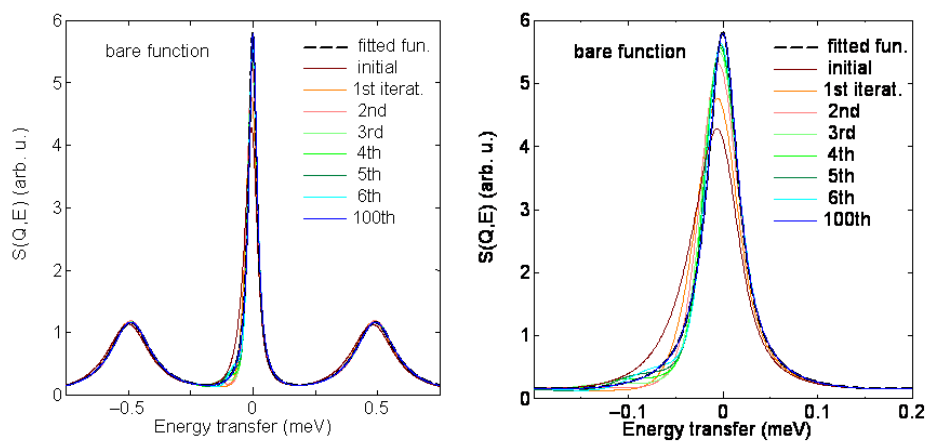
Logarithmic scale



reproduce well even a tail part with lowest intensity

MEM results for PG mirror

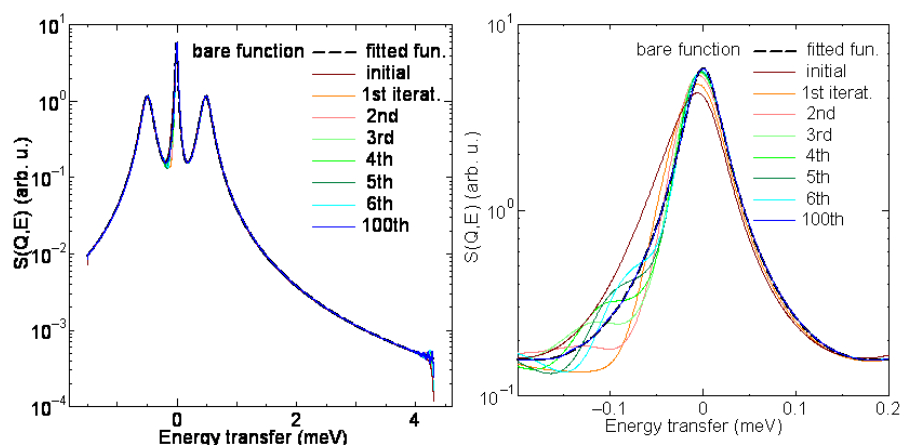
Bare function without convolution of res. fun.



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

Summary

The decoupling procedure using MEM is effective when
the resolution function has a wide long tail,
characteristic peaks in measured spectrum has
a narrow energy width similar to the resolution.

The resolution function of BS-TOF neutron spectrometer
is a much better than that in IXS.

But when a user desires model independent analysis,
the resolution decoupling by MEM will be a good tool.

MEM can resolve a problem on asymmetrical shape of res. fun in DNA,
& also analytic difficulties on energy-dependent resolutions for
every TOF-inelastic neutron spectrometer in the world.

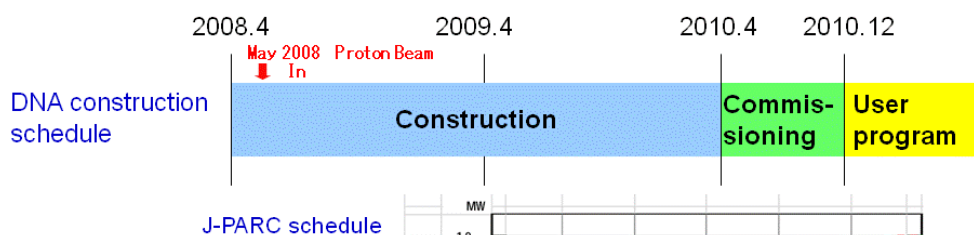
2.7 Cost estimation & Schedule & Support Group

Kaoru Shibata (JAEA)

6. Cost estimation & Schedule & Support Group(sub)

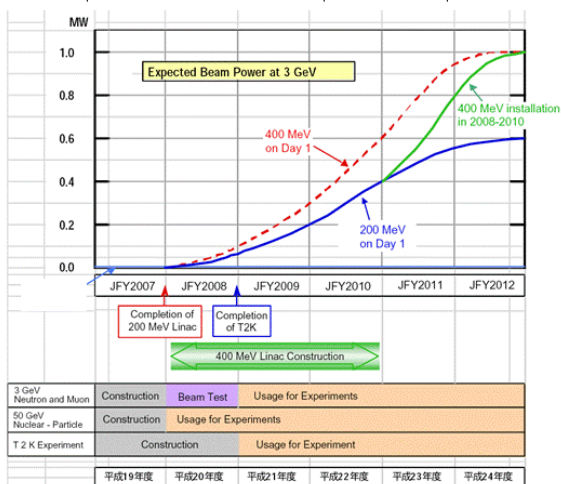
- / cost estimation
- / construction schedule, budgets
- / Construction and Science support group

Schedule



Cost

~1000M. JPY



DNA Proposal Members

Construction & Research Group Construction K. Shibata (JAEA) N. Takahashi (JAEA) T. J. Sato (Univ. of Tokyo) S. Fujiwara (JAEA) I. Tsukushi (Chiba Inst. of Tech.) Y. Kawakita (Kyushu Univ.) Science Y. Jochi (Univ. of Tokyo) H. Nakagawa (JAEA) M. Nakasako (Keio Univ.) M. Kataoka (Nara Inst. Sci. Tech., JAEA) Adviser M. Arai (JAEA) T. Kanaya (ICR, Kyoto Univ.) A. Inaba (Osaka Univ.) S. Takeda (Hokkaido Univ.) F. Mezei (HMI, LANL)	Support Group Biology N. Go (JAEA) N. Niimura (Ibaraki Univ.) A. Kitao (Univ. of Tokyo) S. Ikura (Tokyo Ikashika Univ.) S. Saruwatari (Kitazato Univ.) K. Kuwata (Gifu Univ.) Y. Sugawara (Kitazato Univ.) K. Maenaka (Kyushu Univ.) K. Wakabayashi (Osaka Univ.) H. Urabe (Tokyo Kasei Univ.) Dieter Middelndorf (Univ. of Oxford) A. Sokolov (Univ. of Akron) Physics D. Yamazaki (JAEA) Y. Takeda (JAEA) T. Matsumura (Tohoku Univ.) K. Iwasa (Tohoku Univ.)
--	---

2.8 Issues for homework from the International Advisory Committee International Advisory Committee (Chair: Dan Neumann)

1. Estimate performances of Si analyzer case without choppers.

Nobuaki Takahashi

2. Why are two instruments in series necessary?

Kaoru Shibata

3. What is the real request of sample environment space?

Yukinobu Kawakita

4. Who are the supposed users of DNA?

Kaoru Shibata

5. How much is the expecting flux of the disc chopper instrument of J-PARC AMATERAS?

Taku J. Sato

2.9 Answers to the issues

Kaoru Shibata (JAEA), Nobuaki Takahashi (JAEA), Yukinobu Kawakita (Kyushu Univ.), Taku J. Sato (Tokyo Univ.)

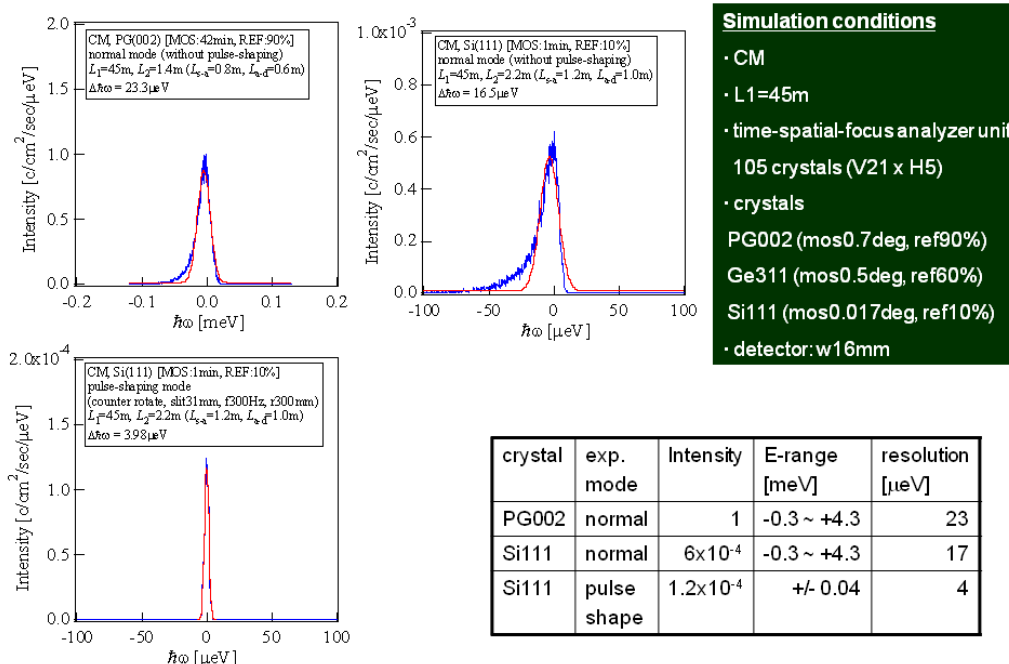
Answers to the homework



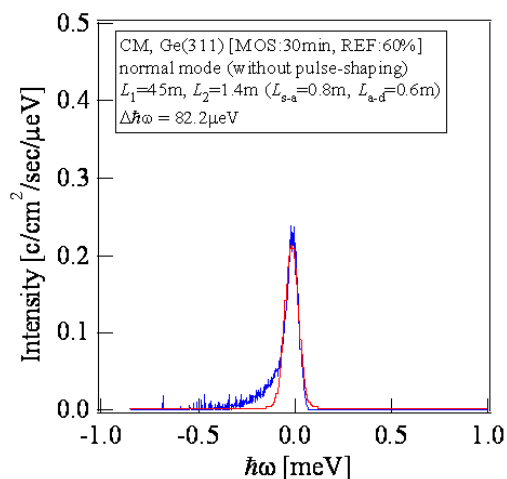
DNA Construction Team (J-PARC)

1. Performances of Si case without pulse-shape choppers
2. Why we need two instruments, in series?
3. Real request of sample environment space.
4. Users

1. Performances of Si case without pulse-shape choppers



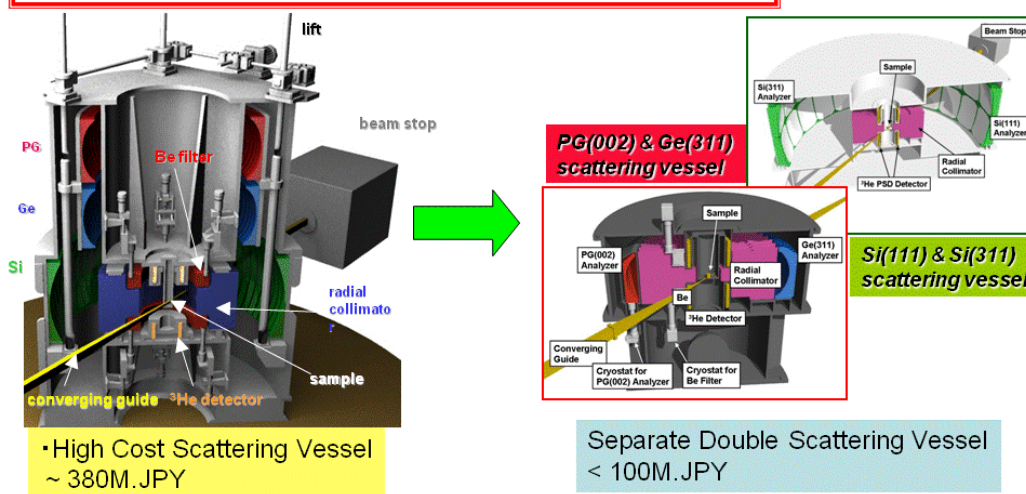
appendix1. Ge311



2. Why we need two instruments, in series?

Background:

Due to the Scientific demand from users group of biophysics, originally, DNA spectrometer includes 3 analyzers in one vessel.



Required Specification for DNA

- Wide Energy Range at Around Several 10~100 μeV

➡ We need 4 analyzers in two vessel in series.

2. Why we need two instruments, in series?

The Scientific demand from bio-physist group is to measure very noble bio-molecules with only small amount around a few mg with various energy resolution and wide energy and Q ranges.

Especially they have a few of experience of neutron inelastic measurement. We expect their use of this instrument that, at the first time use, they will check the sample with very, very few amount of the sample by using PG mirror because of high intensity.

After that they will make much strategic plan using neutron which includes preparation of the sample with more volume.

In the next measurement, they will check once the sample by PG analyzer for checking the sample and focus their interesting region with high resolution of Si analyzer. We expect this is a sequence of the measurement for bio-molecule.

That's why we intended, at first, that we should realize this demand with one instrument, because we feel this demand is essential for bio-molecule.

According to their demands, we need very intense instrument using PG or Ge analyzer and Si analyzer with high resolution, and we supply a chance measuring both simultaneously.

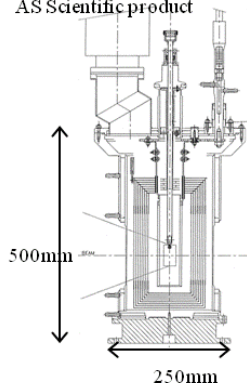
3. Real request of sample environment space.

The diameter of sample flange in Si scattering vessel:
D = 280 mm

Almost all standard sample environment accessories will be able to install in DNA

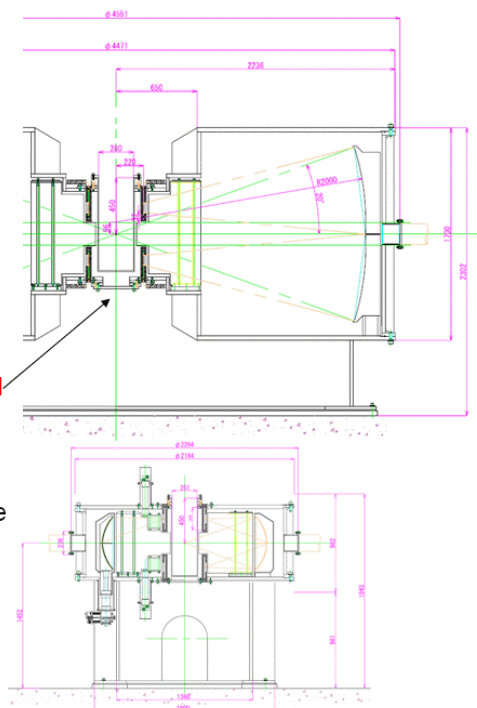
Example

ILL 1800°C furnace
AS Scientific product



Special devices install from the bottom of instrumental vessel.

Example:
laser photo guide tube



4. Users

Users in the polymers field: power users are existing in DNA Group, already

T. Kanaya (ICR, Kyoto Univ.)

Adviser in DNA Construction & Research Group

I. Tsukushi (Chiba Inst. of Tech.)

A member of DNA Construction Group

Another users in the Polymers field will be increase.

Potential biophysics users group is various.

•Workshop for study of dynamics in biopolymer by inelastic neutron scattering was held on September 08, 2003 in KEK (afternoon)

Participant: 18 members in biophysics field + 4 members in neutron instrumentation = Total 22 members

•LOI of DNA

When we made LOI of DNA in 2004, the number of the proposals of experiment on DNA spectrometer is 13 in biophysics field, 8 in soft matter and chemistry field and 3 in magnetism field.

appendix2. DNA Proposal Members

Construction & Research Group Construction

K. Shibata (JAEA)
N. Takahashi (JAEA)
T. J. Sato (Univ. of Tokyo)
S. Fujiwara (JAEA)
I. Tsukushi (Chiba Inst. of Tech.)
Y. Kawakita (Kyushu Univ.)

Science

Y. Jochi (Univ. of Tokyo)
H. Nakagawa (JAEA)
M. Nakasako (Keio Univ.)
M. Kataoka (Nara Inst. Sci. Tech., JAEA)

Adviser

M. Arai (JAEA)
T. Kanaya (ICR, Kyoto Univ.)
A. Inaba (Osaka Univ.)
S. Takeda (Hokkaido Univ.)
F. Mezei (HMI, LANL)

Support Group Biology

N. Go (JAEA)
N. Niimura (Ibaraki Univ.)
A. Kitao (Univ. of Tokyo)
S. Ikura (Tokyo Ikashika Univ.)
S. Saruwatari (Kitazato Univ.)
K. Kuwata (Gifu Univ.)
Y. Sugawara (Kitazato Univ.)
K. Maenaka (Kyushu Univ.)
K. Wakabayashi (Osaka Univ.)
H. Urabe (Tokyo Kasei Univ.)
Dieter Middendorf (Univ. of Oxford)
A. Sokolov (Univ. of Akron)

Physics

D. Yamazaki (JAEA)
Y. Takeda (JAEA)
T. Matsumura (Tohoku Univ.)
K. Iwasa (Tohoku Univ.)

5. DNA vs CNDCS

DNA vs CNDCS (Inverted vs direct geometry)

Taku J Sato

2008/02/28

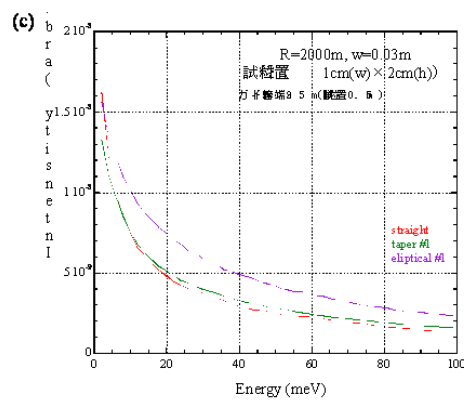
(DNA IAC meeting at JAEA)

Handwritten argument

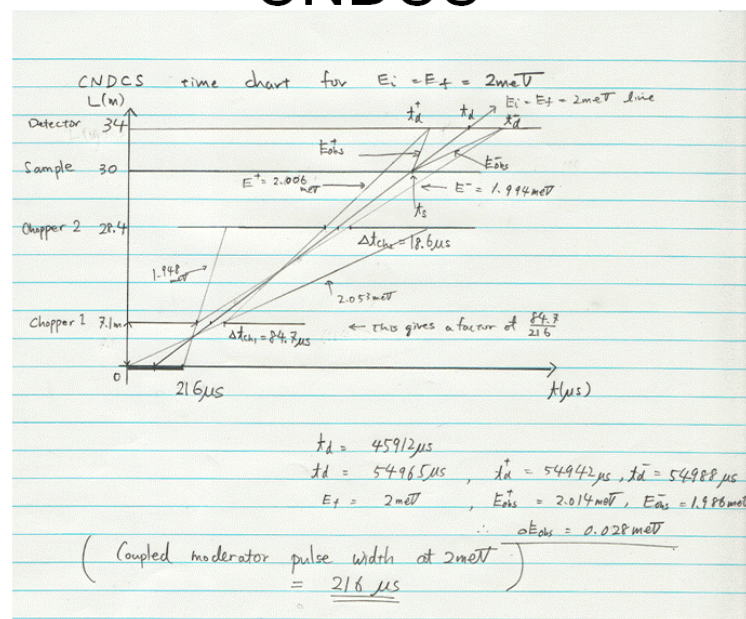
	CNDCS	f	DNA	f
source	1	1	1	1
guide tube cross section	3cm(W)X9cm(H)	0.27	10cm(W)X10cm(H)	1
gain by elliptic guide	1(?)	1	1(?)	1
chopper slit	3cm -> 2cm	0.67	n/a	1
energy resolution	20ueV	1	20ueV	1
pulse shaping	84.7us/216us	0.39	n/a	1
total		0.07 (1)		1 (14)

elliptical guides

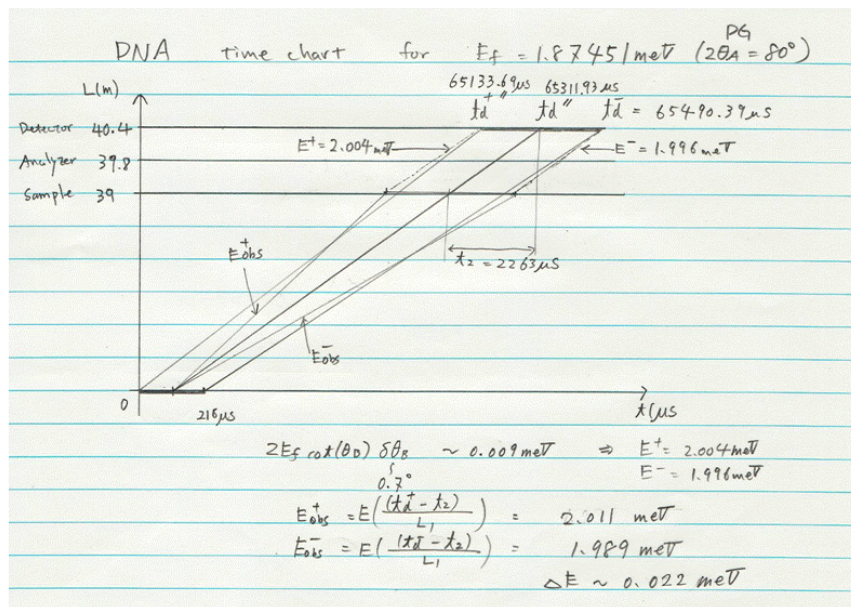
- elliptical guide simulation (CNDACS)
 - not much gain at 2meV (K. Nakajima)



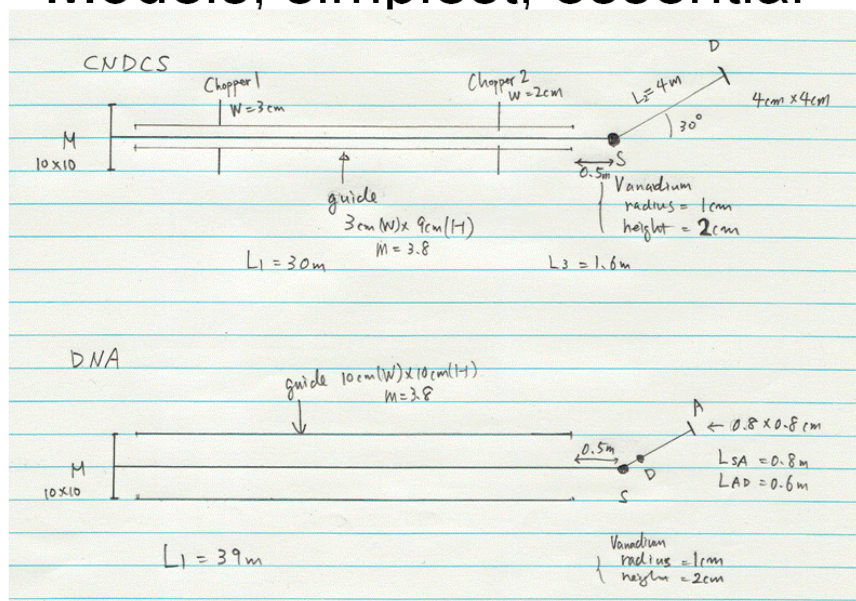
CNDACS



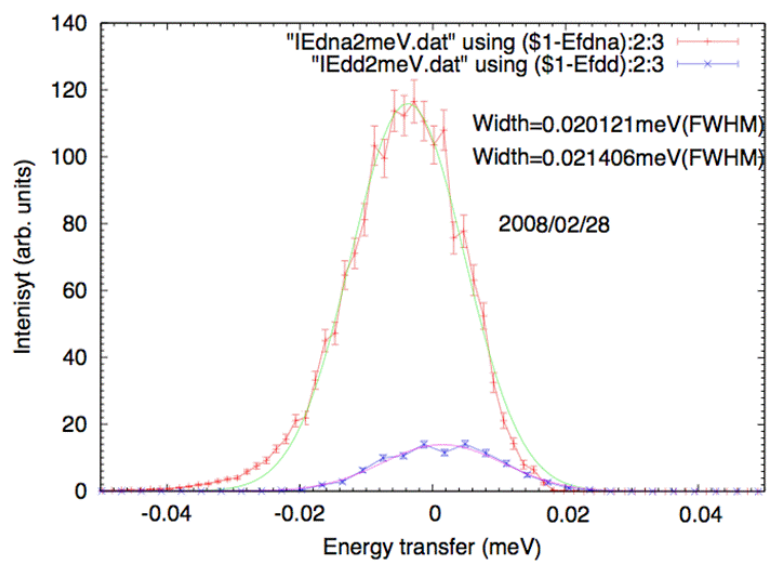
DNA



Models; simplest, essential



McStas results



2.10 Advice from the International Advisory Committee International Advisory Committee (Chair: Dan Neumann)

Advices from the advisory committee

IAC

Dan Neumann (Chair)

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 $\sim 4 \mu\text{eV}$ 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.

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.

Comments on Instrument Functionality

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.

Comments on Cost and Schedule

1. Not enough information was presented for a reliable cost estimate and funding is not in hand.
2. Schedule seems quite optimistic.

Summary

DNA will be an excellent instrument, building on the pioneering efforts and distinguished experience on pulsed-source, inverted geometry instruments on pulsed sources in Japan.

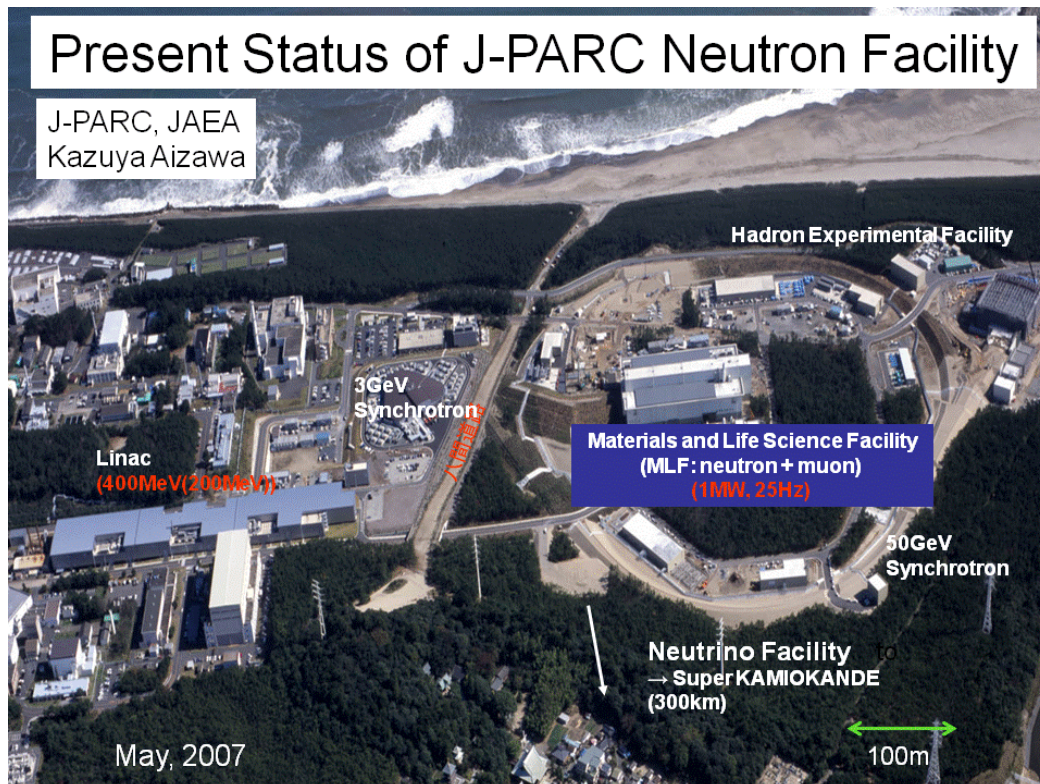
Thanks to all for the hospitality, the excellent presentations, and fruitful discussions.

Good luck with the instrument.

3. Proceedings of the Workshop on “Biomolecular Dynamics Backscattering Spectrometers”

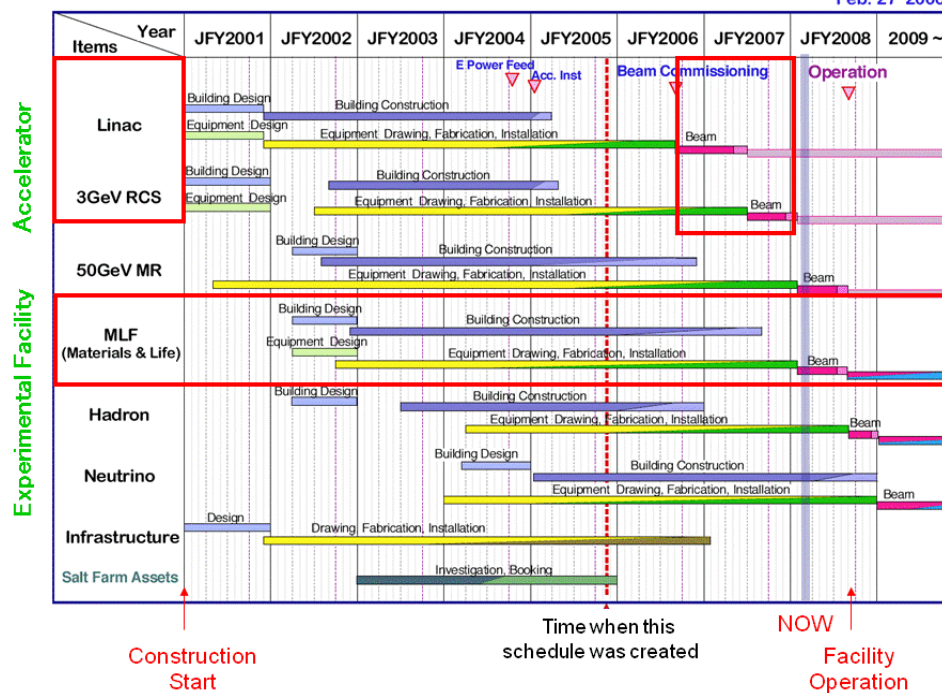
3.1. Present Status of J-PARC Neutron Facility

Kazuya Aizawa (J-PARC)



J-PARC Construction Schedule

Feb. 27 2006



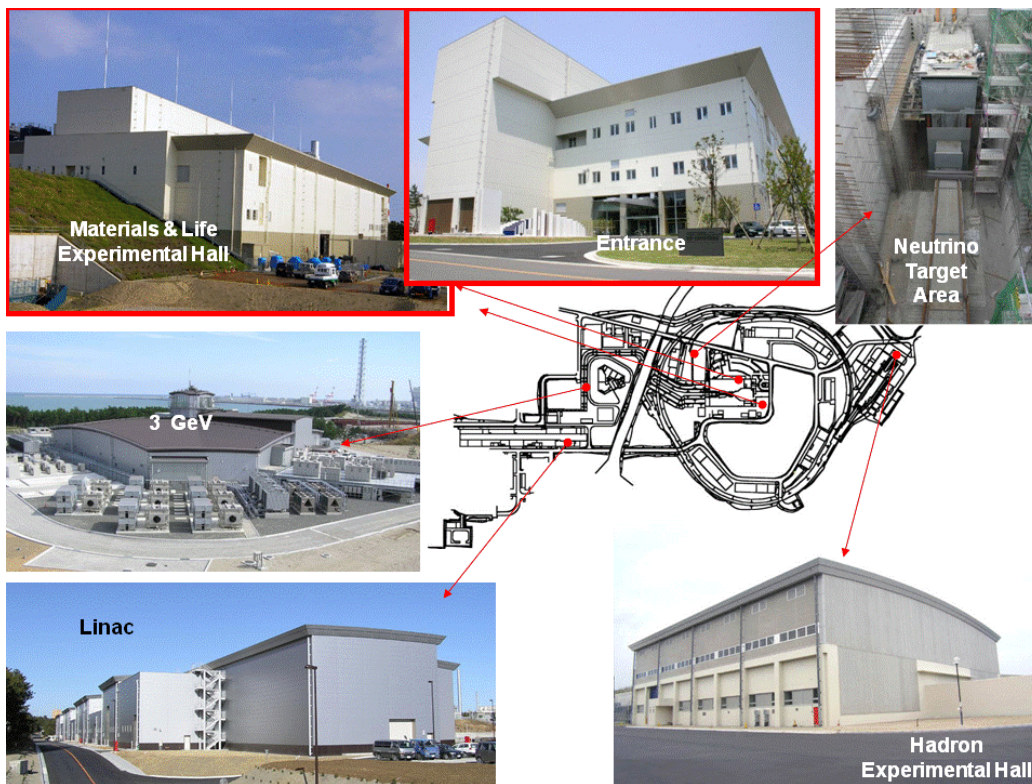
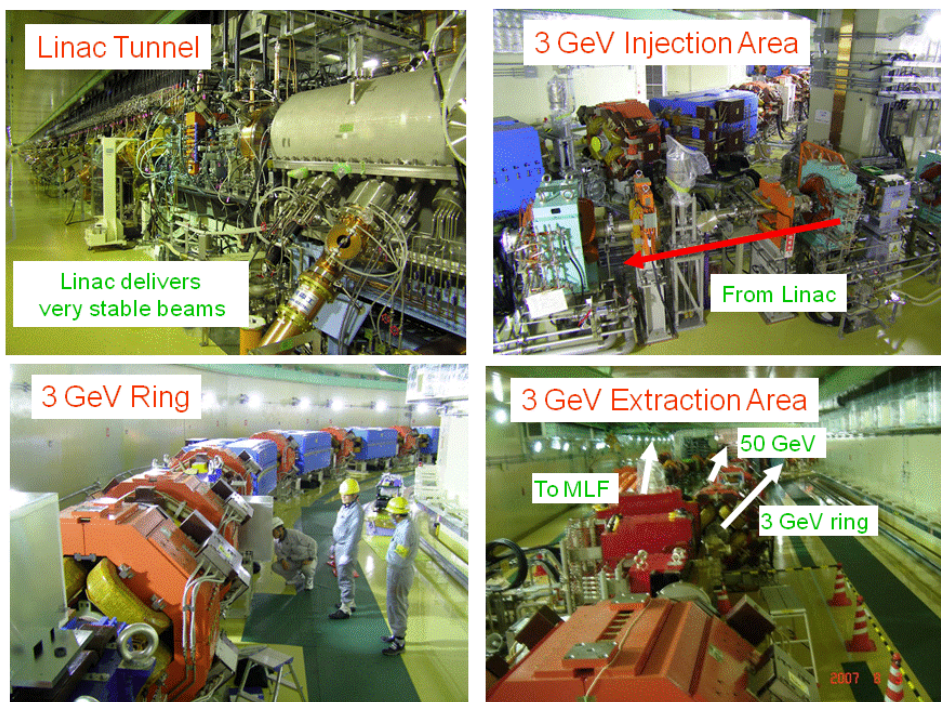


Photo tour of accelerators

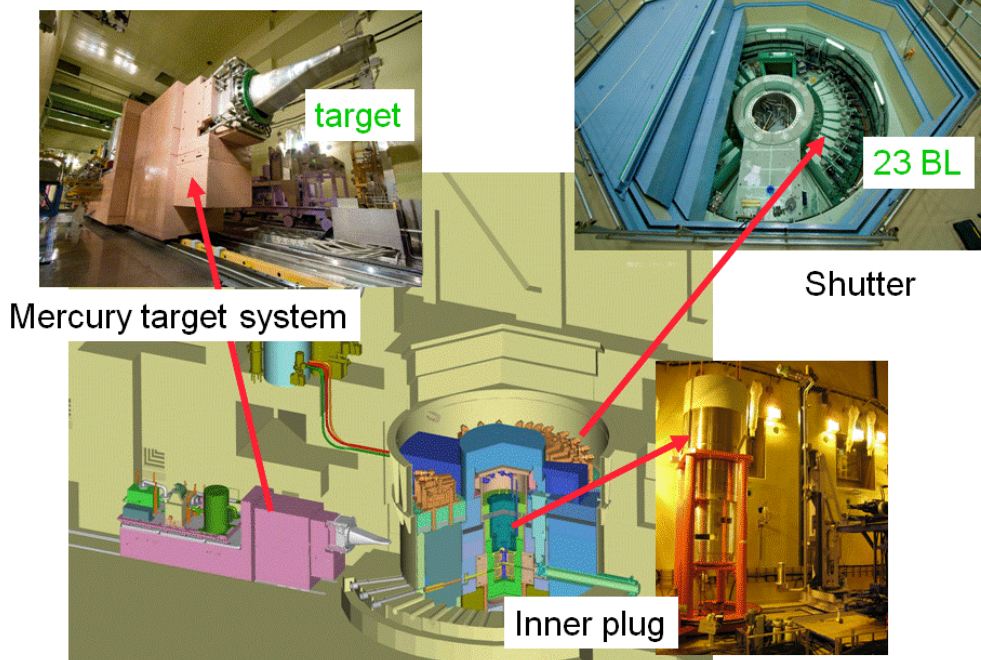
Status : On beam commissioning





Target station (JSNS)

Status : Off beam commissioning



Beam Line / Instruments Status

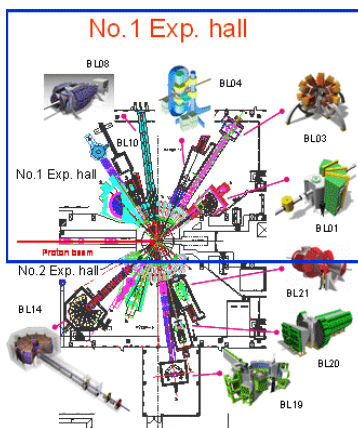
		FY2006												FY2007												FY2008											
		2007.1	2	3	4	5	6	7	8	9	10	11	12	2008.1	2	3	4	5	6	7	8	9	10	11	12	2009.1											
		Linac acceleration Jan.24, 2007												3GeV RCS acceleration Oct.31, 2007												The 1st neutron beam, May 2008											
1st Hall	BL01 4-SEASONS	Grant (JAEA, KEK, Tohoku U.)												Construction												commissioning											
	BL03 Bio-Molecule Diff.	Ibaraki Pref.												Construction												commissioning		User Op.									
	BL04 Neutron Cross-section measurement	Grant (Hokkaido Univ., etc)												Construction												commissioning		User Op.									
	BL05 NOP	Grant (KEK)												Construction												commissioning											
	BL08 High-Resolution Powder Diff.	KEK												Construction												commissioning		User Op.									
															completion																						
2nd Hall	BL14 AMATERAS (low E chopper)	JAEA												Construction												commissioning											
	BL19 TAKUMI (stress analysis)	JAEA												Construction												commissioning		User Op.									
	BL20 Versa. Powder Diff.	Ibaraki Pref.												Construction												commissioning		User Op.									
	BL21 Versa. Total Scatt. Diff.	Grant (KEK)												Construction												commissioning											
															completion																						

● Safety patrol for constructions at MLF : two persons twice / day

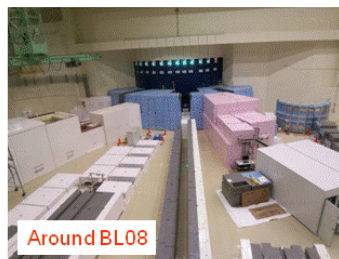


Neutron instruments : No.1 Experimental Hall

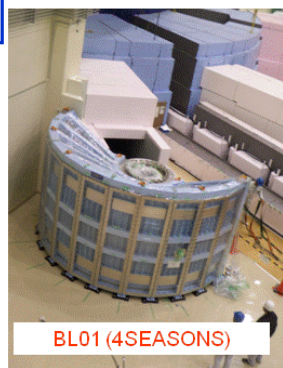
Status : Constructing



Around BL03



Around BL08



BL01 (4SEASONS)

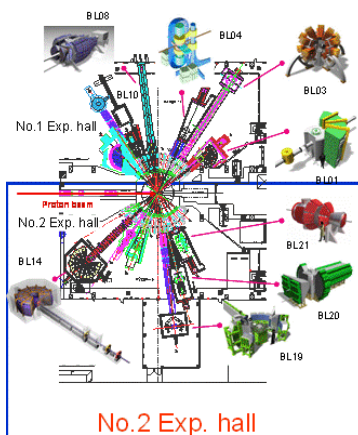


BL08 (SHRPD) Guide Hall with base shield



Neutron instruments: No.2 Experimental Hall

Status : Constructing



BL20 (iMATERIA)



BL14 (AMATERAS) beam line shield



BL14 (AMATERAS) with Fe Shield



BL19 (TAKUMI)



4SEASONS (BL01)

High-Intensity Chopper Spectrometer

JAEA, KEK, Tohoku Univ.

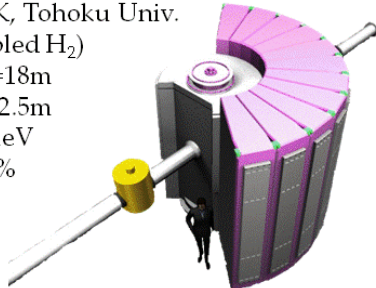
BL01(coupled H₂)

$L_{\text{mod-sample}}=18\text{m}$

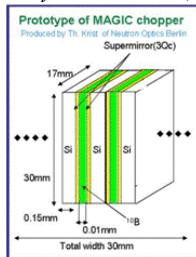
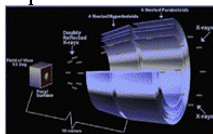
$L_{\text{sample-det.}}=2.5\text{m}$

$E_i=5\sim 300\text{meV}$

$\Delta E/E_i=5\sim 6\%$

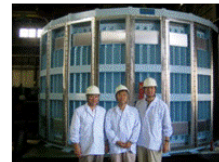
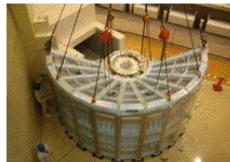


- Supported by MEXT, Grant-in-Aid for **Specially Promoted Research** (JFY2005-2009)
- Dedicated to **Oxide high- T_c superconductor**
- High Intensity & High Efficiency (**MAPSx100**)
- Multi E_i ability by **MAGIC** Chopper
- Sophisticated design of beam transport device



What were done in JFY2007

Fabrication & Installation of Main Chamber



Fabrication & Installation of Shielding



Re-use of clearance iron from decommissioned atomic power station to reduce the cost.

Fabrication of Guide Jacket

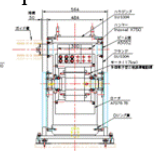
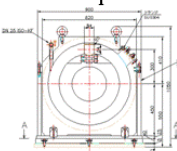
200 detector tubes have been ordered

Development of Choppers is continued...

Fermi by SFK, T₀ & Disc-chopper by KOBELCO

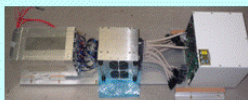
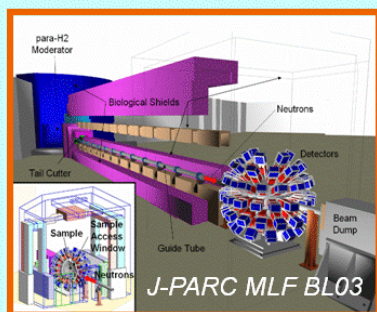
Development of Software is continued...

Development of Spin Filter is continued...

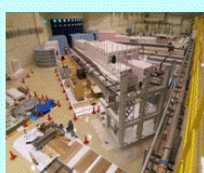


will be Ready in Autumn of 2008

IBARAKI Biological Crystal Diffractometer (iBIX) (BL03)



2-Dim. WLSF
Scintillation
Detector under
Development



The Latest Setting
of Biological Shields
(Feb. 19, '08)



Guide Tube Jackets
on Adjustable Motors

- Hydrogen and hydration structure of biological molecules
- Efficiency more than 50 to 100 times higher than BIX-3 in JRR-3
- Minimum crystal size^(*): 0.5x0.5x0.5mm³
- Maximum measurable No. sample^(*): 100 crystals/yr^(*)
- (*)Both for macromolecules
- (*)In case of 2mm³ in volume
- Structure-based drug design
- Development of functional organic materials

Specifications

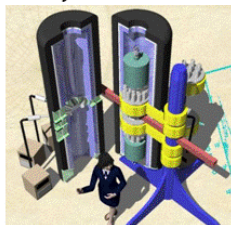
- Moderator : Coupled H₂ 100 X 100mm²
- L1 & L2 : 40m, 0.45m
- Guide Tube : 1~3Qc (70X20~15X15mm curved & focusing)
- Maximum cell dimension : 135 Å
- Minimum d-spacings : <1.2 Å (Macromolecules)
- <0.7 Å (Organic compounds)
- Range of Wavelength : 0.7~3.85 Å
- Detector spatial resolution : Less than 1 X 1 mm²



■ NNRI (BL04)

Neutron-Nucleus Reaction Instrument

Hokkaido Univ., JAEA, Tokyo Int. of Tec.
BL04 (coupled H₂)



- Neutron capture cross section measurement minor actinides & long lived fission products

■ NOBORU (BL10)

Neutron Beam-line for Observation and Research Use

JAEA
BL10 (decoupled H₂)

- JSNS Design Validation
- Test Port



■ What were done in JFY2007 ■

- Construction almost completed



■ What were done in JFY2007 ■

- Ready to welcome the first neutron pulse on Day-1



■ SHRPD (BL08)

High Resolution Powder Diffractometer

KEK
BL08 (decoupled H₂ (poisoned))
Highest resolution $\Delta d/d : 3 \times 10^{-4}$
Total flight path: 100 m
Two banks: BS ($150^\circ \leq 2\theta \leq 170^\circ$)
and WA ($10^\circ \leq 2\theta \leq 100^\circ$)
 d range : $0.3 \leq d(\text{\AA}) \leq 60$

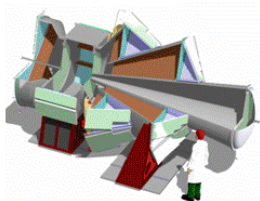
■ Schedule

2007 Dec - : Ground settlement has been continuously measured
2008 Apr: 80 m supermirror guide tube will be aligned in both main & annex buildings
2008 May: Commissioning using a previous vacuum tank of the Sirius diffractometer
2008 Dec: Test experiments will start with the Sirius tank
2009 Aug: Install the SHRPD chamber and commissioning will start

■ High Intensity Total Diffractometer (BL21)

High Intensity Total Diffractometer

NEDO, KEK
BL21 (decoupled H₂)
Highest resolution
 $\Delta Q/Q : 3 \times 10^{-3}$
 Q range
 $0.01 \leq Q(\text{\AA}^{-1}) \leq 100$



■ What were done in JFY2007 ■

- East annex building dedicated to SHRPD



completed in Dec. 2007

■ What were done in JFY2007 ■

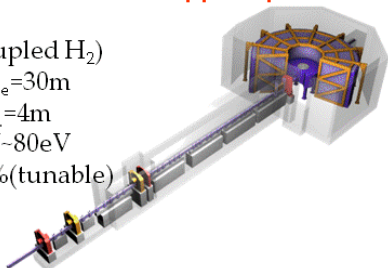
- Construction on Fabrication of major Components
- Shieldings is partly installed (March 2008)
- Schedule
2008 May: Biological shields will be constructed
2008 Nov: Vacuum tank will be installed
2008 Dec: Commissioning will be started



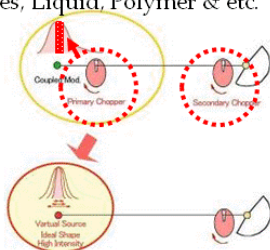
AMATERAS (BL14)

Cold-Neutron Disk-Chopper Spectrometer

JAEA

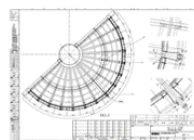
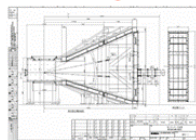
BL14(coupled H₂) $L_{\text{mod-sample}}=30\text{m}$ $L_{\text{sample-det.}}=4\text{m}$ $E_i=1\text{meV}\sim 80\text{eV}$ $\Delta E/E_i \sim 1\%$ (tunable)

- 3-years construction, JAEA (JFY2006-JFY2008)
- Fine and Tunable Resolution by Disk Choppers
- High-Intensity & High-Resolution at Cold Neutron Region
- Inelastic and Quasi-elastic measurements on Single Crystals, Glasses, Liquid, Polymer & etc.



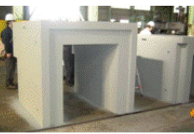
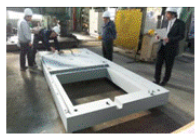
■ What were done in JFY2007 ■

- Contraction on Fabrication of major Components have been made in JFY2006. Scattering Chamber, Shielding, Choppers, Neutron Guide, Detectors (266 tubes), Utility, Cryostat...
- Detail Design of Scatt. Chamber was finished



- Detail Design of Shielding was finished.

Fabrication & Installation has been started ~May 2008



- First User Meeting December 20-21, 2008



- Detail Design of other components are progressing....

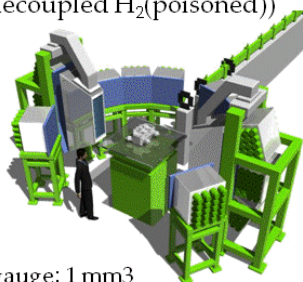
will be Ready by the end of 2008



TAKUMI (BL19)

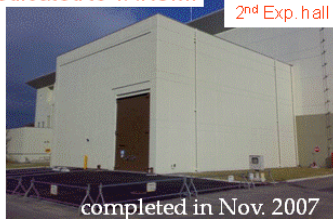
Engineering Materials Diffractometer

JAEA

BL19 (decoupled H₂(poisoned))

- lowest gauge: 1 mm³
- 2 × 2 × 2 mm³, 30 mm path in Fe: ~3 min
- stress resolution: ~ ± 15 MPa (Steel)

West annex building dedicated to TAKUMI



■ What were done in JFY2007 ■

- Beamline and main shields were almost installed

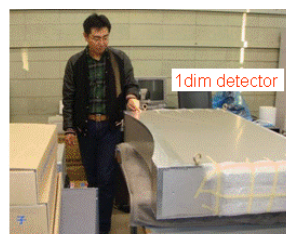


Beamline shields



main shields (trial assembly)

- ISIS type Scintillation Detectors have been tested



1dim detector

- Schedule

2008 April: main parts will be installed

2008 Aug: all parts will be completed

2008 Sep: Commissioning using prototype software

2008 Dec: Test experiments will start



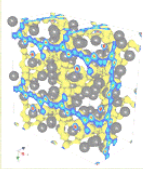
iMATERIA BL20

- IBARAKI Materials Design Diffractometer -

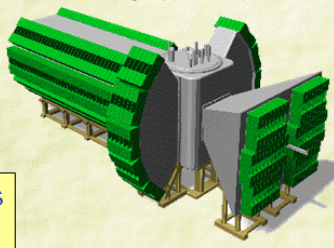



• Versatile powder diffractometer

The Ibaraki Prefecture; the local government for J-PARC site decided to build diffractometers to promote a **industrial application** for neutron beam in J-PARC



Contact: Toru Ishigaki (Ibaraki Univ.)

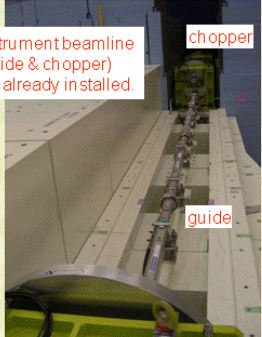


• High throughput >
(100 x KENS-Sirius)
20,000 samples/year

Sample exchange robots
One button analysis



Vacuum chamber is installed



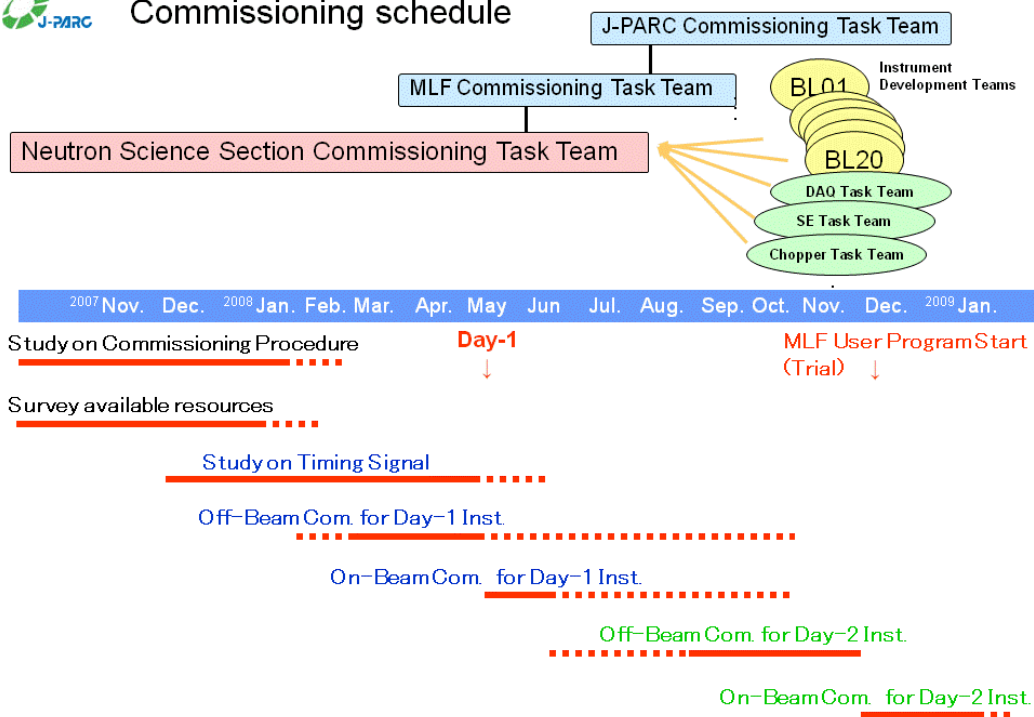
Instrument beamline (guide & chopper) are already installed.

chopper

guide

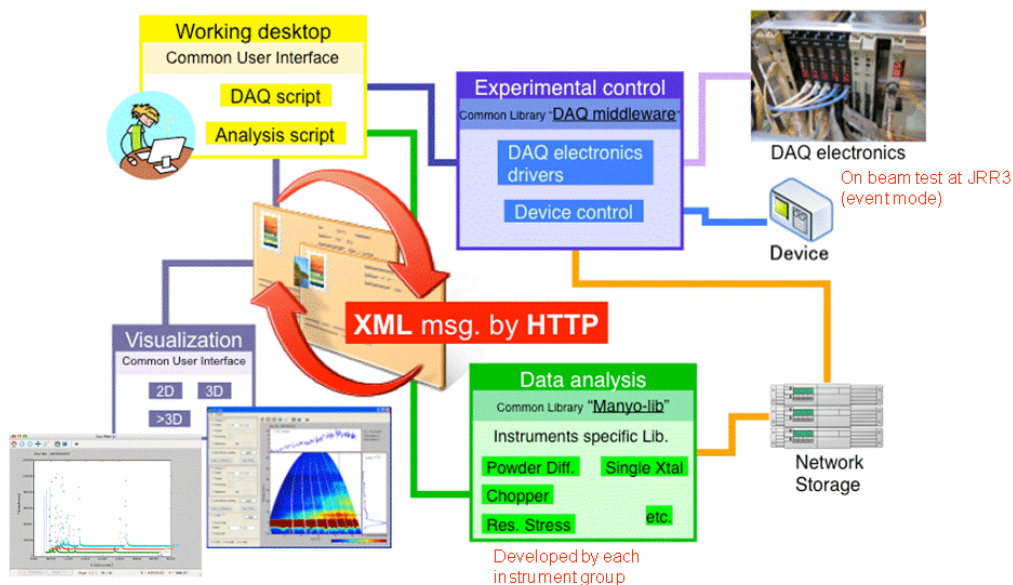


Commissioning schedule





MLF software framework : integration of software components

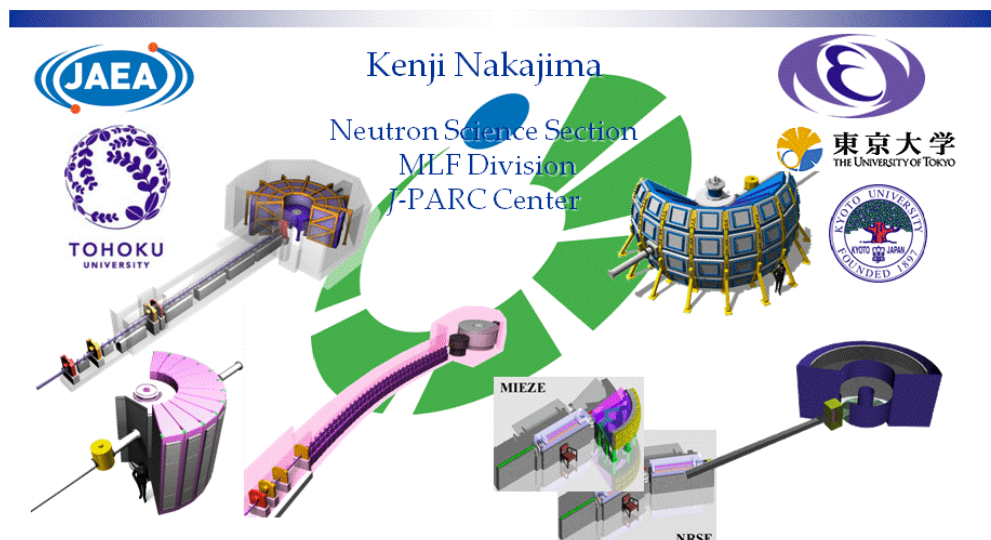


- Commissioning will start from April 2008

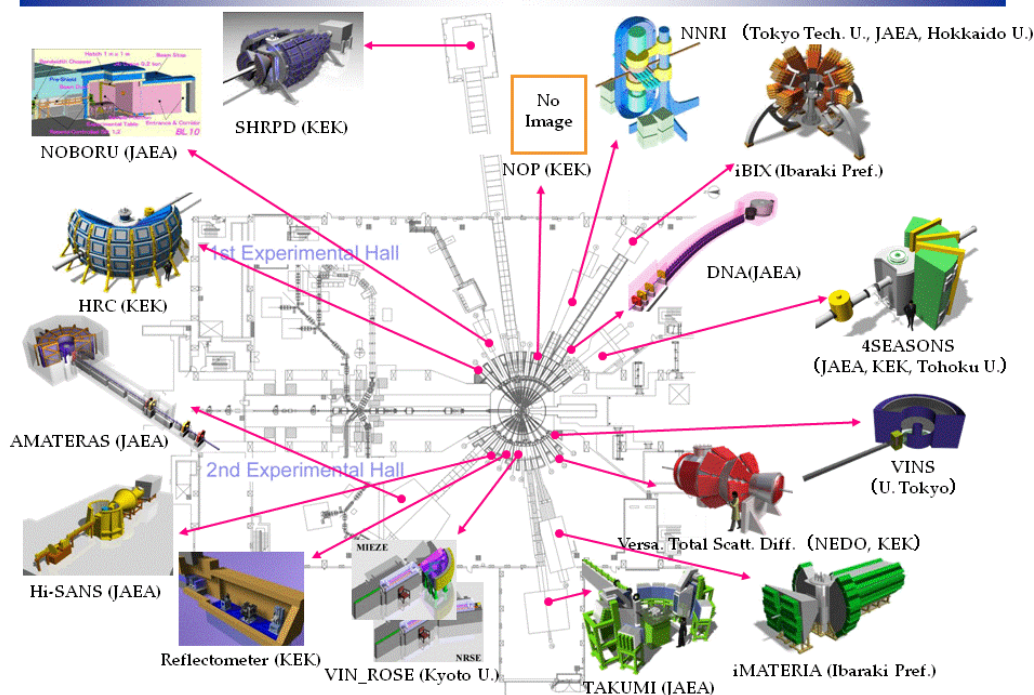
3.2. Inelastic Instrument Suite in MLF, J-PARC Kenji Nakajima (JAEA)



Inelastic Instrument Suite in MLF, J-PARC



Inelastic Instrument Suite in MLF, J-PARC





Inelastic Instrument Suite in MLF, J-PARC

Inelastic Spectrometers @ MLF

6 Inelastic Spectrometers @ J-PARC

4SEASONS (Hi-Intensity Chopper Spectrometer)

JAEA, KEK, Tohoku U.
Ready in Autumn of 2008

AMATERAS (Disk-Chopper Spectrometer)

JAEA
Ready in the End of 2008

HRC (Hi-Resolution Chopper Spectrometer)

KEK
Under Construction

VIN_ROSE (Resonance SE Suite)

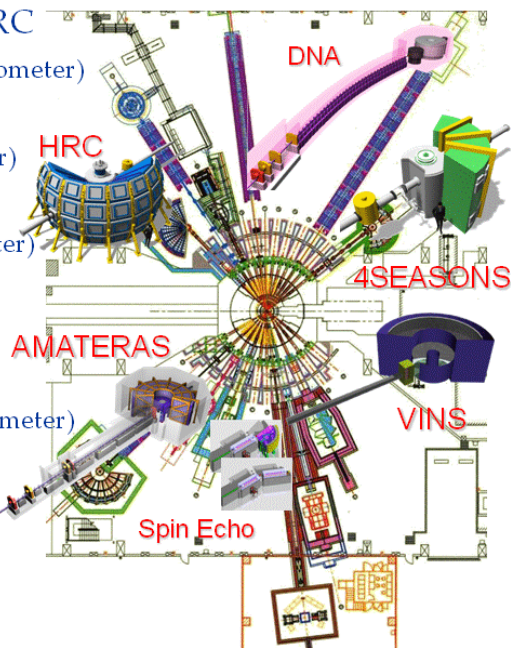
Kyoto U.
Under Development

VINS (Versatile Inelastic Neutron Spectrometer)

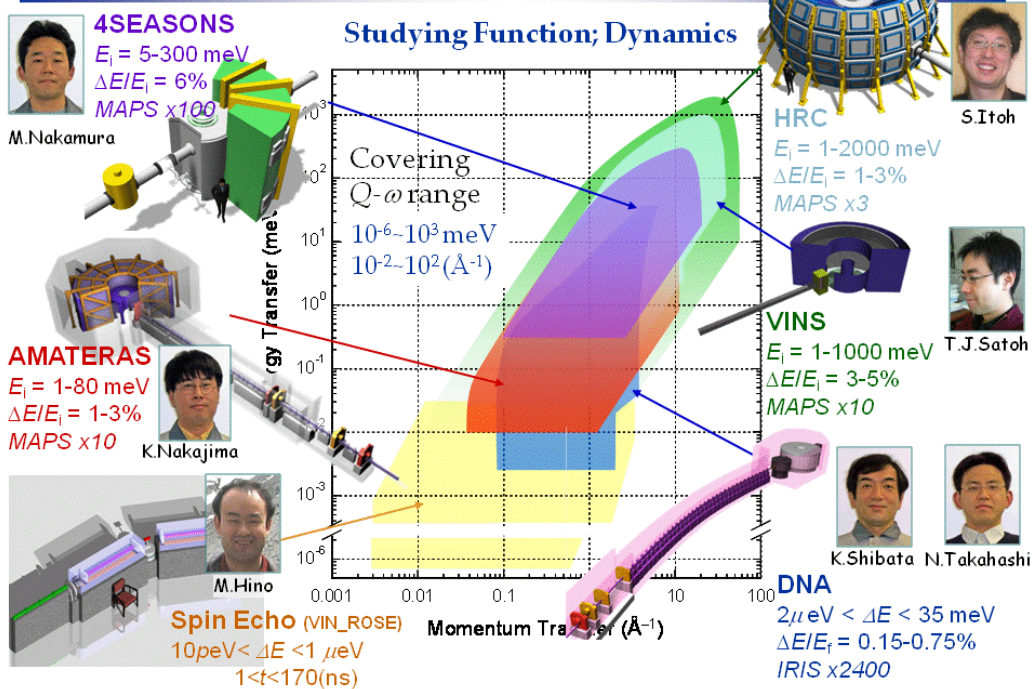
U. of Tokyo (ISSP)
planned

DNA (Inverted Geometry Spectrometer)

JAEA
Ready in 2010



Inelastic Spectrometer Suites in MLF, J-PARC





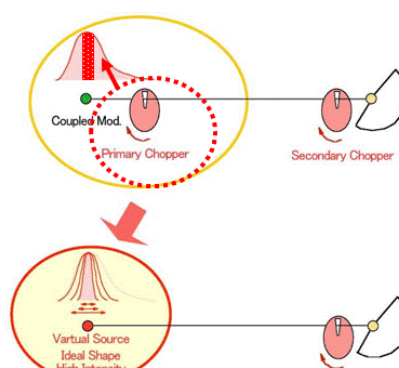
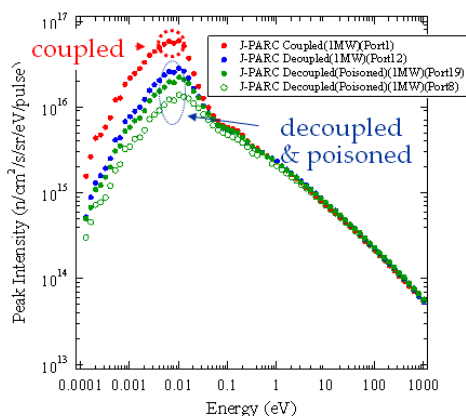
Coupled Moderator & RRM

- To Enhance the Measuring Efficiency



Coupled Moderator + Multi-Incident Energy (E_i) Measurements
AMATERAS, 4SEASONS, **DNA**

- Coupled Moderator + Pulse Shaping Chopper (AMATERAS, DNA)



Coupled Moderator & RRM

- To Enhance the Measuring Efficiency

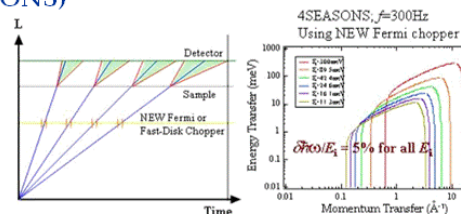


Coupled Moderator + Multi-Incident Energy (E_i) Measurements
AMATERAS, 4SEASONS, **DNA**

- Multi- E_i Measurements (AMATERAS, 4SEASONS, DNA)

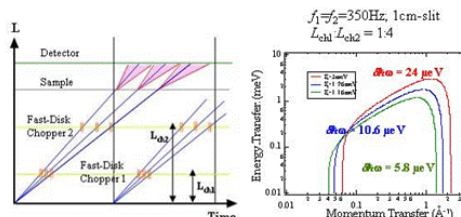
■ High-Energy Mode (AMATERAS, 4SEASONS)

- Utilizing Multi- E_i Beam Established from the Monochromating Chopper
- Covers Relatively Higher Energy Region with Moderate Resolution
- *Without Pulse-Shaping Chopper on AMATERAS
- *Using New Fermi-chopper for 4SEASONS



■ High-Resolution Mode (AMATERAS)

- Coherent Operation of Both Pulse Shaping Chopper & Monochromating Chopper ($L_{mod-ch1} \cdot L_{mod-ch2} = 1.4$ on AMATERAS)
- Covers Lower Energy Region with Fine Resolution
- *Dynamic Range is Narrow

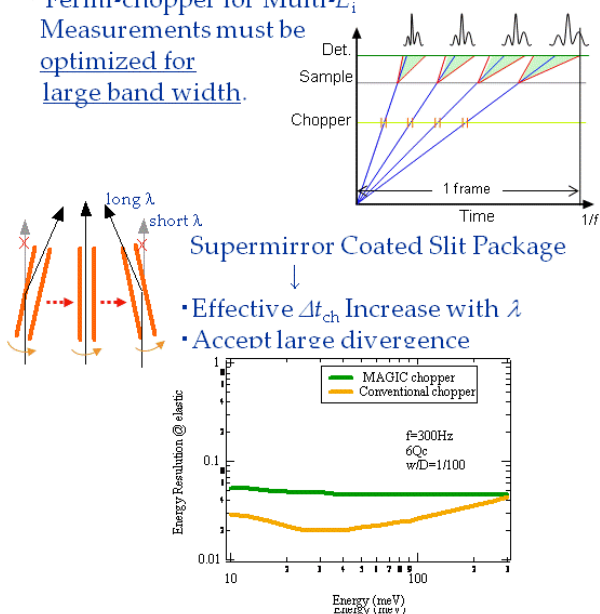




Coupled Moderator & RRM

Multi- E_i Measurements & MAGIC Chopper on 4SEASONS

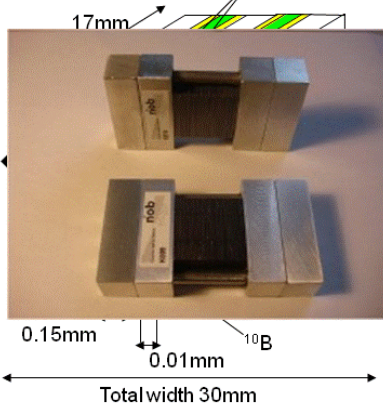
- Fermi-chopper for Multi- E_i
Measurements must be optimized for large band width.



Prototype of MAGIC chopper

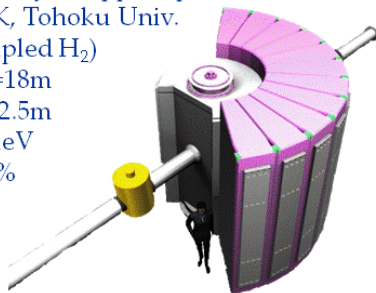
Produced by Th. Krist of Neutron Optics Berlin

Supermirror(3Qc)

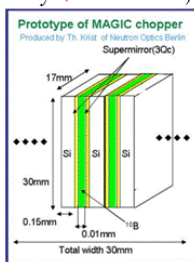
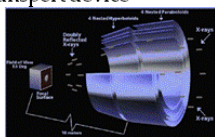


4SEASONS

High-Intensity Chopper Spectrometer
JAEA, KEK, Tohoku Univ.
BL#01(coupled H₂)
 $L_{mod-sample}=18m$
 $L_{sample-det.}=2.5m$
 $E_i=5\sim300meV$
 $\Delta E/E_i=5\sim6\%$

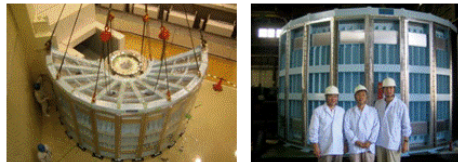


- Supported by MEXT, Grant-in-Aid for **Specially Promoted Research** (JFY2005-2009)
- Dedicated to **Oxide high- T_c superconductor**
- High Intensity & High Efficiency (**MAPSx100**)
- Multi- E_i ability by **MAGIC** Chopper
- Sophisticated design of beam transport device



Current Status

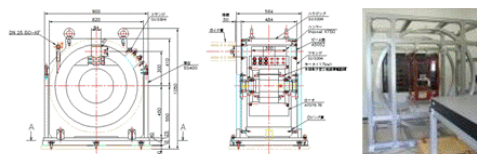
Fabrication & Installation of Main Chamber



Fabrication & Installation of Shielding



- 200 detector tubes have been ordered
- Development of Choppers is continued...
Fermi by SFK, T₀ & Disc-chopper by KOBELCO
- Development of Software is continued...
- Development of Spin Filter is continued...



will be Ready in Autumn of 2008

AMATERAS

Cold-Neutron Disk-Chopper Spectrometer JAEA

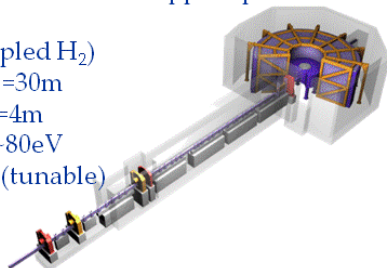
BL14(coupled H₂)

$L_{\text{mod-sample}}=30\text{m}$

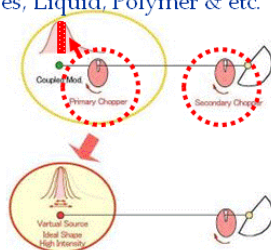
$L_{\text{sample-det.}}=4\text{m}$

$E_i=1\text{meV}\sim 80\text{eV}$

$\Delta E/E_i \sim 1\%$ (tunable)

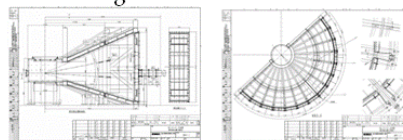


- 3-years construction, JAEA (JFY2006-JFY2008)
- Fine and Tunable Resolution by Disk Choppers
- High-Intensity & High-Resolution at Cold-Neutron Region
- Inelastic and Quasi-elastic measurements on Single Crystals, Glasses, Liquid, Polymer & etc.

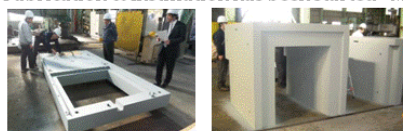


Current Status

- Construction on Fabrication of major Components have been made in JFY2006. Scattering Chamber, Shielding, Choppers, Neutron Guide, Detectors (266 tubes), Utility, Cryostat...
- Detail Design of Scatt. Chamber was finished



- Detail Design of Shielding was finished. Fabrication & Installation has been started ~May 2008



- First User Meeting December 20-21, 2008



- Detail Design of other components are progressing....

will be Ready by the end of 2008

HRC

High-Resolution Chopper Spectrometer

KEK

BL#12(decoupled H₂)

$L_{\text{mod-sample}}=15\text{m}$

$L_{\text{sample-det.}}=4\text{m}$

$E_i=1\text{meV}\sim 2\text{eV}$

$\Delta E/E_i \sim 1\%$



Current Status

- Construction is going slowly but steadily.
 - Insertion Devices (front end beam transport)
 - Part of Shieldings
 - Development of Fermi Choppers.



VIN_ROSE

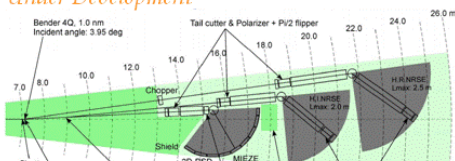
Neutron Spin Echo (MIEZE&NRSE)

Kyoto Univ., JAEA

BL: not yet assigned

Covering wide dynamic range combining three types of neutron spin echo technique

Under Development



VINS

Hi-Intensity Chopper

Univ. of Tokyo (ISSP)

BL#23(decoupled H₂)

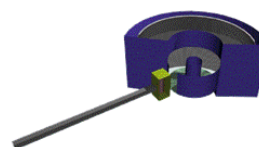
$L_{\text{mod-sample}}=11.8\text{m}$

$L_{\text{sample-det.}}=2.5\text{m}$

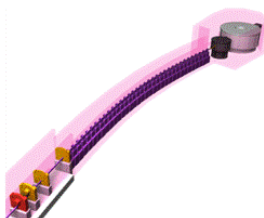
$E_i=1\text{meV}\sim 1\text{eV}$

$\Delta E/E_i \sim 5\%$

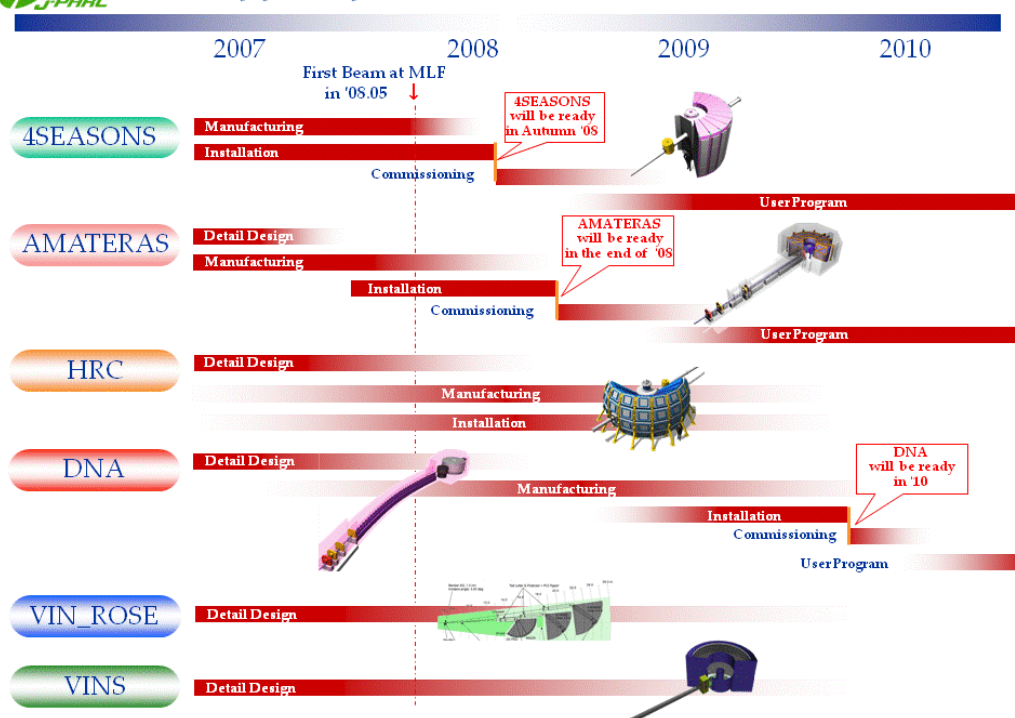
Planned



DNA
 Indirect-geometry Spectrometer
 JAEA
 BL#02(decoupled H₂)
 $L_{\text{mod-sample}} = 39 \text{ \& } 43\text{m}$
 4 analyzers:
 PG(002), Ge(311), Si(111), Si(311)
 $2 \text{ micro-eV} < \Delta E < 35 \text{ meV}$



4 Chopper Spectrometers at MLF, J-PARC





Thank You for Your Attention!

■ Contact Persons ■

4SEASONS

M. Nakamura & M. Arai (JAEA)

AMATERAS

Kenji Nakajima (JAEA)

HRC

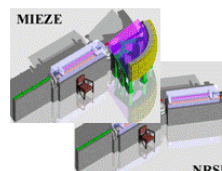
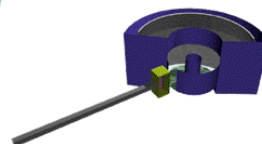
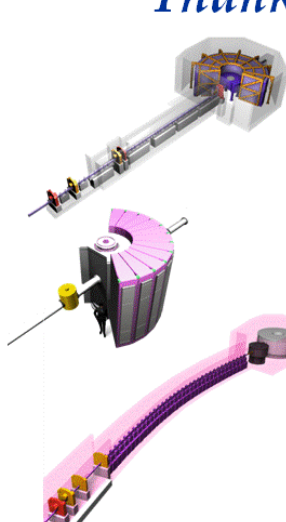
Shinichi Itoh (KEK)

VIN ROSE

Masahiro Hino (KURRI, Kyoto Univ.)

VINS

Taku J. Satoh (ISSP, Univ. of Tokyo)

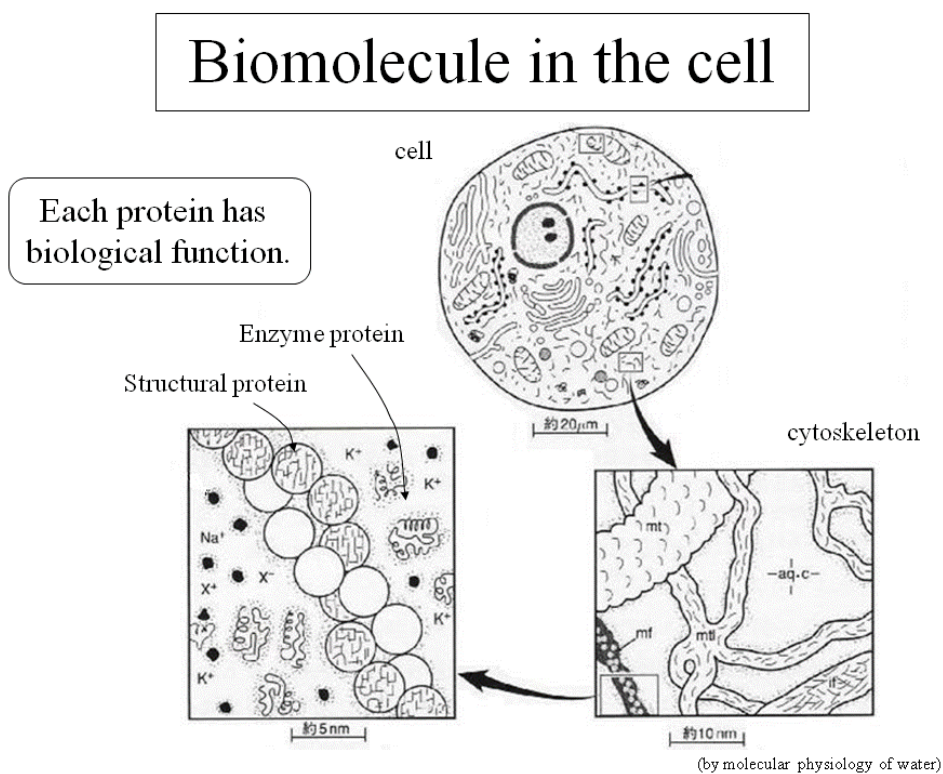


3.3. Required Spectrometer Specification from Biomolecular Dynamics Studies

Hiroshi Nakagawa (JAEA)

Required Spectrometer Specification from Biomolecular Dynamics Studies

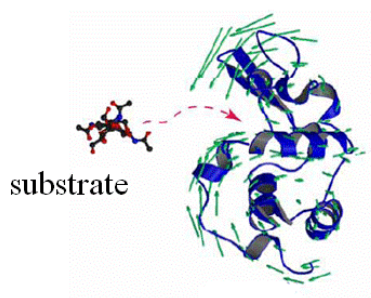
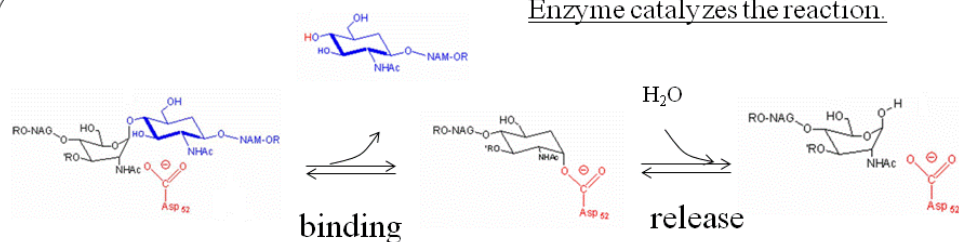
Hiroshi Nakagawa (JAEA)



Enzyme function ~Lysozyme~

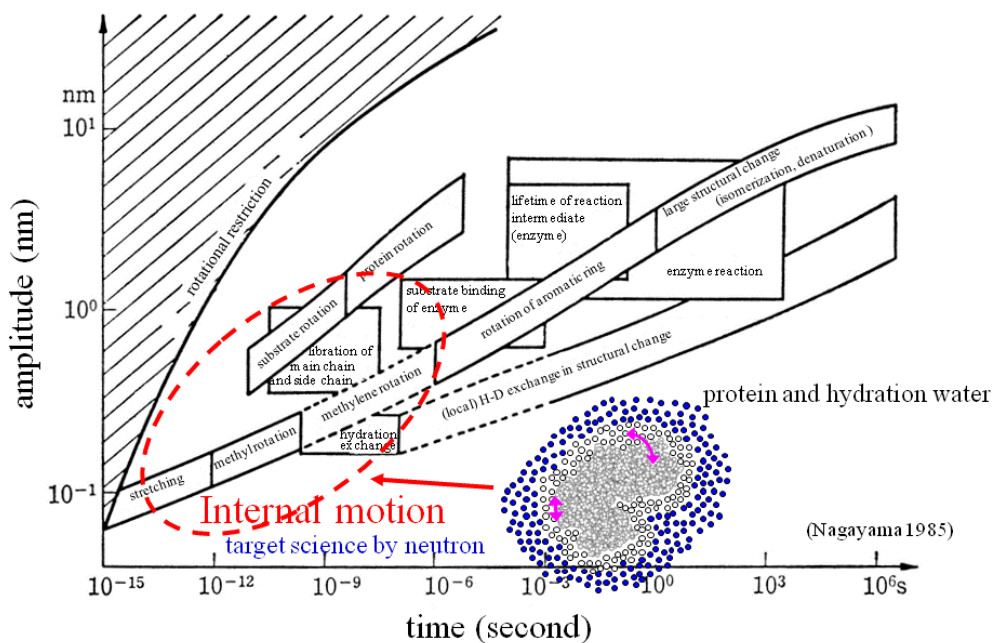
(chemical reaction in the cell)

Enzyme catalyzes the reaction.



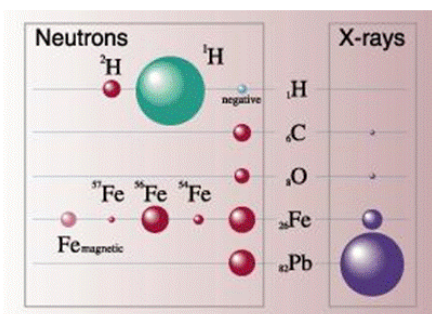
Biological function accompany structural change of biomolecule.

Space and time scale in functional dynamics

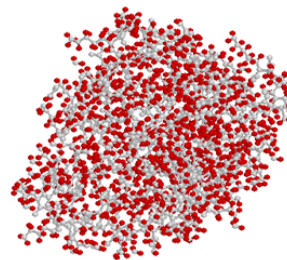


Incoherent neutron scattering

scattering cross section of neutron



● hydrogen atom



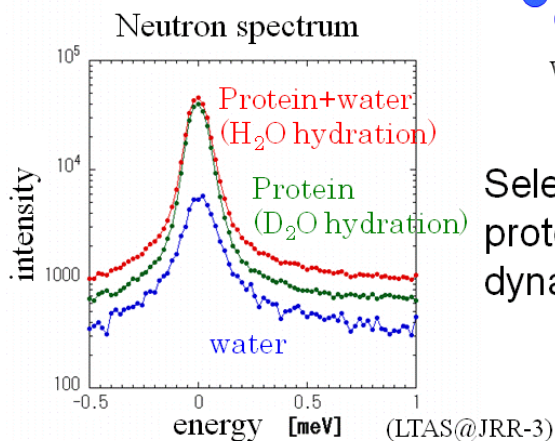
H atoms are distributed over protein.

Observation of hydration water by isotope labeling

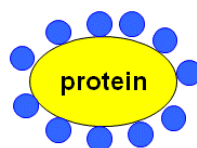
Cross section (10^{-28}m^2)

H atom (●) **80.2**

D atom (○) **2.0**

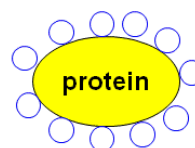


H₂O hydration



Water visible

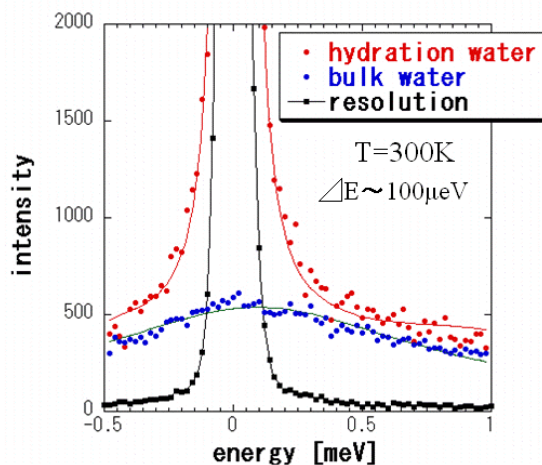
D₂O hydration



Water invisible

Selectively observation of protein and hydration water dynamics by isotope labeling

Quasielastic scattering of hydration water



(LTAS@JRR-3)

Dynamics of hydration water is restricted.

↓ next step

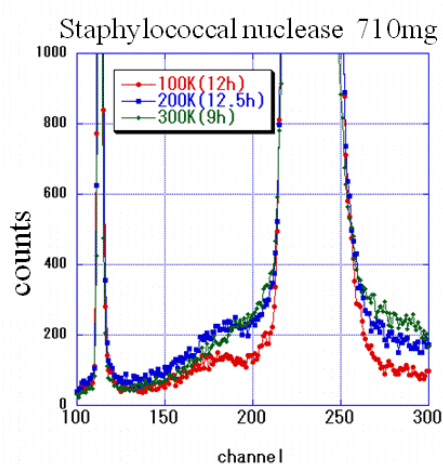
Slow dynamics

$\Delta E \sim 1 \mu\text{eV}$

Q-dependence of QNS

Symmetrical spectrum is important for the data analysis.

Sample amount and data statistics



LAM-40 gave us the high quality spectrum of protein. But, large amount of sample and long experimental time was required.

→ a kind of experimental sample is limited.

(LAM-40)

intensity $1/10 \times \text{IN6@ILL}$

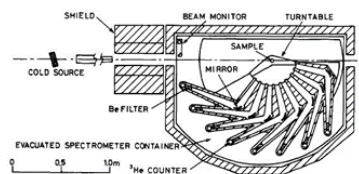
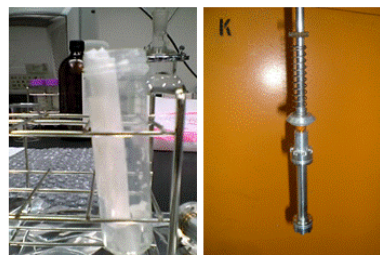
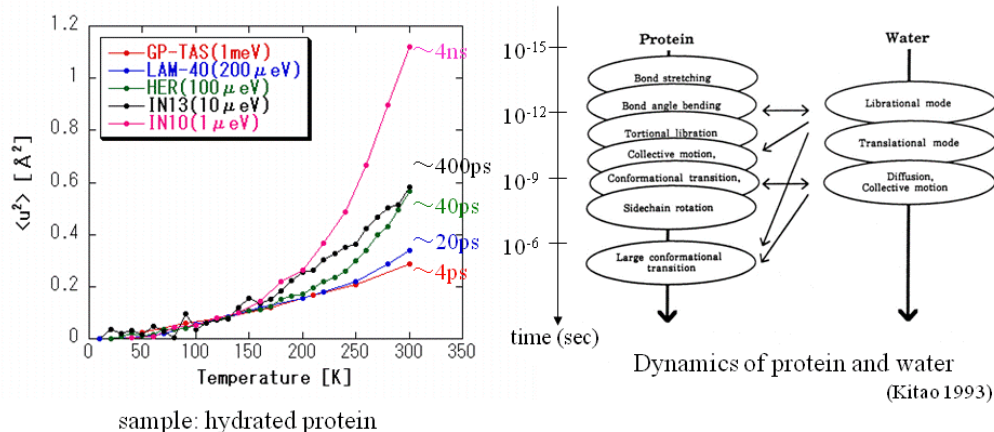


Fig. 7. The conventional resolution quasielastic spectrometer (LAM-40).



Hierarchy in protein-water dynamics

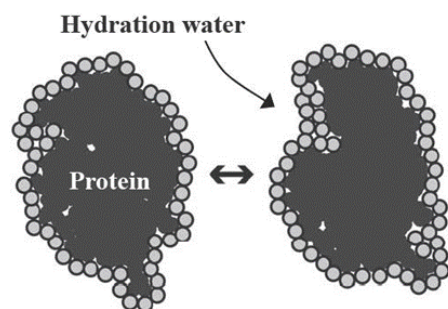
Time scale and temperature dependence of protein dynamics



Variable energy resolution experiment is important!

High-resolution experiment is essential!

Hydration-coupled slow dynamics of protein

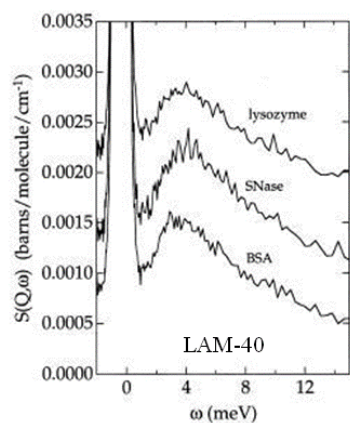


Hydration-coupled slow dynamics

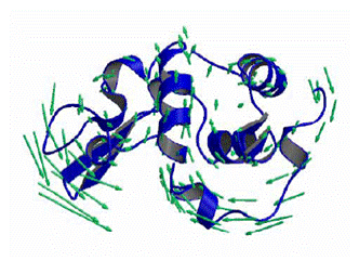
(~ns)

Quasi elastic scattering experiment with high resolution is required.

Protein low-energy dynamics (Boson peak)



M.Kataoka et al(1999)



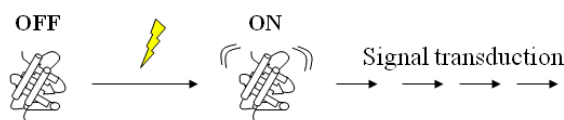
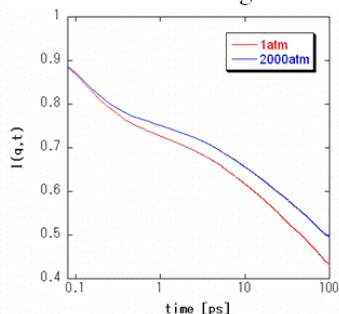
Collective motion

“Coherent” inelastic scattering in the wide q range is essential.

Sample environment

- Under high pressure
- Activation dynamics by light, laser,,,

Intermediate scattering function by MD



Biological molecules response the stimulations.

The response is related to the biological function.

Required specification

- High resolution and wide q range (analysis of QNS)
 - Slow dynamics
 - Geometry of dynamics
 - Symmetrical spectrum
- Variable energy resolution
 - Hierarchy of protein-water dynamics
- Small amount sample and neutron focusing
 - Expansion of species of target sample
- Sample environment
 - Functional dynamics by various stimulation

Acknowledgment

- Mikio Kataoka (NAIST & JAEA)
- Nobuhiro Go (JAEA)
- Yasumasa Joti (Univ. of Tokyo)
- Akio Kitao (Univ. of Tokyo)
- Kaoru Shibata (JAEA)
- Naoto Metoki (JAEA)
- Kouji Kaneko (JAEA)
- Toshiiji Kanaya (Kyoto Univ.)
- Itaru Tshukushi (Chiba Institute)
- Atsushi Tokuhisa (NAIST)

3.4. The Backscattering Spectrometer HFBS at NIST

Dan Neumann (NIST)

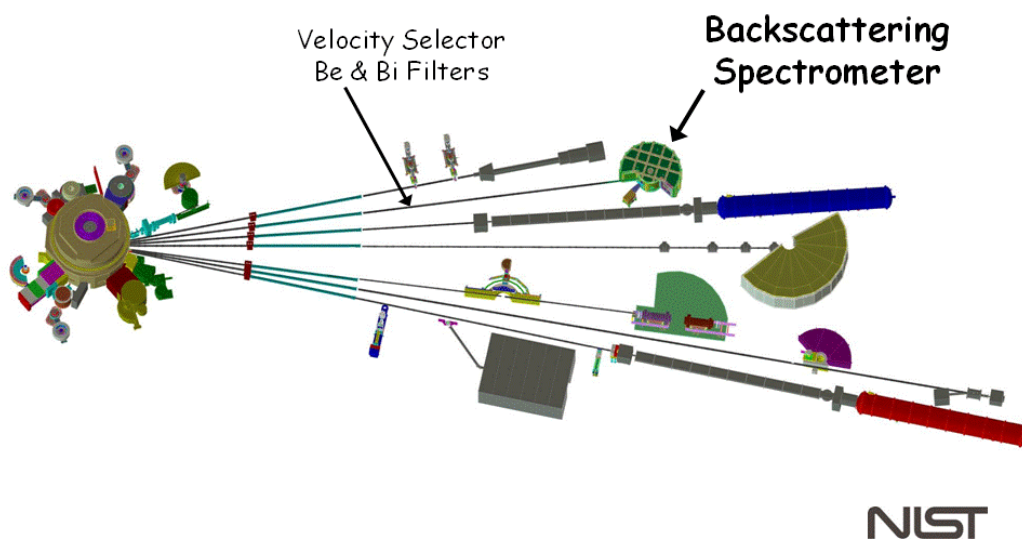
Backscattering at NIST

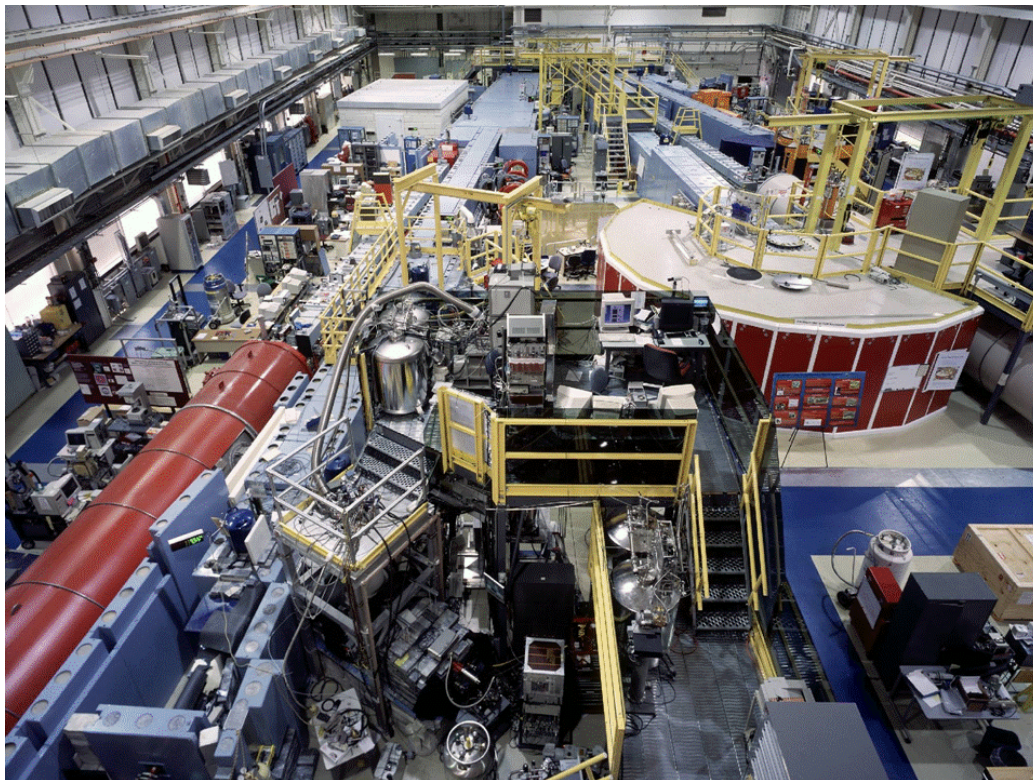
Dan Neumann
NIST Center for Neutron Research

dan@nist.gov www.ncnr.nist.gov

NIST

Instrument Layout at the NCNR



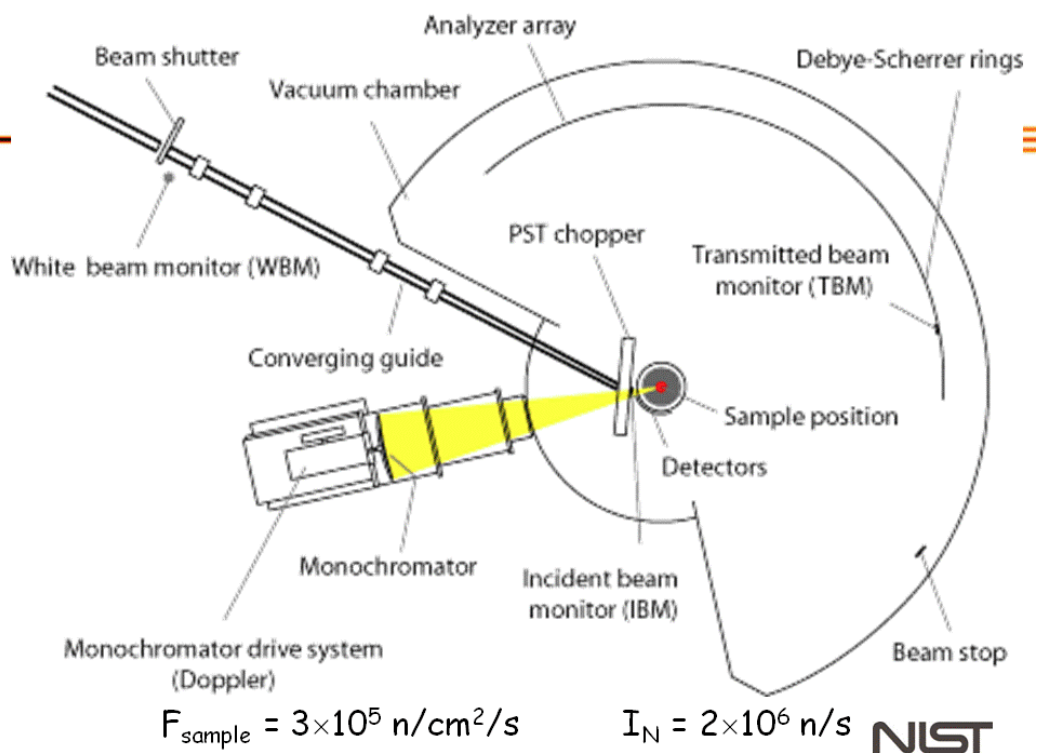


Backscattering Spectrometer

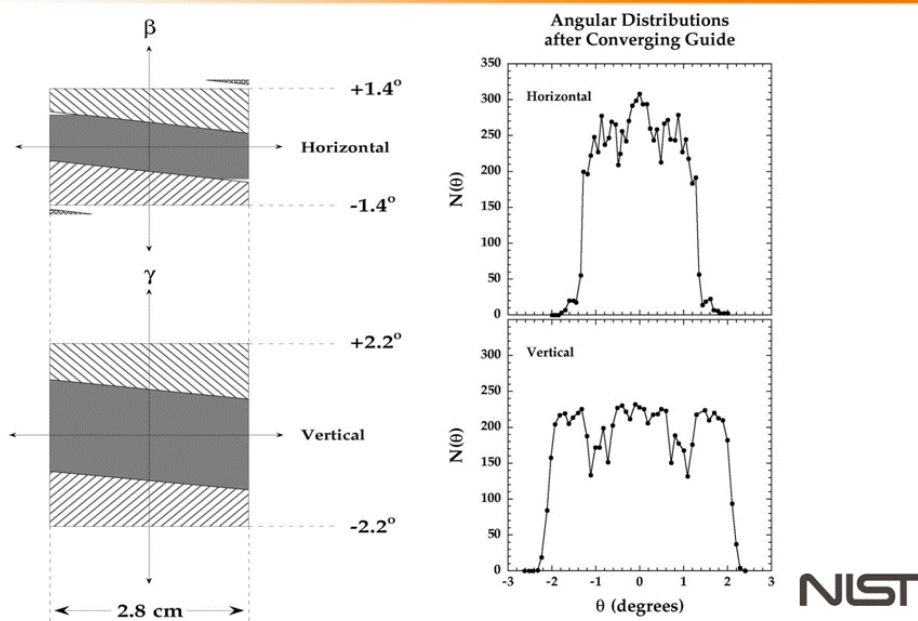


Analyzer covers 20% of 4π sr
(12 m²)

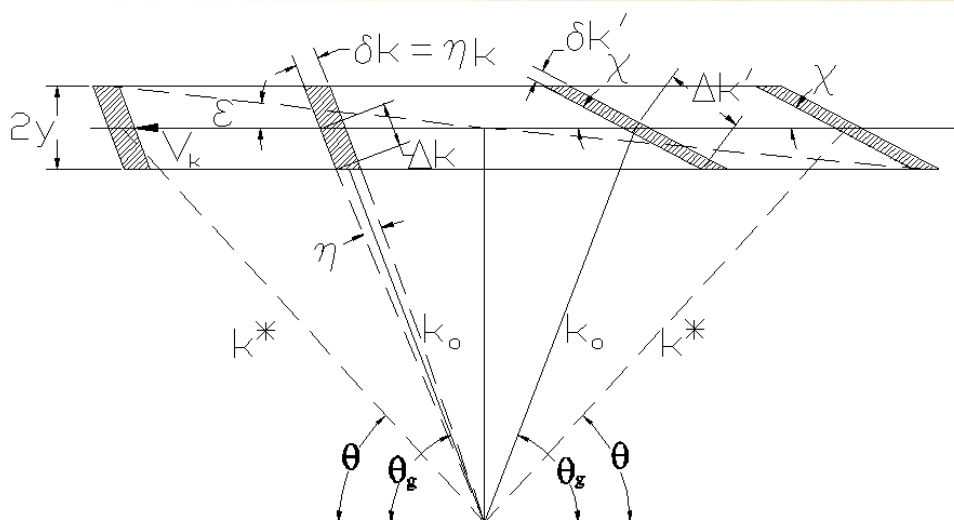
NIST



After Converging Guide



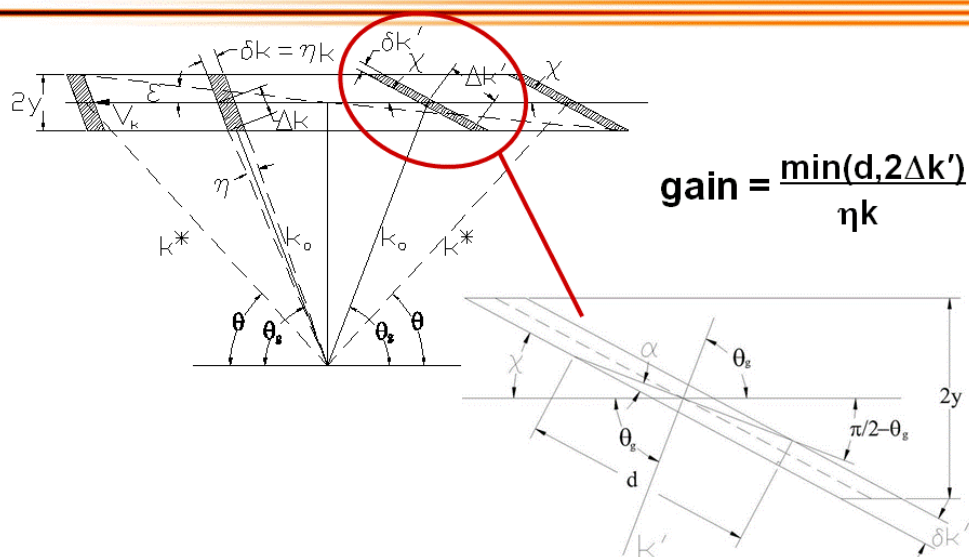
Phase Space Transform



Schelton & Alefeld

NIST

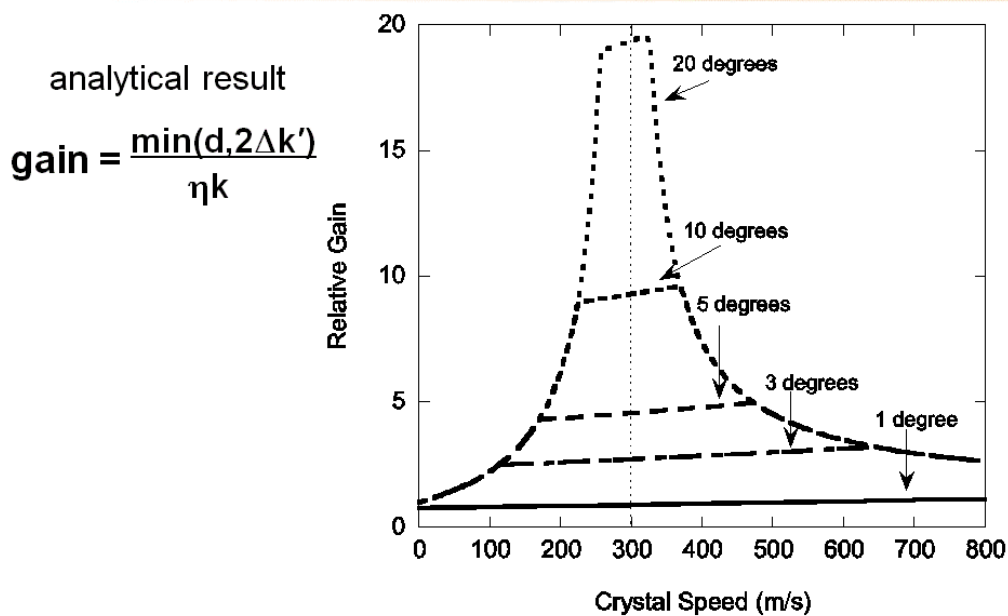
Phase Space Transform



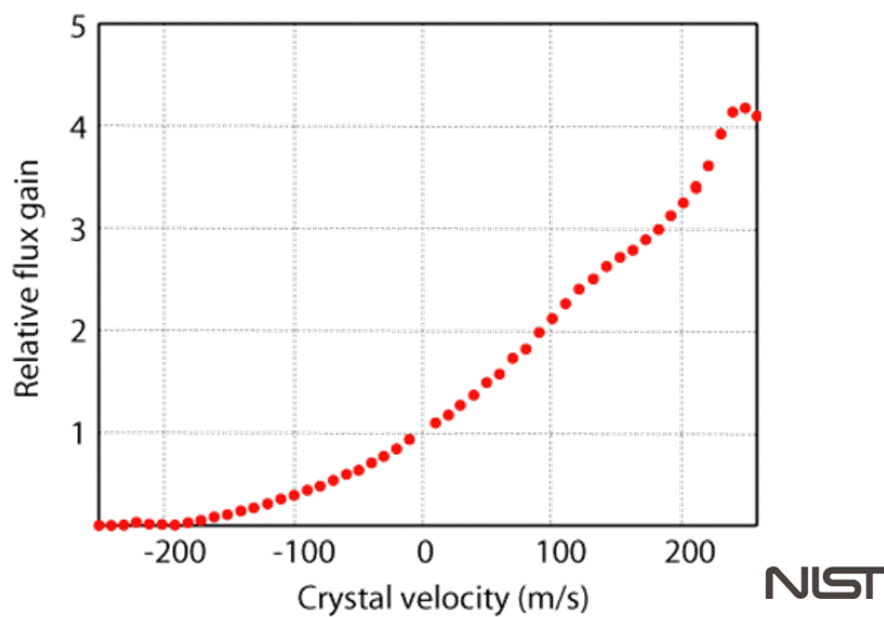
$$\text{gain} = \frac{\min(d, 2\Delta k')}{\eta k}$$

NIST

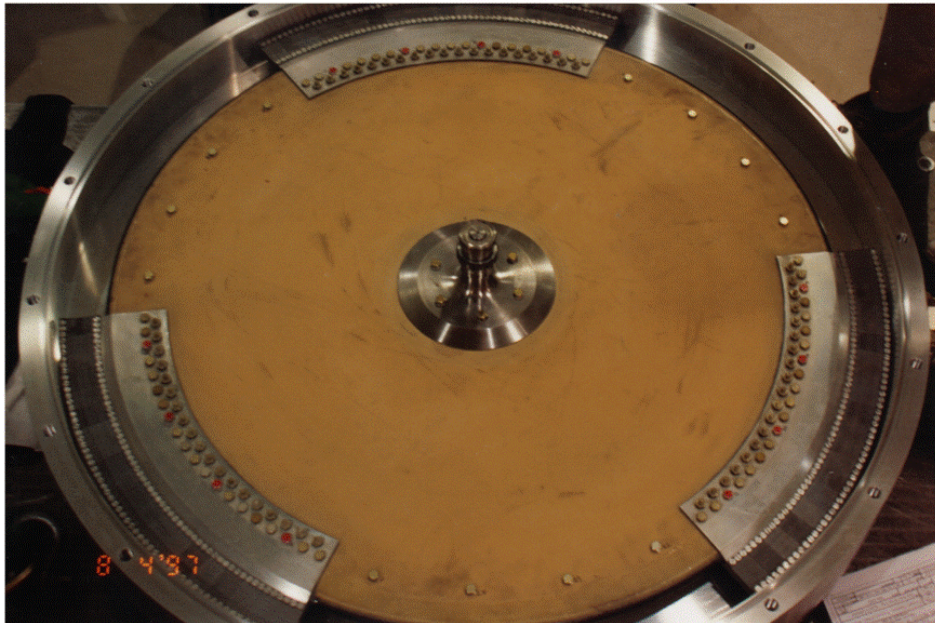
Phase Space Transform



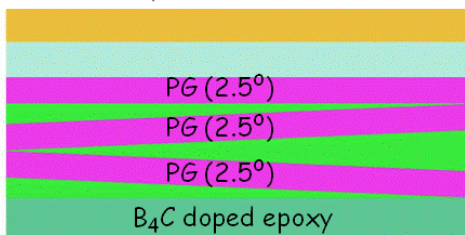
Phase Space Transform



Phase Space Transform



Layout of Cassettes



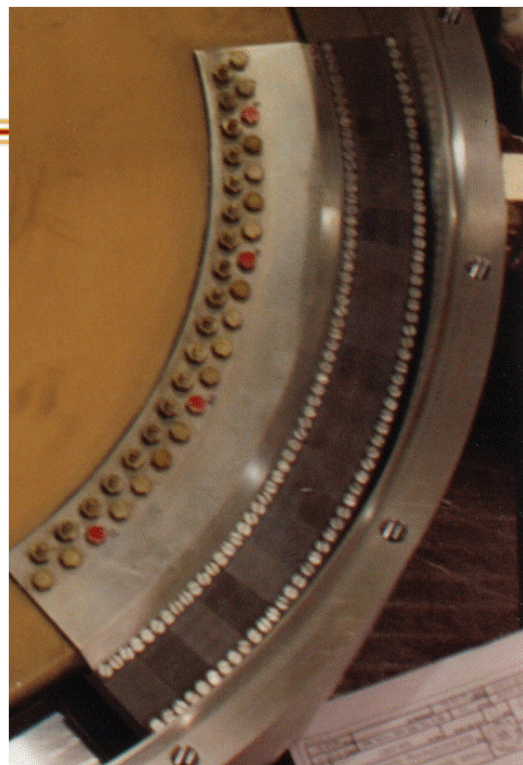
Disk has diameter of 1 m and rotates at 4780 rpm

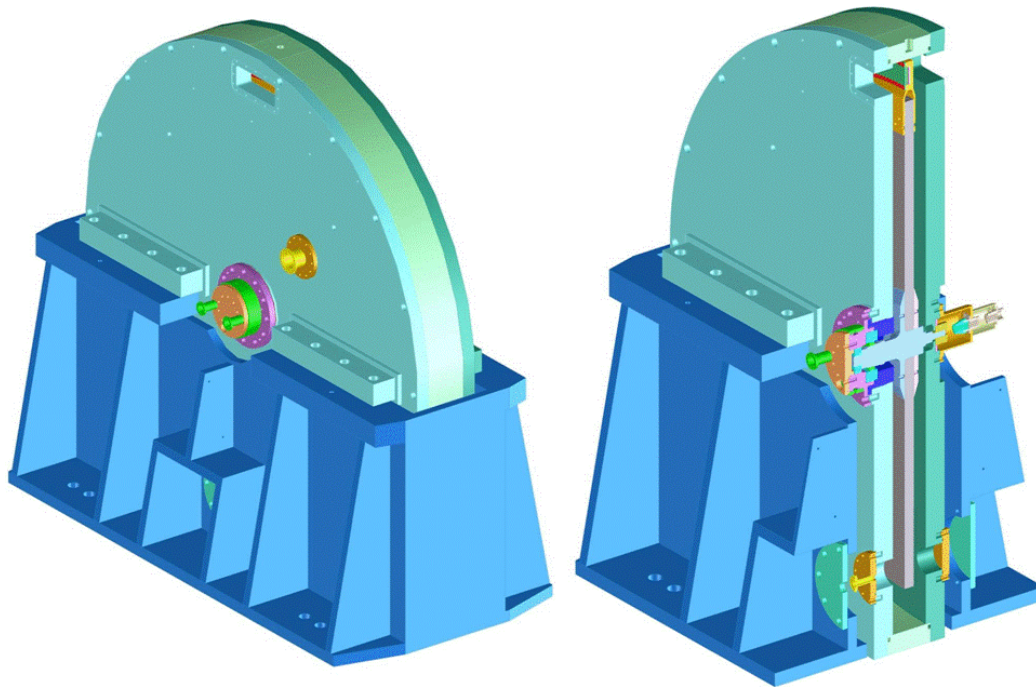
$$\omega = 500 \text{ rad/sec}$$

$$v = r\omega = 250 \text{ m/s}$$

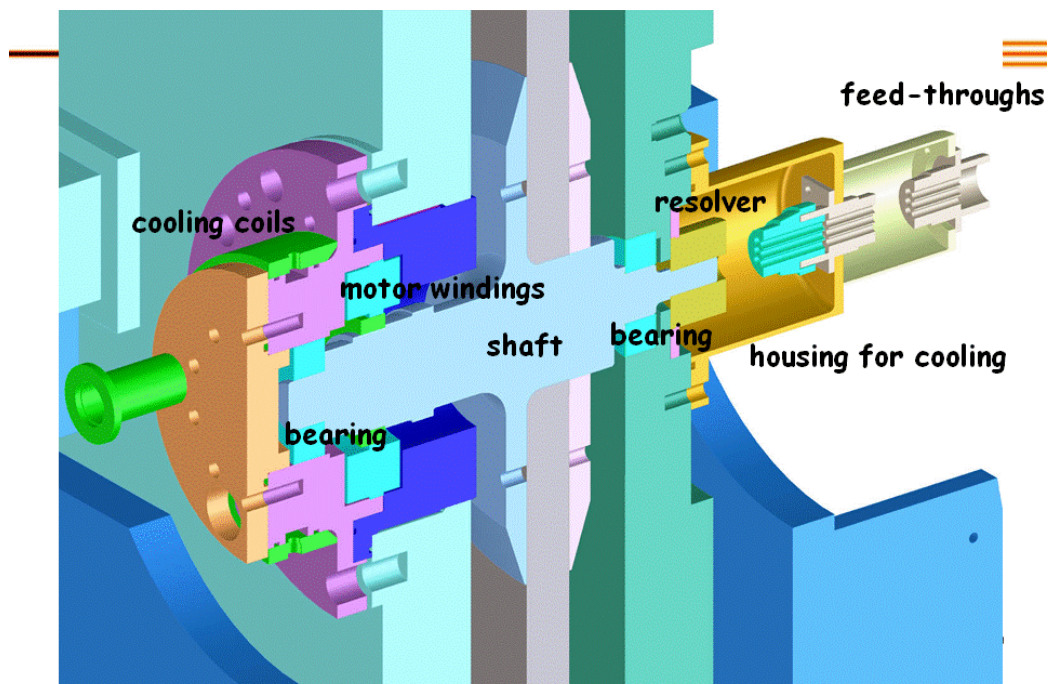
$$a = r\omega^2 = 125 \text{ km/s}^2$$

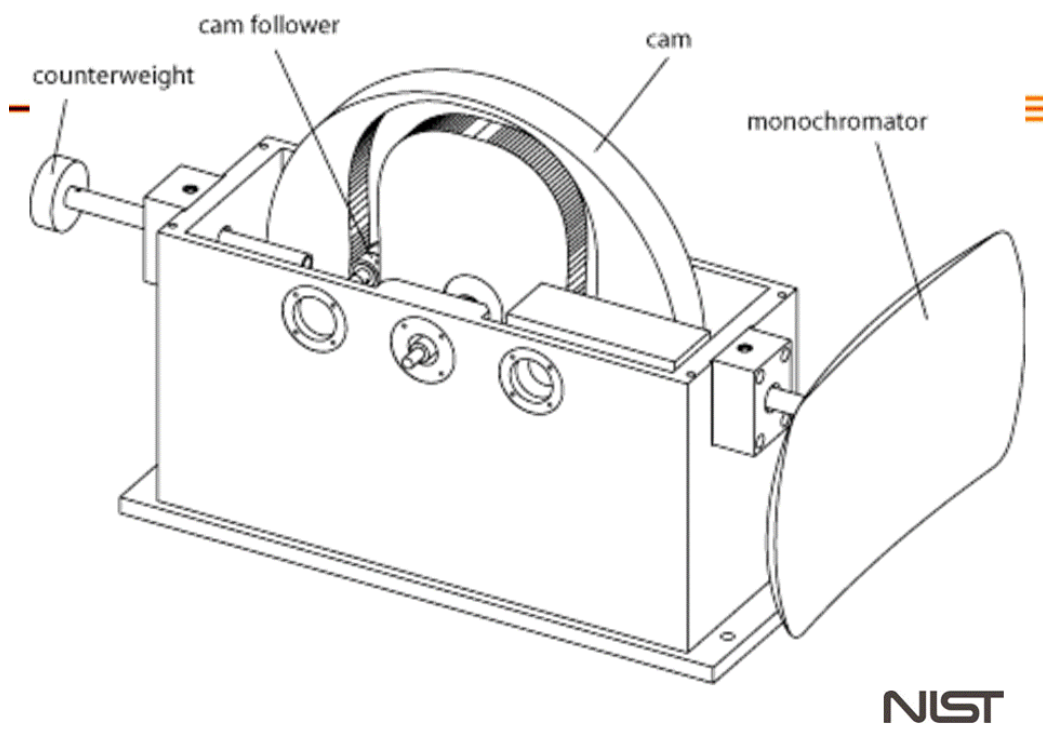
Before building the PST, we tested to twice this acceleration



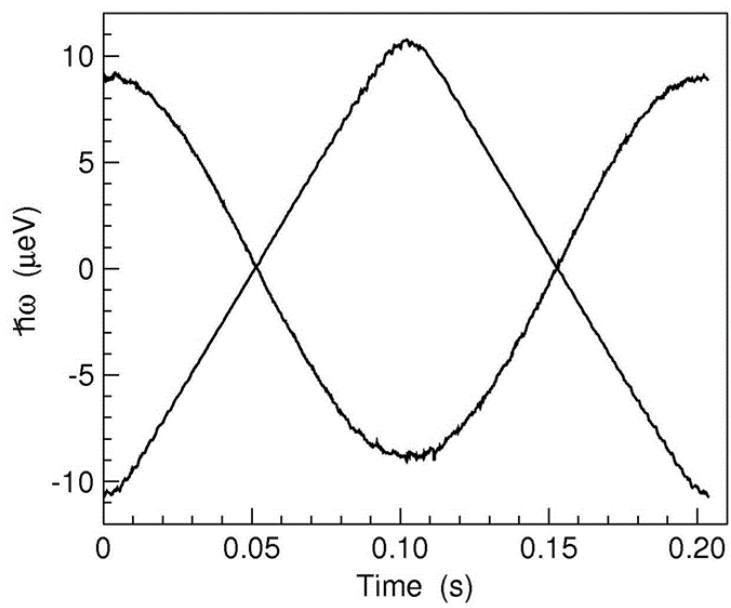


Shaft is AISI 4140, harden 38-42 Rockwell C



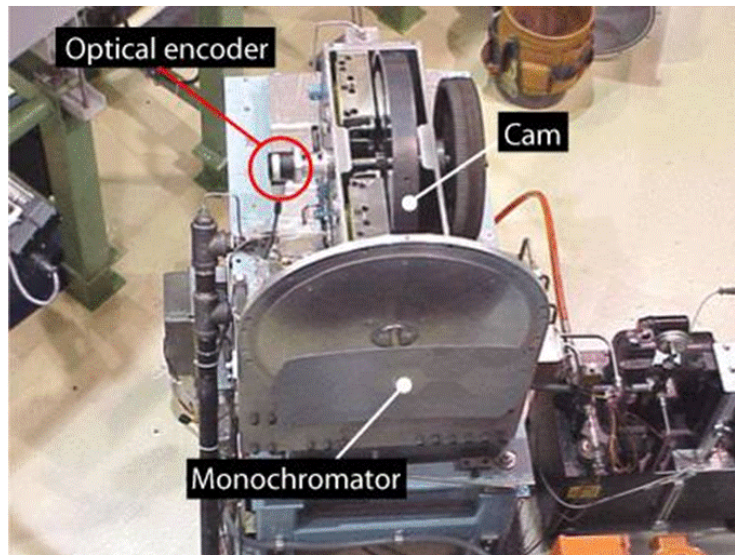


Velocity Profile

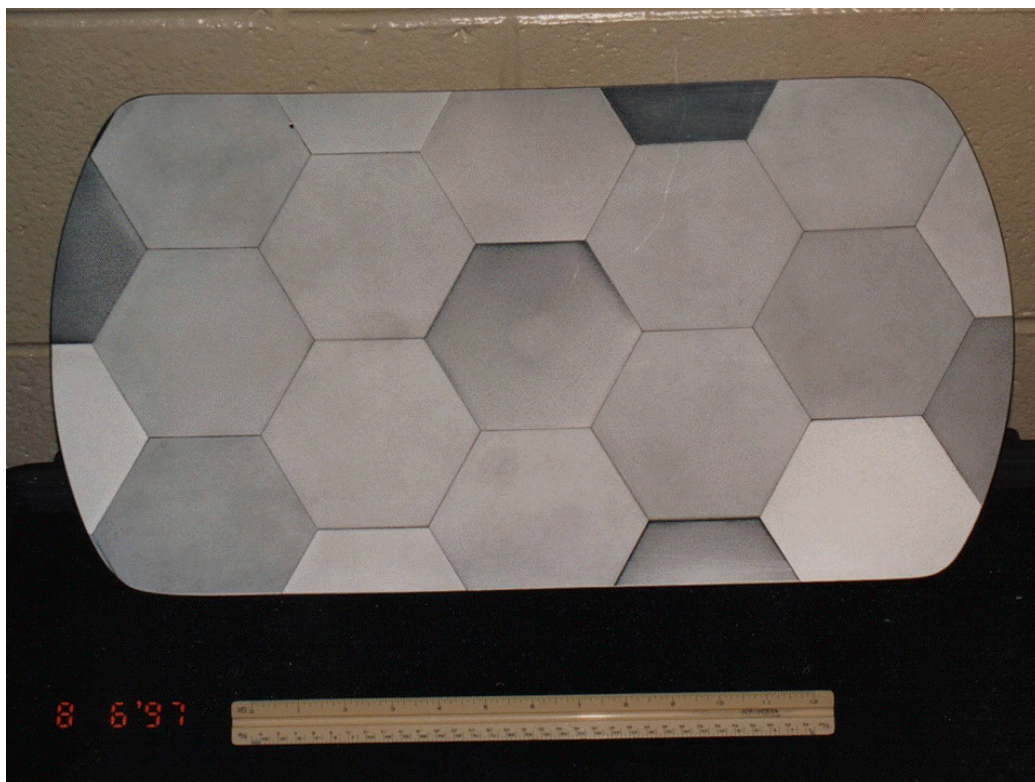


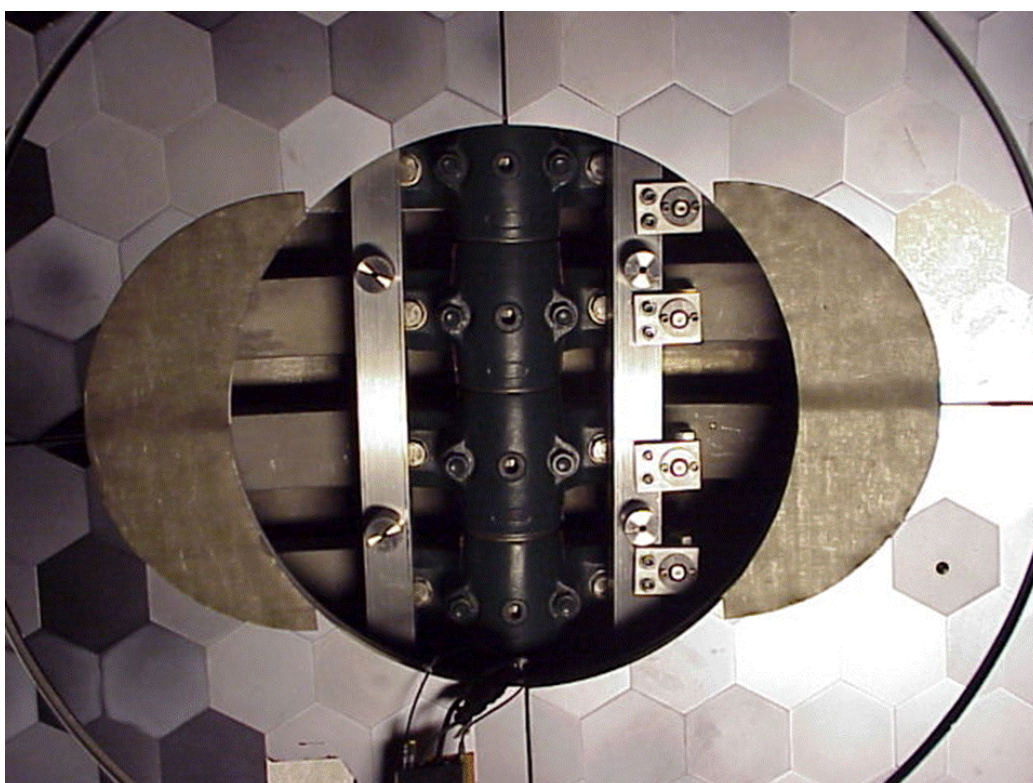
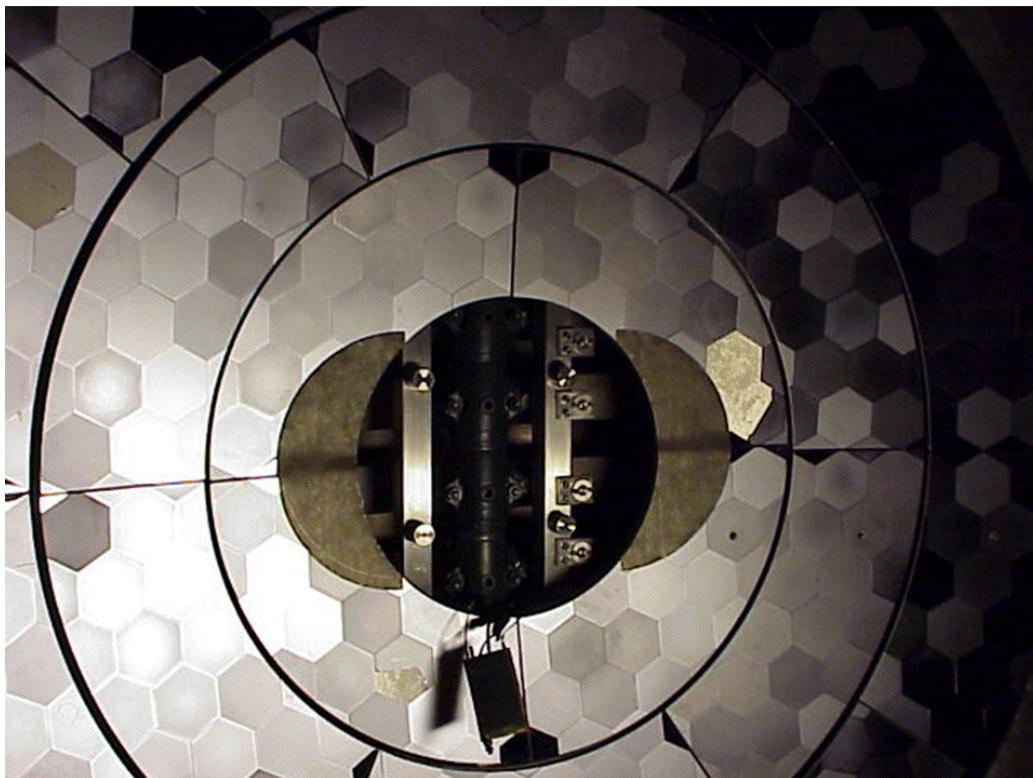
NIST

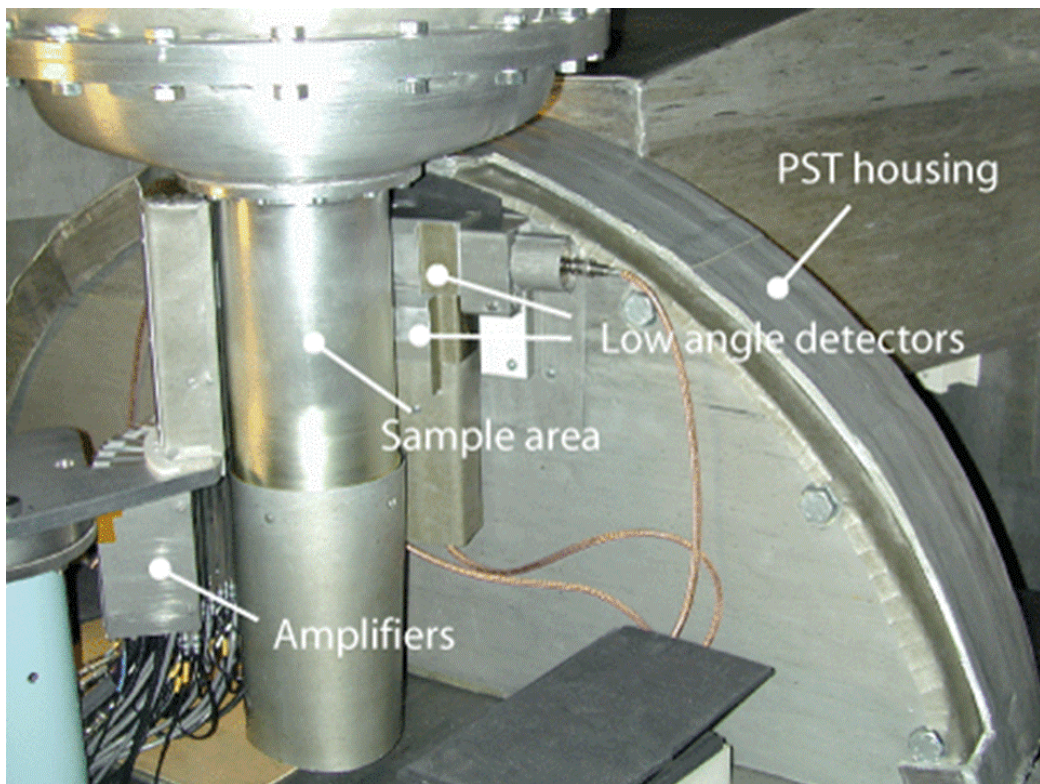
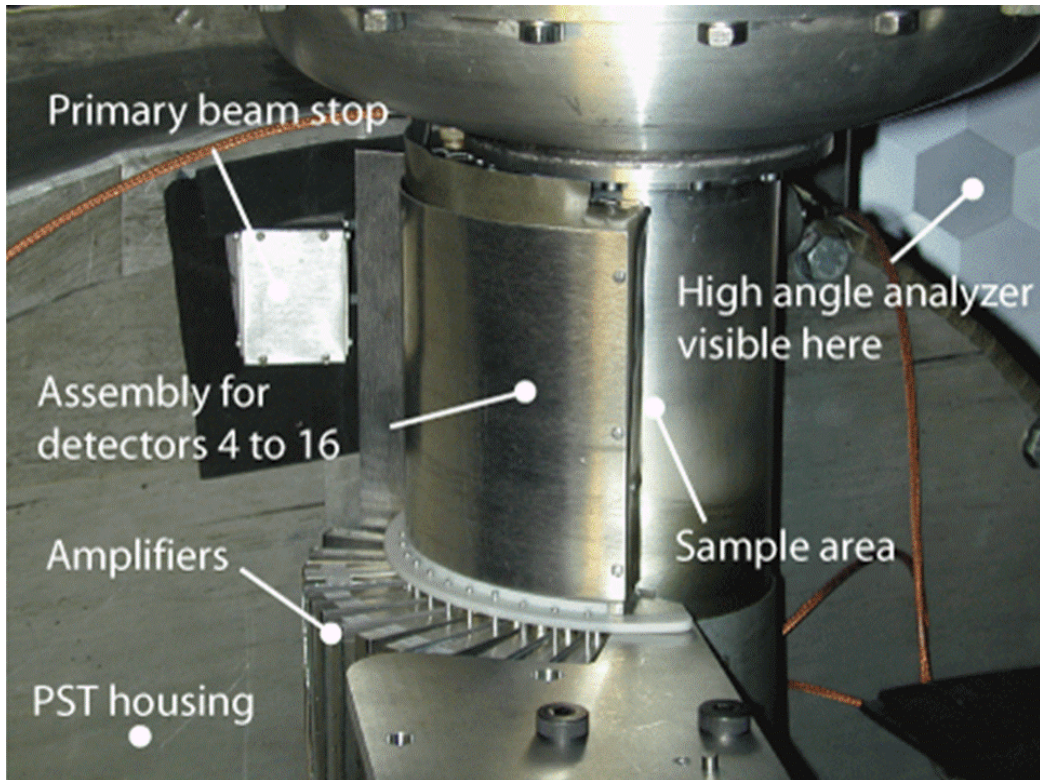
Doppler Drive

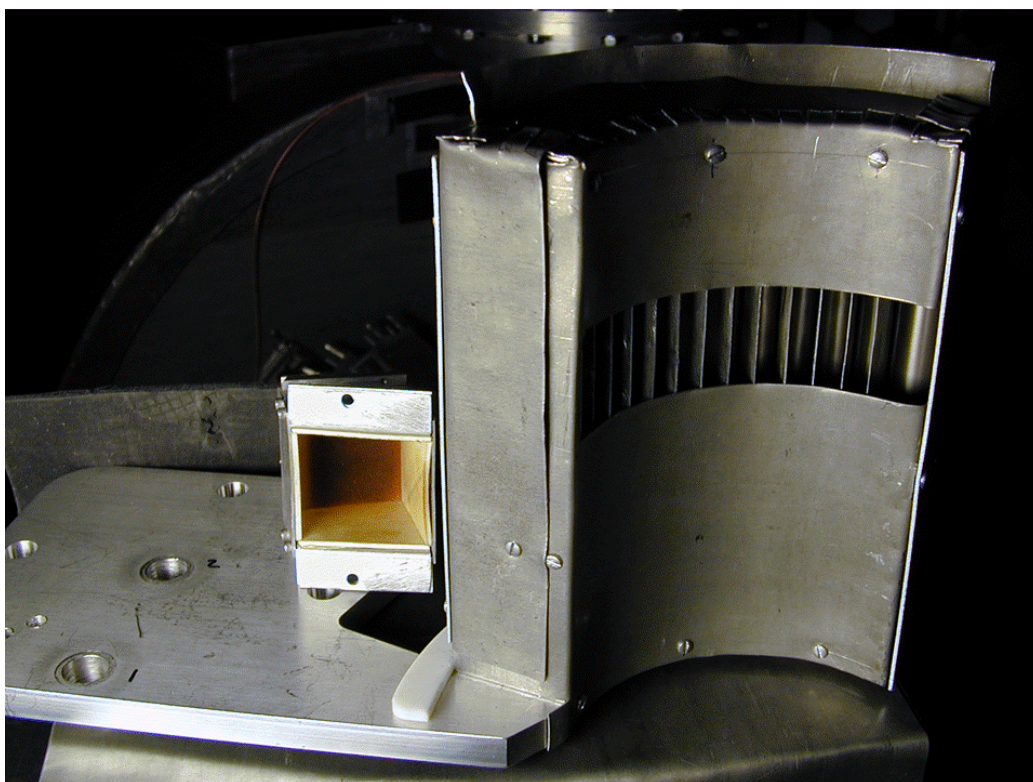
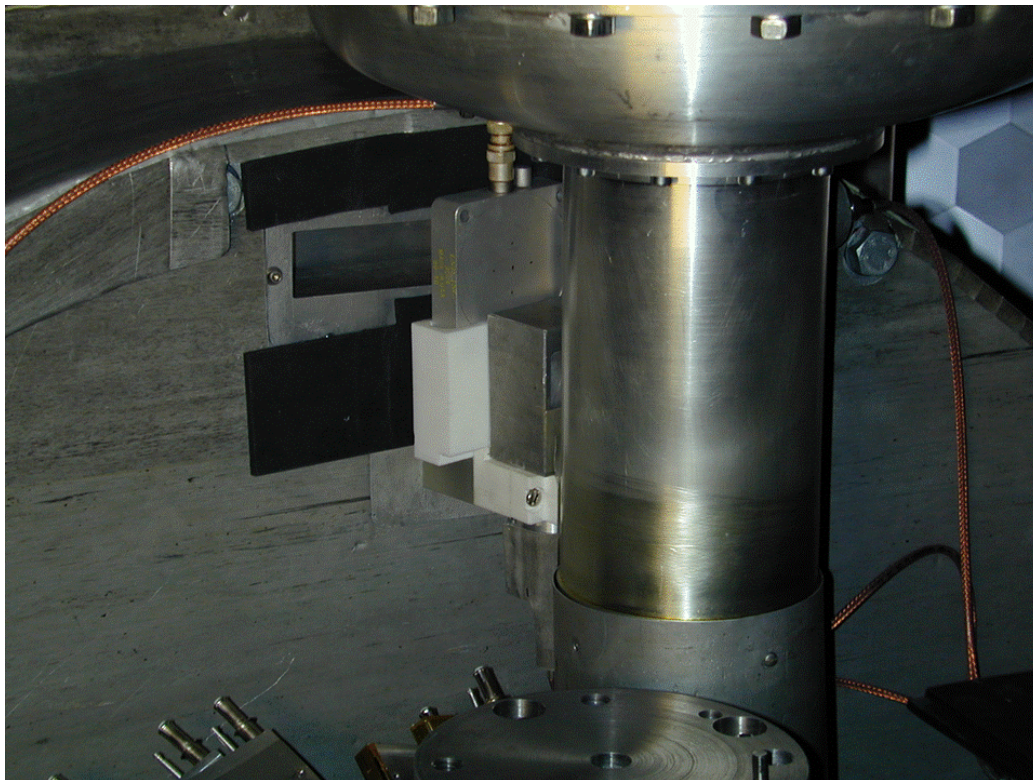


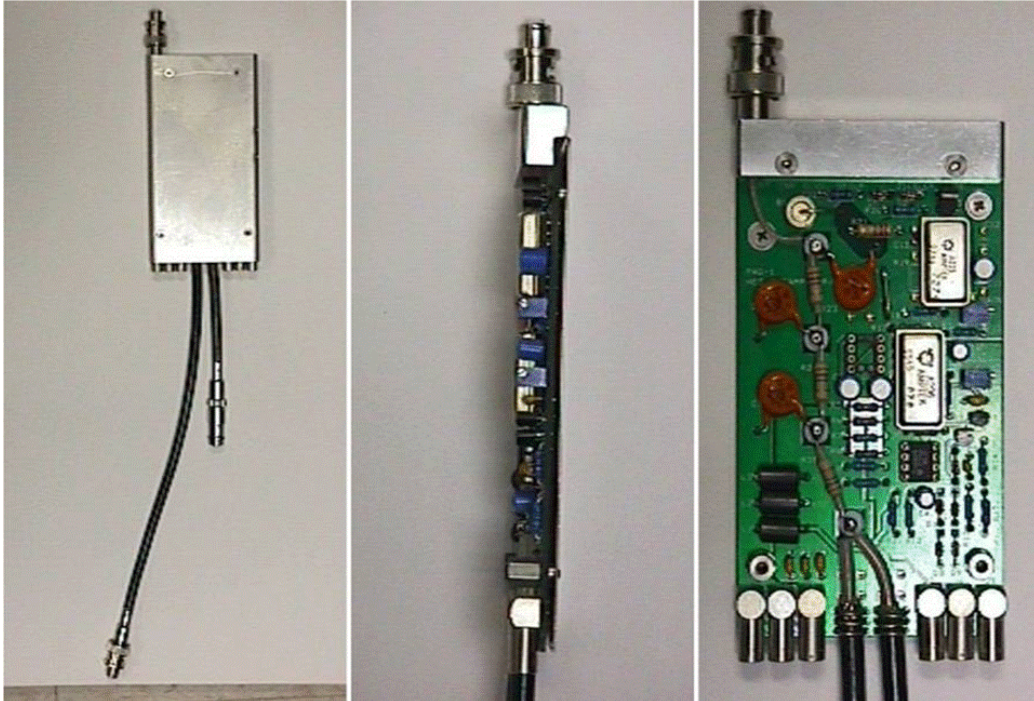
NIST



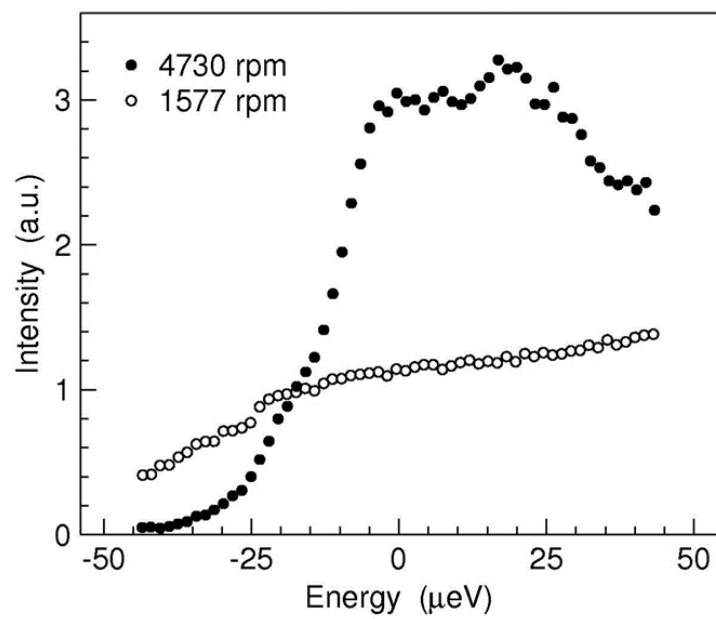






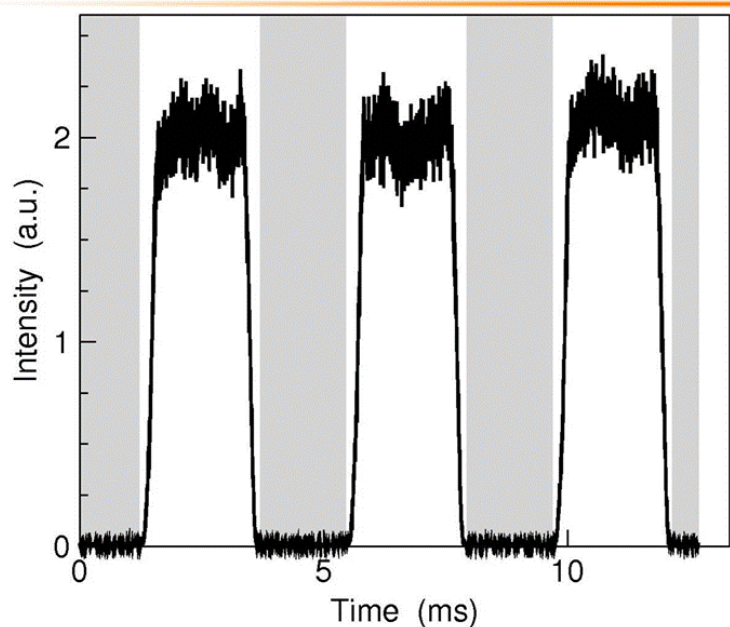


Monitor Rate



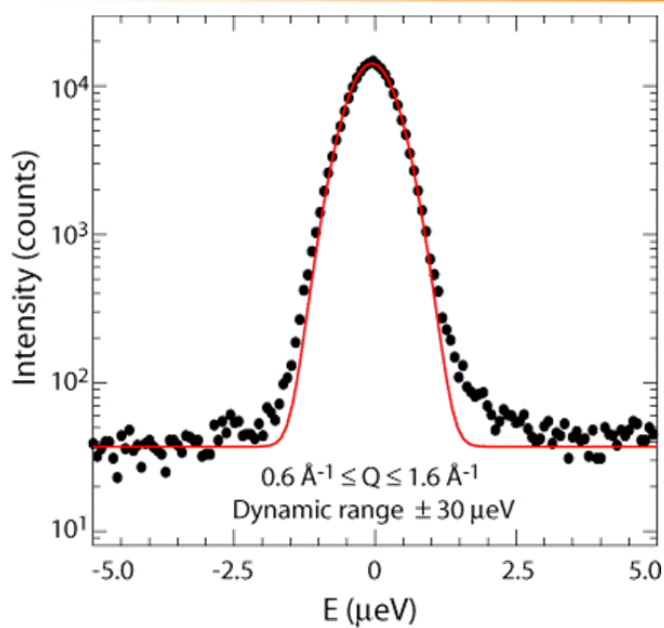
NIST

Data Binned vs. PST Chopper



NIST

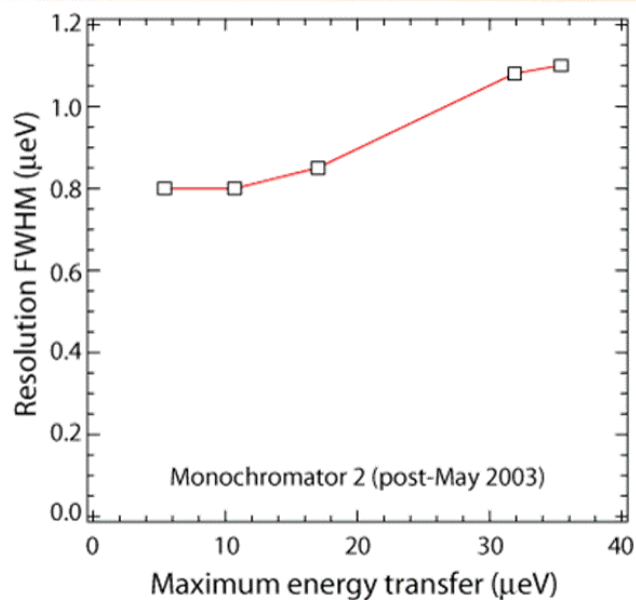
Vanadium Scan



Signal-to-Noise
400 to 1

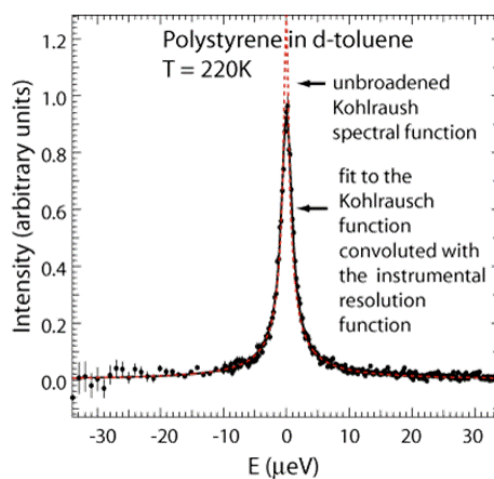
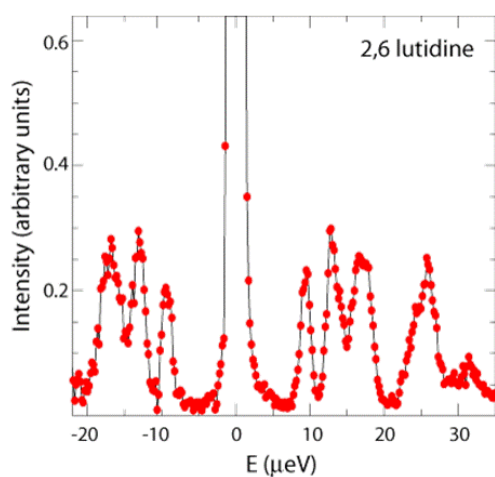
NIST

Energy Resolution



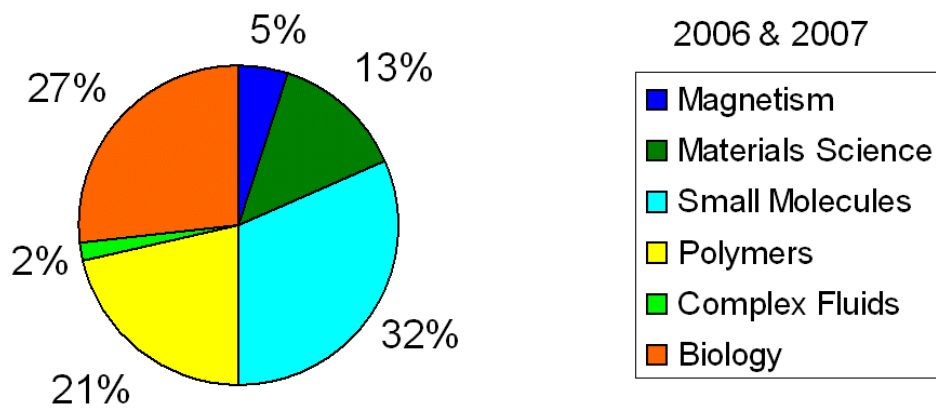
NIST

Sample Scans



NIST

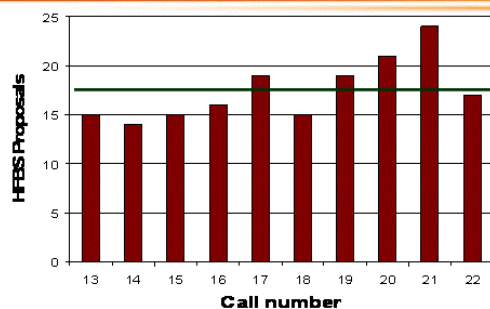
Backscattering Spectrometer



Year	Reliability
2006	95%
2007	94%

NIST

HFBS

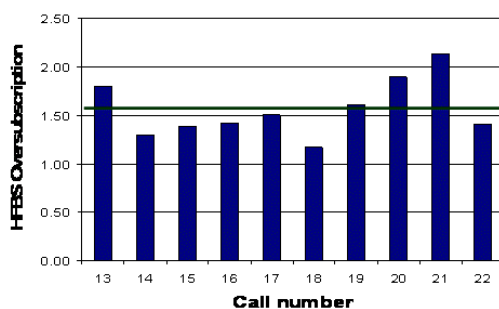


Our last 10 "Calls for Proposals"

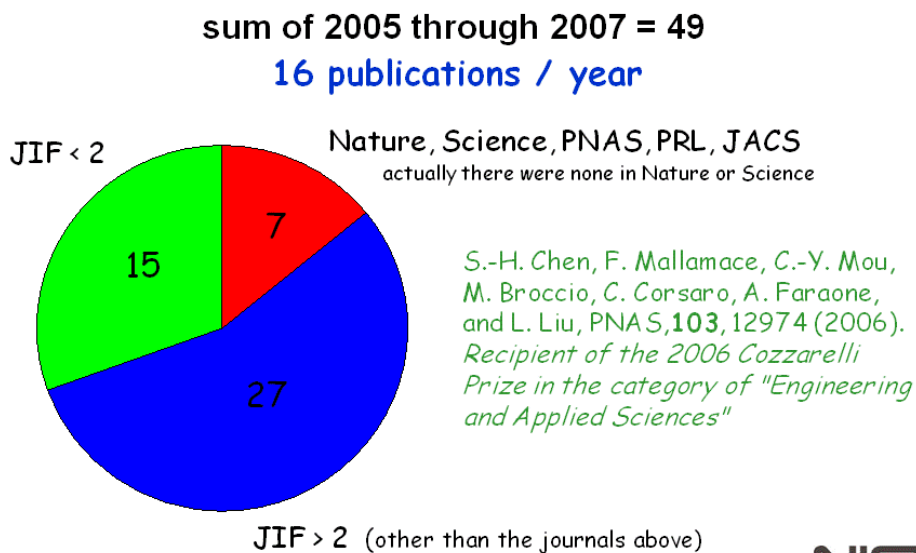
Ave. Proposals : **17**

Ave. Oversubscription : **1.6**

Days per approved prop : **5½** (2007)



Publications



NIST

Summary

Our Backscattering Spectrometer has been successful
Publish 16 papers per year

Most of the information in this presentation is available on the
instrument website:

<http://www.ncnr.nist.gov/instruments/hfbs/>

or in the instrument papers:

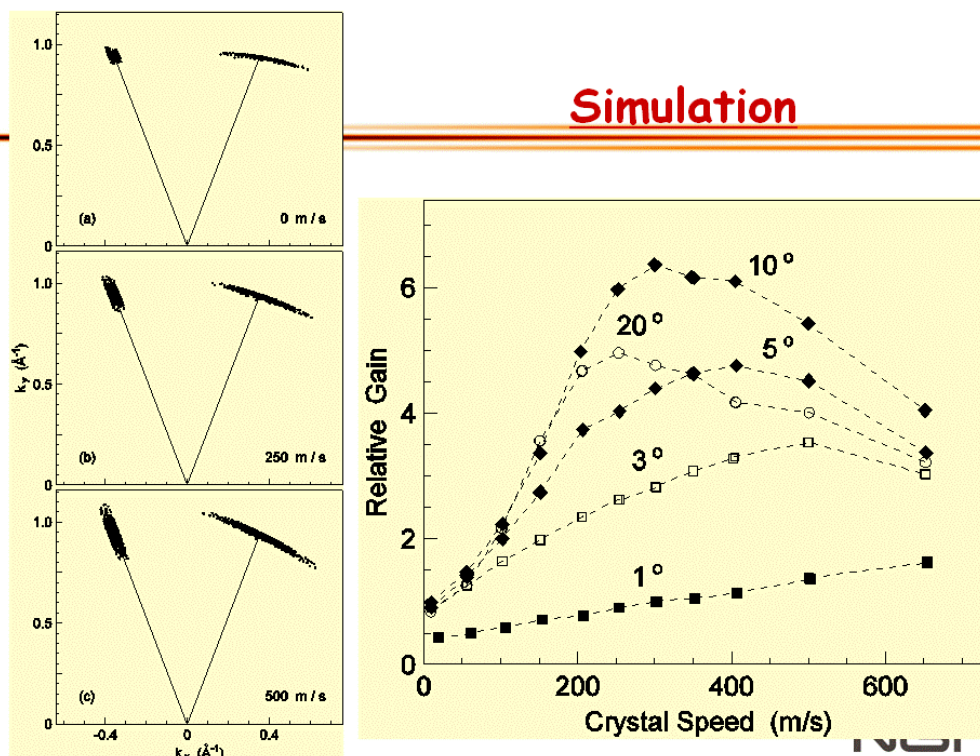
The High Flux Backscattering Spectrometer at the NIST Center for Neutron Research, A. Meyer, R.M. Dimeo, P.M. Gehring, and D.A. Neumann, Rev. Sci. Instrum. **74**, 2759 (2003).

and

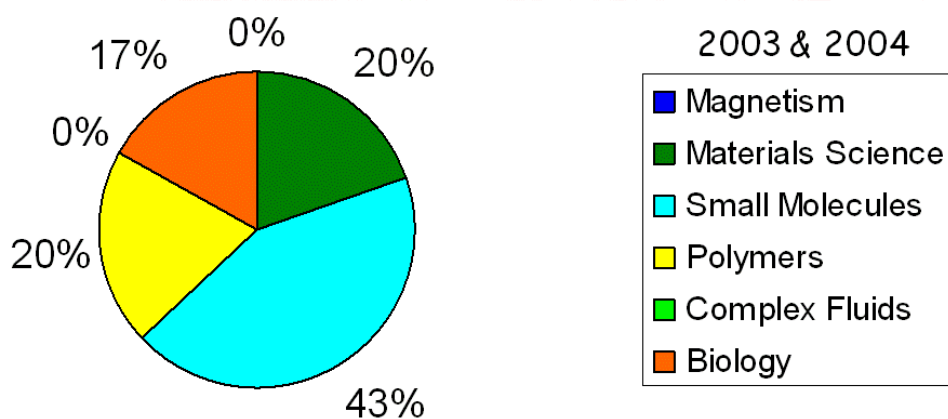
Backscattering Spectroscopy at the NIST Center for Neutron Research, P.M. Gehring and D.A. Neumann, Physica B **241**, 64 (1998).

NIST

Simulation



Backscattering Spectrometer



Year	# of Users	# of Publications	Reliability
2002	50	8 (1)	96%
2003	60	6	87%
2004	74	13* (2)	96%

* incl. in press

NIST

3.5. The New Spectrometer MARS at PSI Philip Tregenna-Piggott (PSI)

Laboratorium für Neutronenstreuung



Eidgenössische Technische Hochschule Zürich

Paul Scherrer Institut Würenlingen & Villigen



Introducing MARS -
MICA Analyser High Resolution
Inverted Time-of-Flight Spectrometer

Philip L.W. Tregenna-Piggott

The Paul Scherrer Institut
Villigen, Switzerland

MARS: MICA Analyser High Resolution
Inverted Time-of-Flight Spectrometer



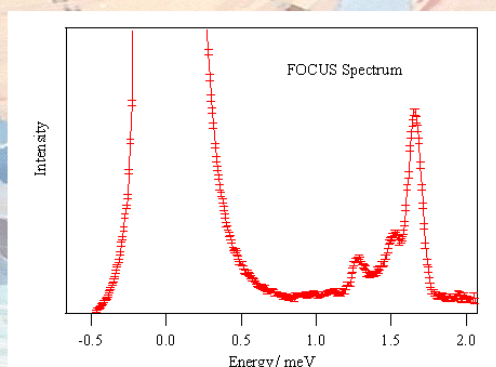
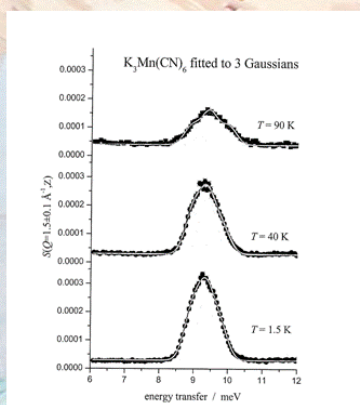
Outline of Talk

- The Purpose of MARS
- Characteristics of MARS
- User Software
- First Results
- Further Developments

MARS: MICA Analyser High Resolution Inverted Time-of-Flight Spectrometer



Recently Collected Direct Geometry TOF Data



Need to Focus in on spectral region of interest and obtain
High resolution Spectrum, with high-intensity, and wide range of Q

MARS: MICA Analyser High Resolution Inverted Time-of-Flight Spectrometer

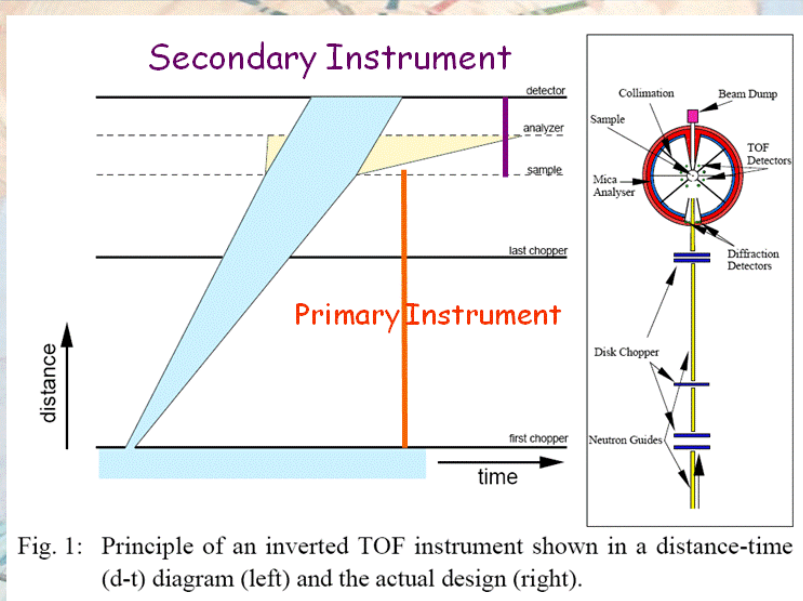
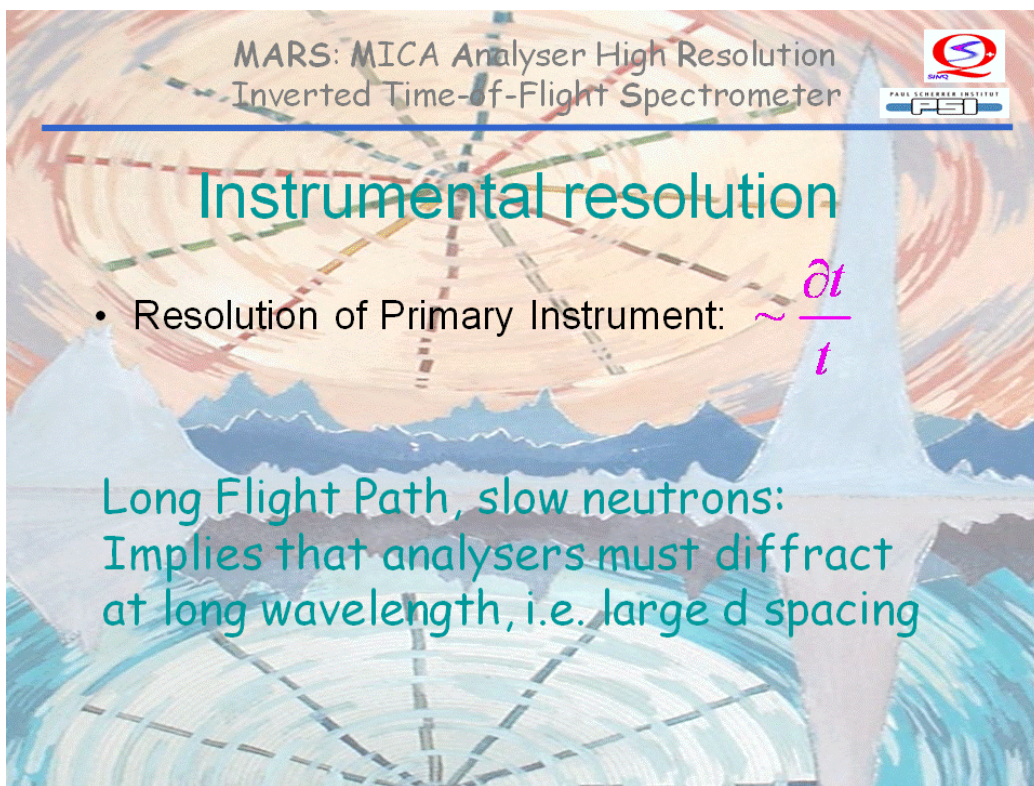


Fig. 1: Principle of an inverted TOF instrument shown in a distance-time (d-t) diagram (left) and the actual design (right).

After Allenspach – MARS – A Concept Study



MARS: MICA Analyser High Resolution
Inverted Time-of-Flight Spectrometer

Instrumental resolution

- Resolution of Primary Instrument: $\sim \frac{\partial t}{t}$

Long Flight Path, slow neutrons:
Implies that analysers must diffract
at long wavelength, i.e. large d spacing

Logos: JAEA, Paul Scherrer Institut, FED



MARS: MICA Analyser High Resolution
Inverted Time-of-Flight Spectrometer

MICA: Chemical and Physical Properties

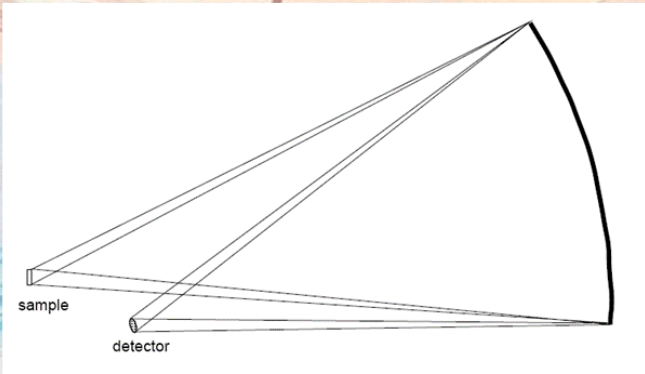
- Chemical Composition of Phlogopite:
 $\text{K}(\text{Mg,Fe,Mn})_3\text{Si}_3\text{AlO}_{10}(\text{F,OH})_2$
- Pliable
- Strong 002 and 006 reflections
- $d_{002} \sim 9.9 \text{ \AA}$

Logos: JAEA, Paul Scherrer Institut, FED

MARS: MICA Analyser High Resolution Inverted Time-of-Flight Spectrometer

Instrumental resolution

- Resolution of Secondary Instrument $\sim \sin \theta \Delta \theta$



Variation of Backscattering Angles

MARS: MICA Analyser High Resolution Inverted Time-of-Flight Spectrometer

Unique Features of MARS

- Moveable Analyser Banks

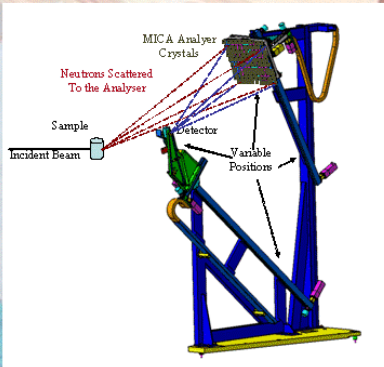
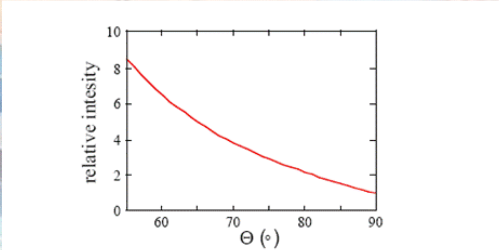
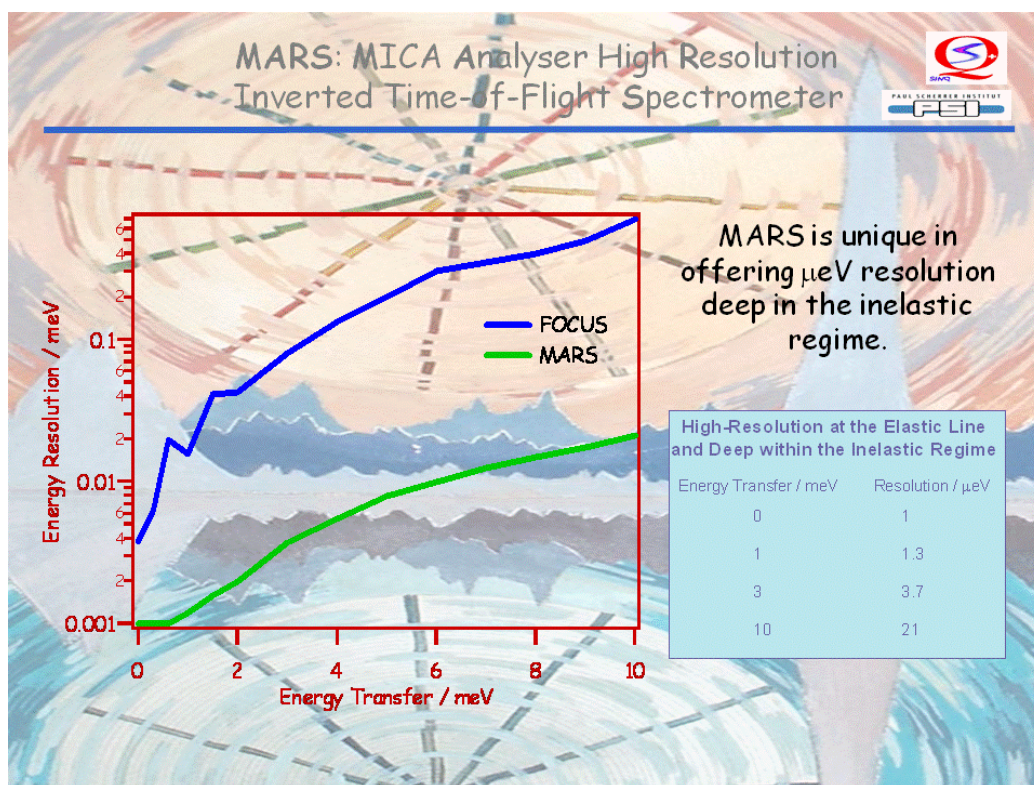



Fig. 25: Relative intensity as a function of "backscattering" angle Θ (normed to 90°)

Adjust Scattering Angle to Match Secondary Resolution to that of the Primary



MARS: MICA Analyser High Resolution Inverted Time-of-Flight Spectrometer



Why is MARS so big? - Avoid Inelastic Overlap

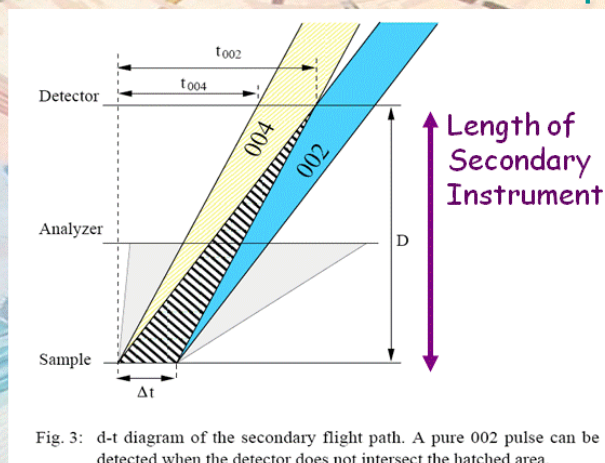


Fig. 3: d-t diagram of the secondary flight path. A pure 002 pulse can be detected when the detector does not intersect the hatched area.

After Allenspach – MARS – A Concept Study

MARS: MICA Analyser High Resolution Inverted Time-of-Flight Spectrometer



Frame Overlap

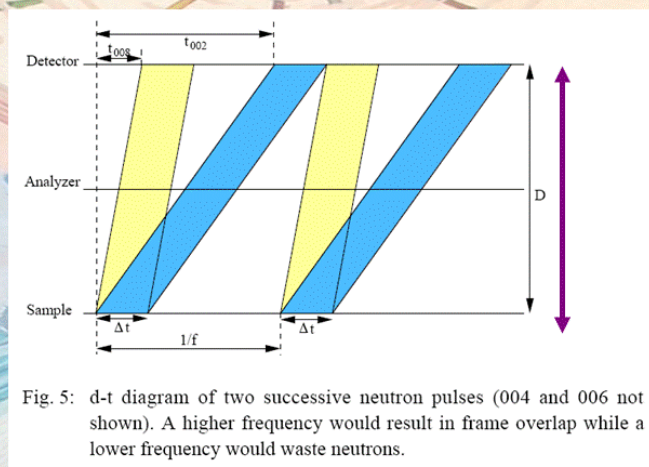
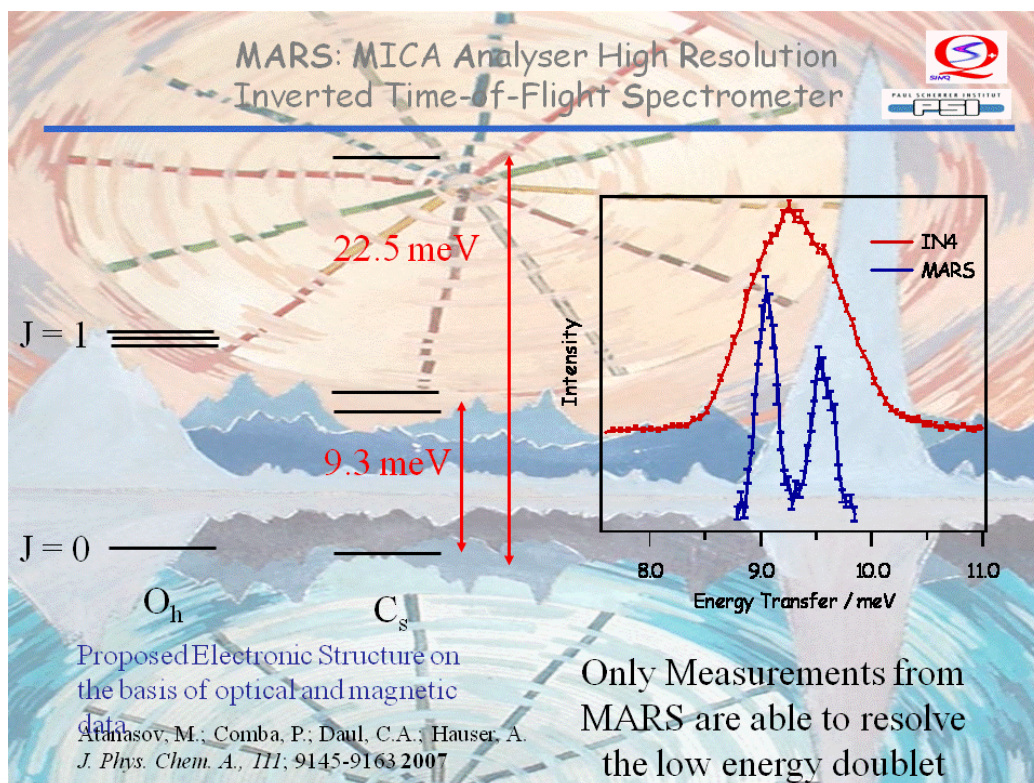
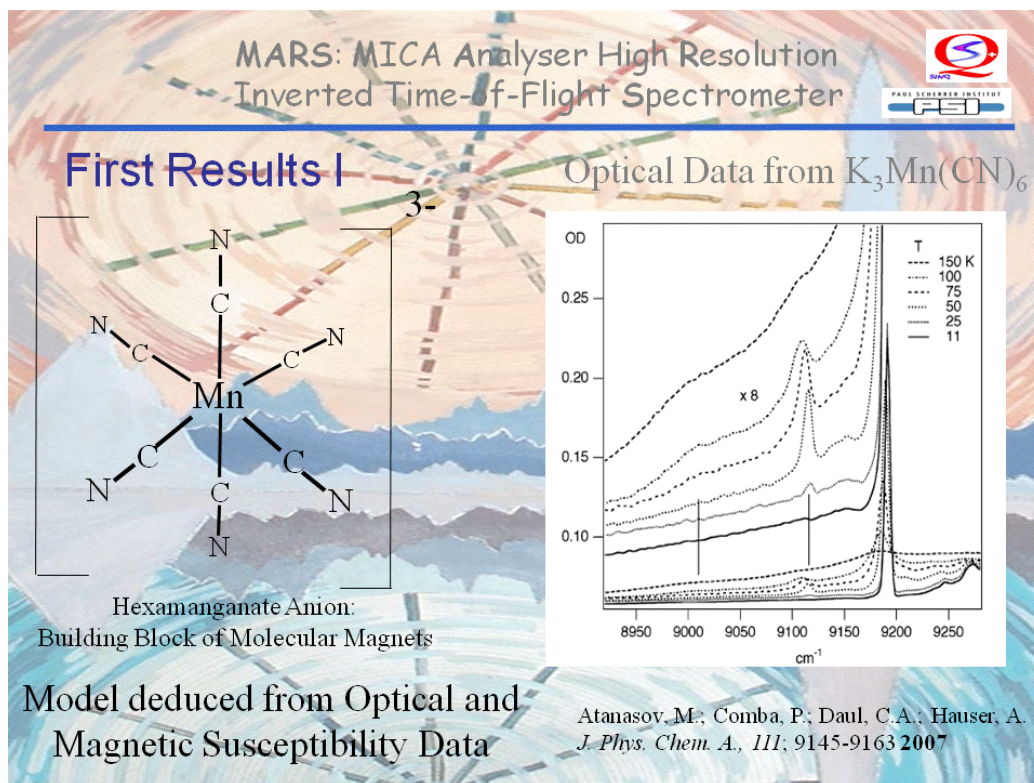
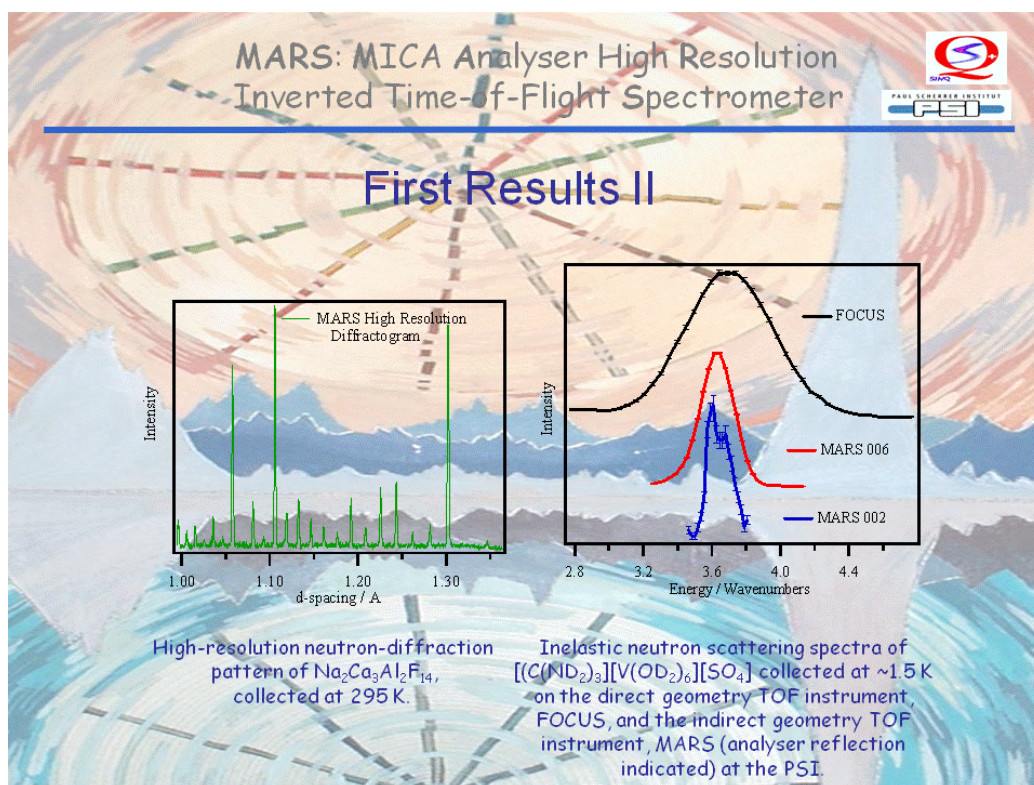


Fig. 5: d-t diagram of two successive neutron pulses (004 and 006 not shown). A higher frequency would result in frame overlap while a lower frequency would waste neutrons.

After Allenspach – MARS – A Concept Study





3.6. Backscattering and Related Capacity at the ILL Hannu Mutka (ILL)



Backscattering and related capacity at the ILL

H. Mutka - personal overview

T-o-F HR Group

- IN4 -thermal cryst. mc
- BRISP th. cryst. mc
- IN5 - cold chopper
- IN6 - cold cryst. mc.
- IN10 - BS
- IN13 (CRG)- BS
- IN16 -BS
- IN11 -NSE
- IN15 -NSE

TAS Group

- IN1BeF - hot

Feb 27 2008, Tokai DNA meeting

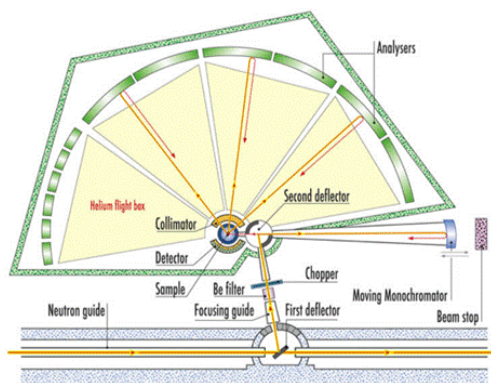
INSTITUT MAX VON LAUE - PAUL LANGEVIN

H. Mutka



IN16 (B. Frick, L. van Eijck)

Resolution $\Delta E \leq 1 \mu\text{eV}$
Q-range $0.02 \dots 1.9 \text{ \AA}^{-1}$



- pro's
- S/N
 - diffraction detector
 - upgraded Doppler drive

- con's
- limited dynamic range
 - very high demand/overload

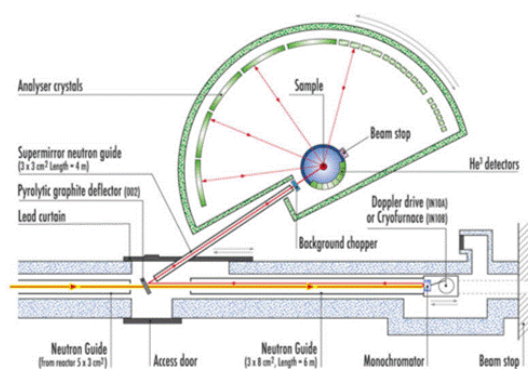
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IN10 (T. Seydel, L. van Eijck)

Resolution $\Delta E \leq 1 \mu\text{eV}$

-offset option



INSTITUT MAX VON LAUE - PAUL LANGEVIN

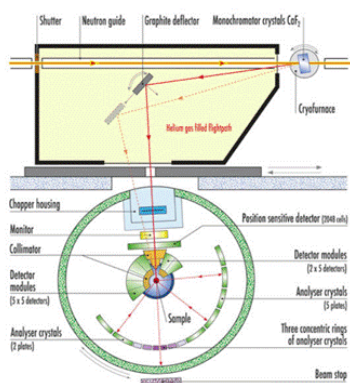


IN13 (F. Natali, J. Peters)

Resolution $\Delta E \approx 10 \mu\text{eV}$
Q-range $\rightarrow 4.9 \text{ \AA}^{-1}$

life sciences driven CRG
(Italian - French)

broad Q-range



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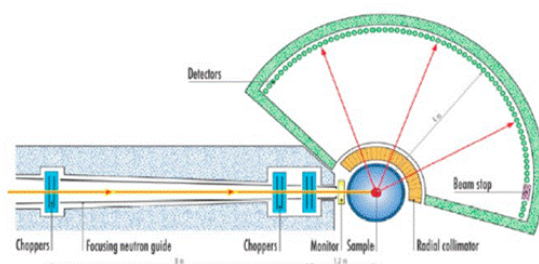
IN5 (J. Ollivier, H. Mutka)

Resolution $\Delta E : \leq 10 \mu\text{eV} \dots \approx 0.5 \text{ meV}$

Incident energy : from below 0.5 meV up to 25 meV (continuous)

pro's

- S/N
- flexibility, resolution lineshape
- upgrade underway



con's

- limited Q-range with high resolution (direct geometry)

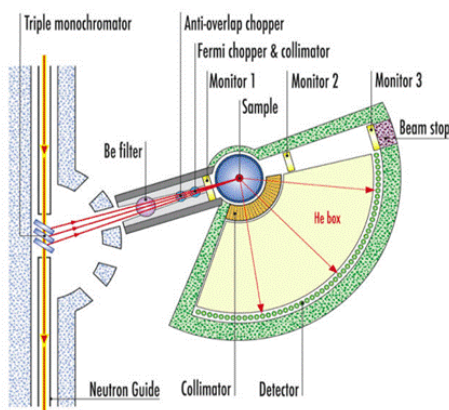
INSTITUT MAX VON LAUE - PAUL LANGEVIN



IN6 (M.M. Koza, M. Plazanet)

Resolution $\Delta E : 40 \mu\text{eV} \dots 0.2 \text{ meV}$

Incident energy : 2.3 meV...4.8 meV (four settings)



pro's

- S/N
- resolution, adjustable focussing
- upgraded Fermi chopper

con's

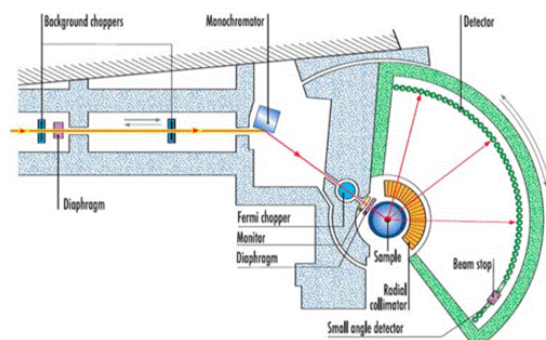
- tedious change of setting
- further upgrades not evident

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IN4 (S. Rols, J.R. Stewart)

Resolution $\Delta E \approx 300 \mu\text{eV} \dots 8 \text{ meV}$
Incident energy 6.5 meV... 120 meV



pro's
- high incident flux
- relatively easy change of setting by order of reflection, continuous Bragg angle

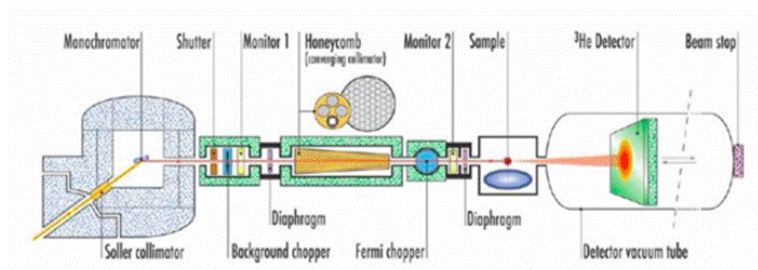
con's
- background (environment & fast neutrons)
- somewhat restricted sample environment

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BRISP (A. De Francesco, A. Lalon, F. Formisano)

Resolution $\Delta E \approx 2.5 \dots 5 \% \text{ of } E_i$
Incident energy 21 meV... 84 meV
Q-range $0.03 \dots 1.7 \text{ \AA}^{-1}$, Q-resolution $0.02 \dots 0.04 \text{ \AA}^{-1}$



CRG (Italian-German collaboration)

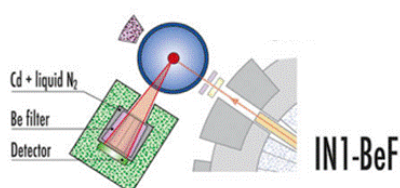
INSTITUT MAX VON LAUE - PAUL LANGEVIN



IN1BeF (A. Ivanov)

Resolution $\Delta E \leq 3$ to 6% of energy transfer meV

Incident energy ≈ 10 meV... 1000 meV



- high sensitivity/ small samples
 - shares the hot beam hole with IN1-TAS and D4
- Proposed upgrade LAGRANGE

INSTITUT MAX VON LAUE - PAUL LANGEVIN



Recent upgrades and new projects

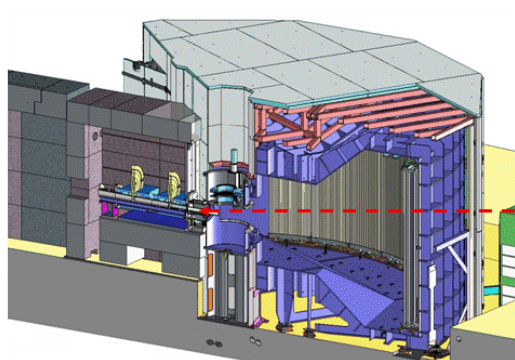
- IN16B - complete rebuild in the pipeline
- IN13 - various upgrades under consideration
- IN5 - secondary spectrometer commissioning soon
- IN6 - new Fermi chopper
- IN4 - beam optics elements, minimizing background
TOPTOF pending
- IN1BeF - 'Lagrange' high sensitivity - better resolution

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IN5 rebuild

The evacuated detector tank is being installed



INSTITUT MAX VON LAUE - PAUL LANGEVIN



Use in materials and life sciences

and for basic problems of physics&chemistry

Dynamics of disordered systems

- Water, confined water, proteins, hydrogen diffusion, polymers, glasses
- **Magnetism**
 - Frustrated magnets, fluctuations, single molecule magnets
- **Molecular spectroscopy**
 - Tunneling states
- **Functional materials**
 - for fuel cells, thermoelectrics
- **Geology, metal physics**
 - melts

Diverse sample environments:
cryostats, furnaces, pressure
cells

INSTITUT MAX VON LAUE - PAUL LANGEVIN

3.7. R&D of Neutron Optical Devices and Neutron Detectors at J-PARC

Kazuhiko Soyama (JAEA)

Research and Development of Neutron Optical Devices and Neutron Detectors in J-PARC

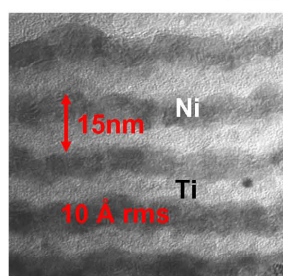
Kazuhiko Soyama

J-PARC Center

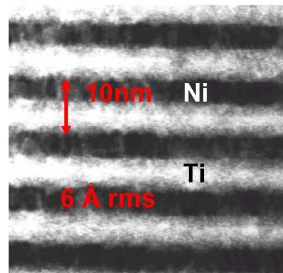


Development of supermirror with sharp interface

TEM images of Ni/Ti multilayers



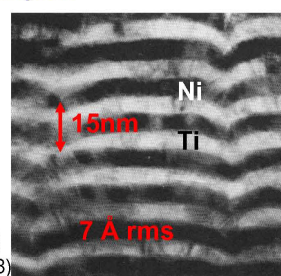
Vacuum evaporation



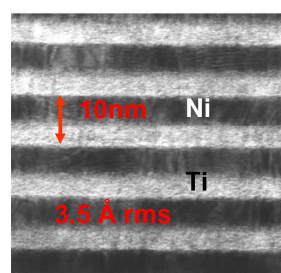
Ion beam sputtering

large crystal grain
inter-diffusion

J.E. Keem, J. Wood
SPIE Vol. 983 (1988)



Magnetron sputtering

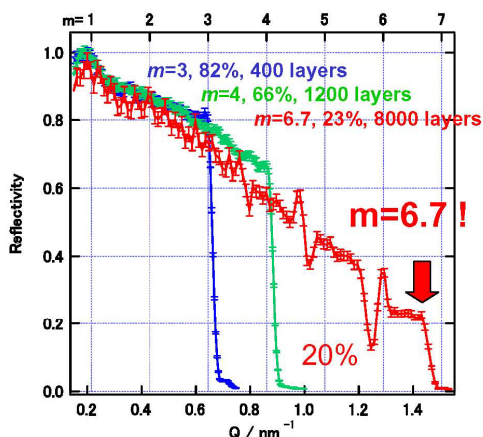


Ion beam sputtering + ion beam irradiation

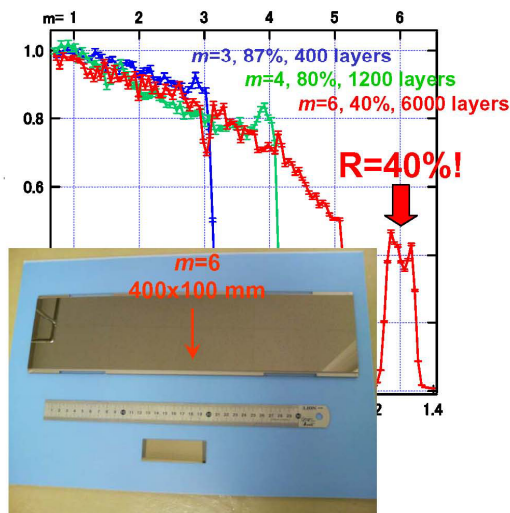


Development of supermirror with large- m , high-reflectivity and large-scale

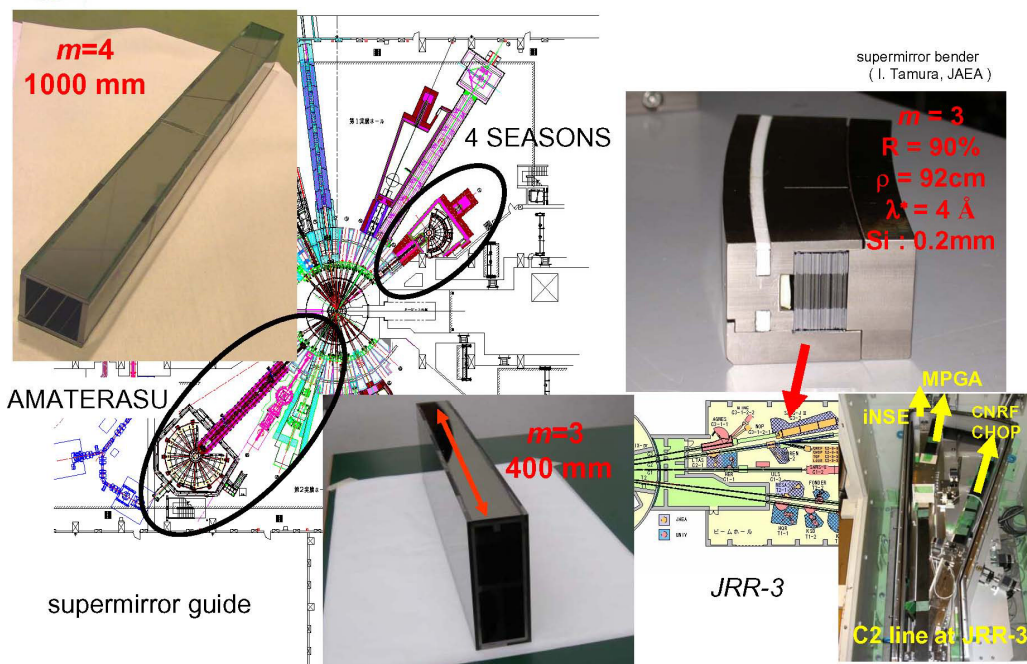
Ni/Ti supermirrors



NiC/Ti supermirrors



Supermirrors with large- m , high- R and large-scale





Fabrication of Ultra-precision Focusing Optics by Numerically Controlled Local Wet Etching



Good substrate

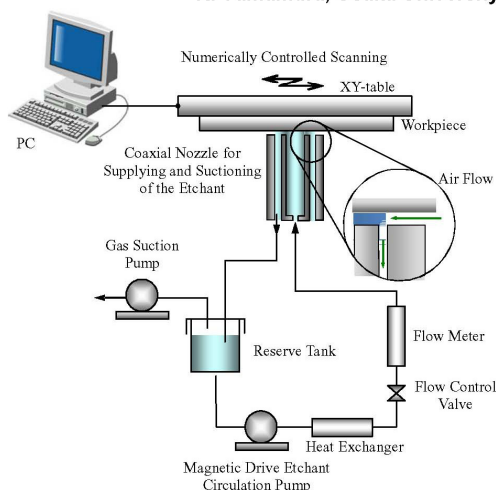
multi-channel
thin substrate
ultra-precise



Ultraprecise fabrication

Thin substrate, No damage

K. Yamamura, Osaka University

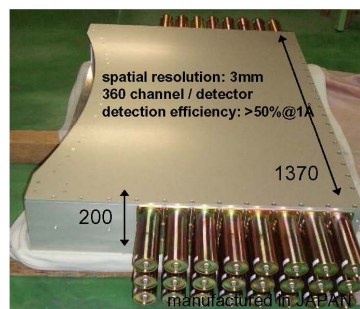
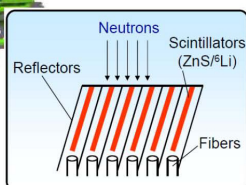
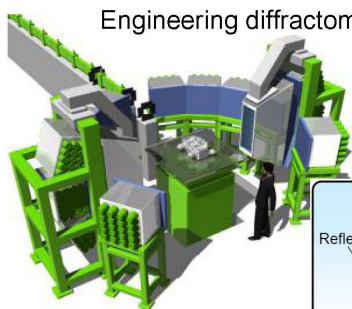


Scintillator Based Large Area One-Dimensional Neutron Detector

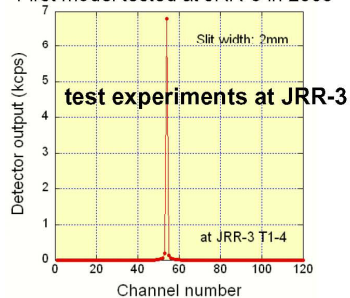


(Under Cooperation Between JAEA and CCLRC)

Engineering diffractometer "TAKUMI"
at BL19



First model tested at JRR-3 in 2008



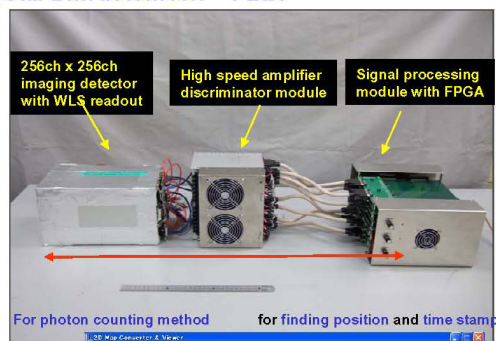
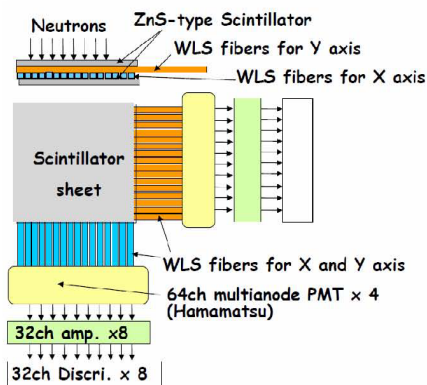
Specifications

- Geometry of detector module: 196 × 1,080 mm
- Position resolution: 3 mm
- Neutron detection efficiency: > 50% at 1 Å
- Gamma sensitivity: < 10⁻⁶ at 1.3 MeV
- Pulse pair resolution: 2.5 μs
- Neutron detection stability: < 1%

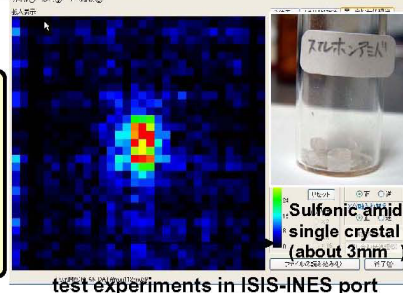
Compact neutron imaging detector with wavelength shifting fiber (WLSF) read-out

ISIS

Biological Single Crystal Diffractometer "i BIX"



For photon counting method for finding position and time stamp



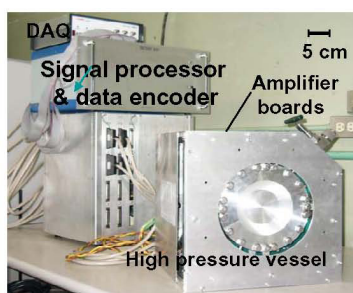
test experiments in ISIS-INES port

Specifications

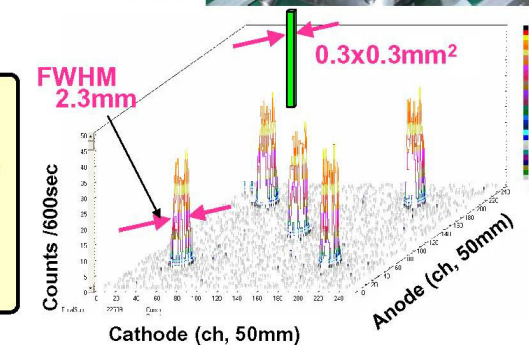
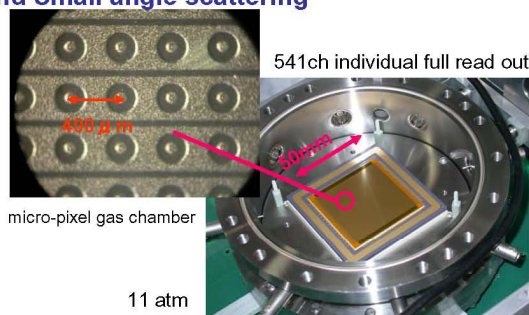
- Geometry of detector module: 160 × 160 mm
- Position resolution: < 1 mm
- Neutron detection efficiency: > 50% at 1.8 Å
- Gamma sensitivity: < 10⁻⁵ at 1.3 MeV
- Pulse pair resolution: < 10 μs

2D MPGC System with Individual Readout

Reflectometer and Small angle scattering



JAERI-MPGC detector system



Performances of JAEA-MPGC

- Spatial resolution: 2 mm
- Detection efficiency: > 80% @ 1.8 Å
- γ/n ratio: < 10⁻⁸
- Double pulse resolution: < 600 ns
- Counting uniformity: < 7%
- Sensitive area: 50x50 mm



SUMMARY

- **Some of key neutron optical devices and detectors for the “Day-1” Instruments have been successfully developed, and constructions should be carefully completed.**
- **Development for the use at full power operation should be started by using existing knowledge as a base and in collaboration with advanced universities and institutes.**
- **Development of neutron devices needs long time and needs keeping funding flow, and the collaboration with advanced universities and institutes are very important.**

3.8. DAQ and software developments at J-PARC/MLF
Takeshi Nakatani (JAEA)

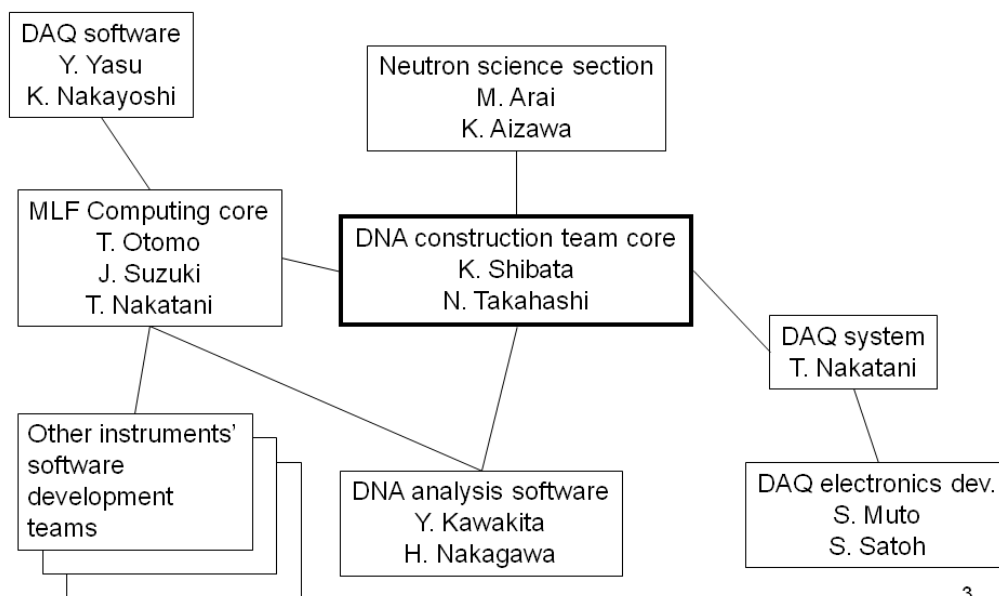
DAQ and software developments at J-PARC/MLF

Takeshi Nakatani
J-PARC Center

Contents

1. Members
2. Data acquisition and analysis system
3. DAQ electronics interface
4. Software framework development
5. DAQ middleware
6. Manyo-Lib
7. Image of use
8. International collaboration
9. Schedule
10. Summary

Members



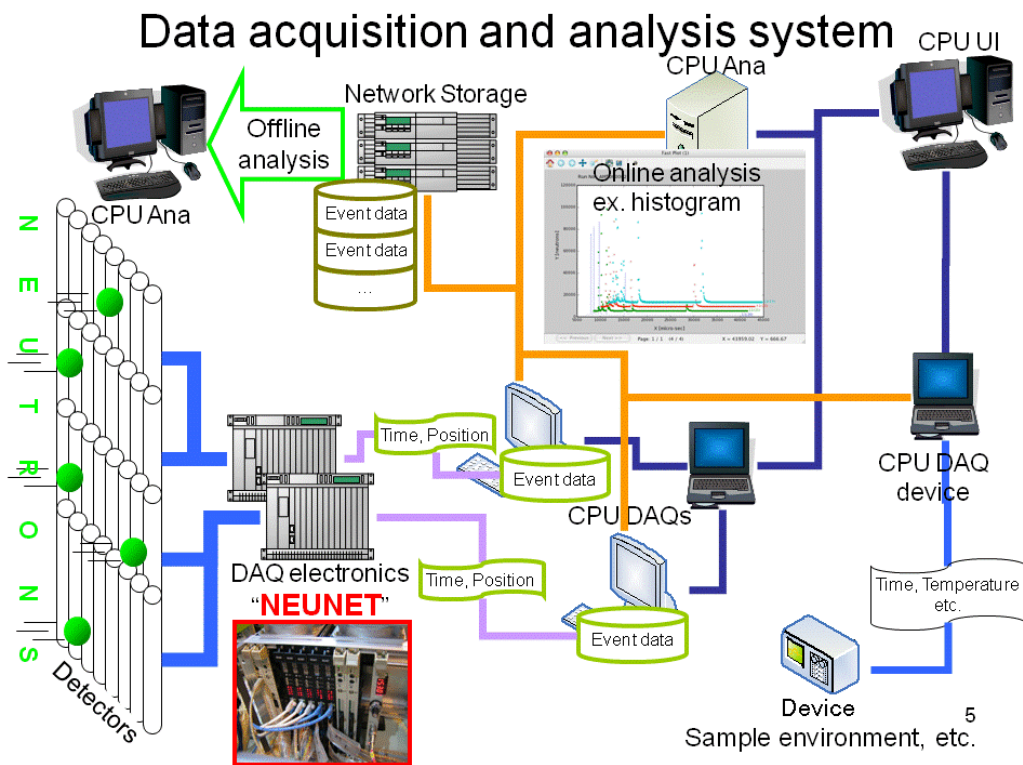
3

Keywords

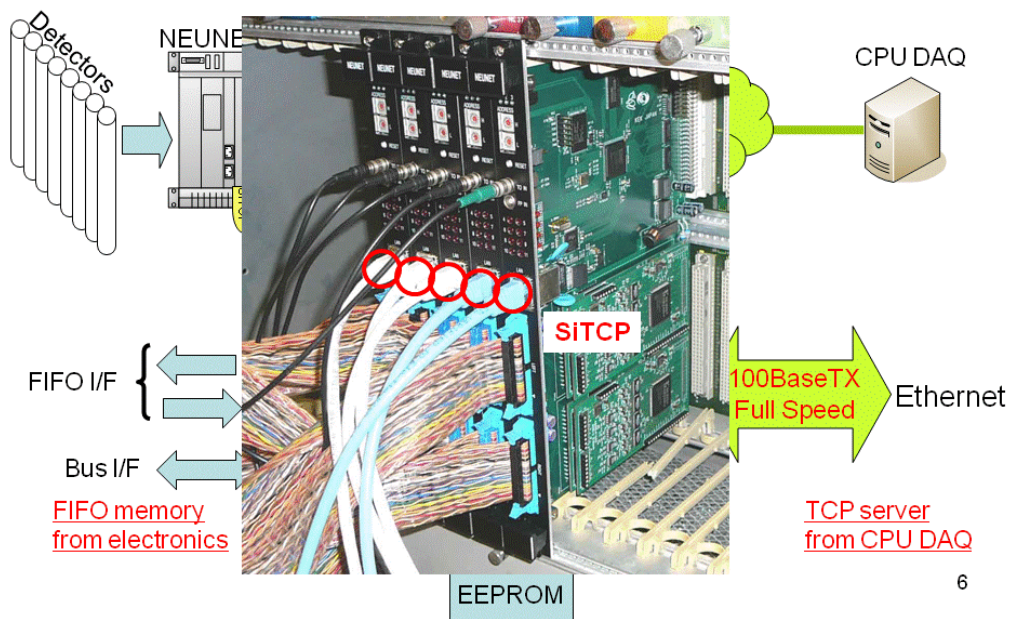
Using conventional Information Technologies

- Ethernet
- Python
- XML (eXtensible Markup Language)
- HTTP (Hyper Text Transfer Protocol)

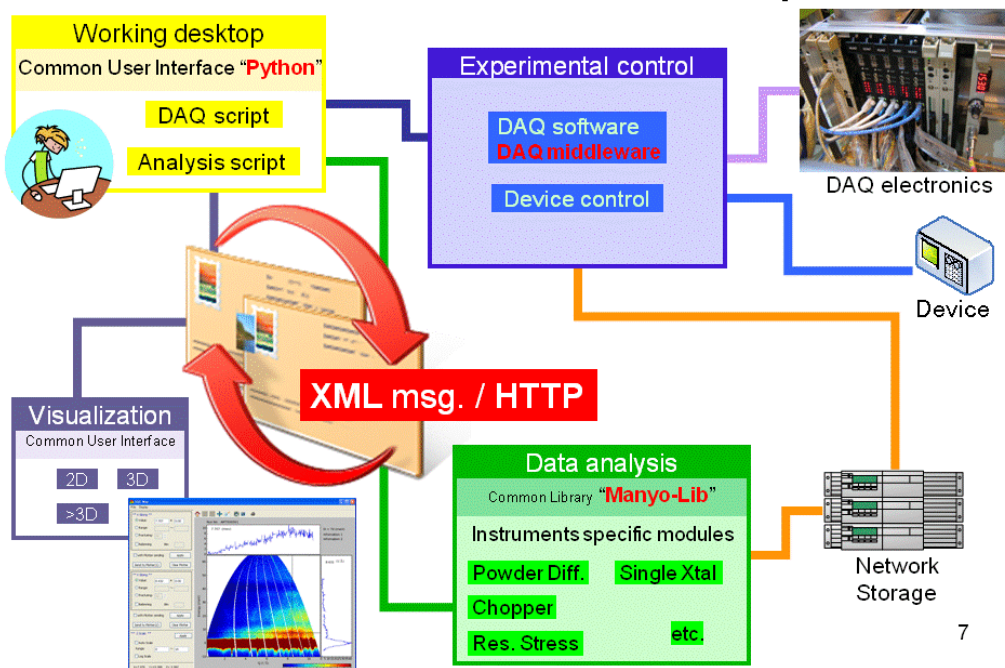
4



DAQ electronics interface “SiTCP”

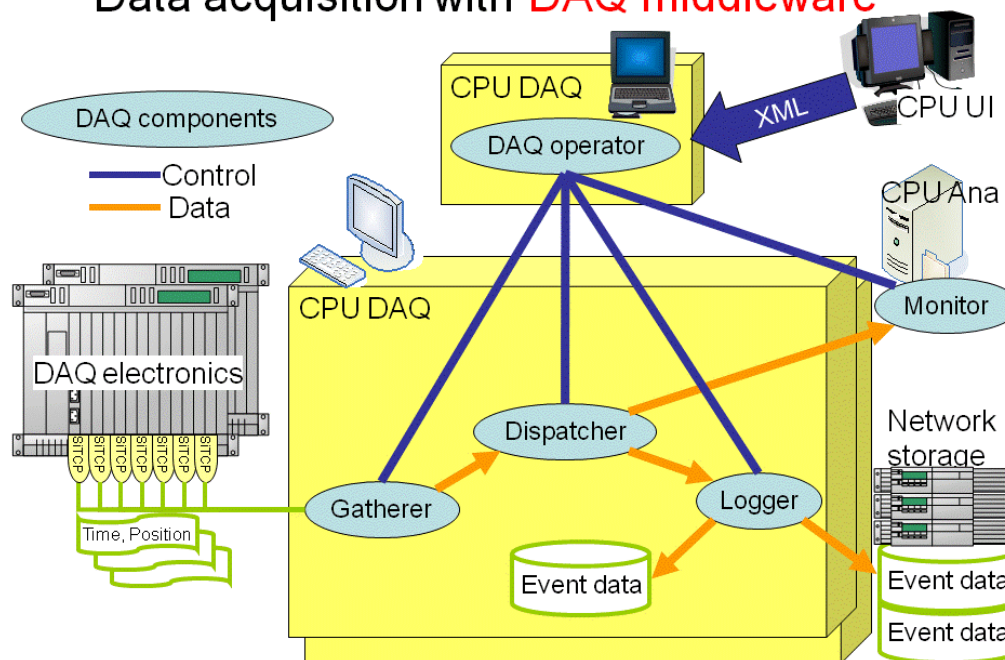


Software framework development



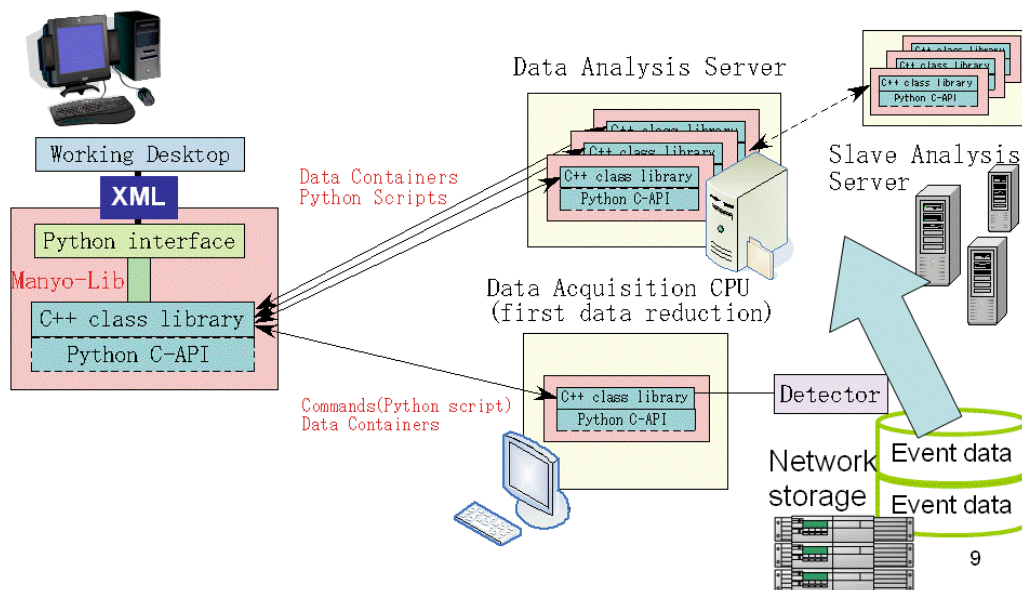
7

Data acquisition with DAQ middleware



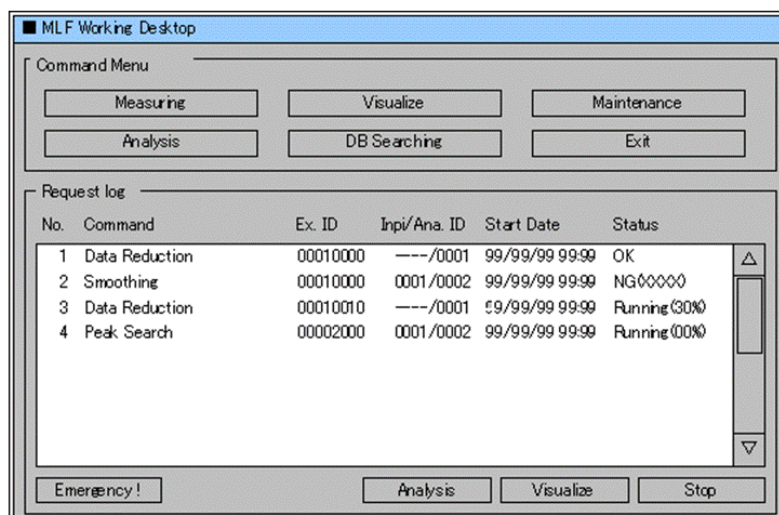
8

Distributed analysis processing with **Manyo-Lib**



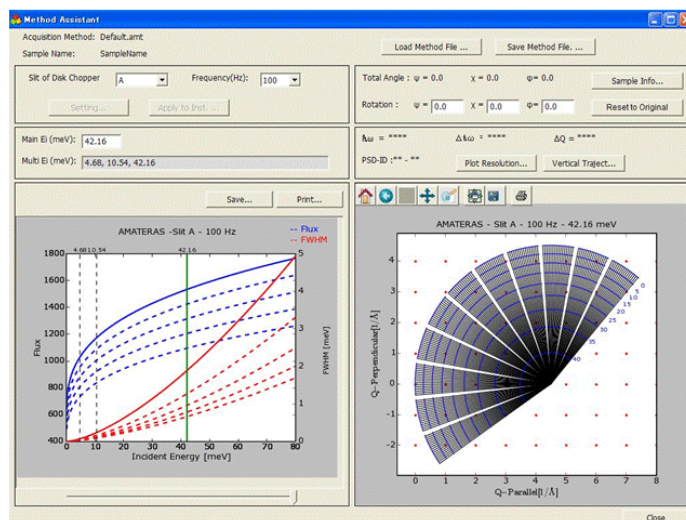
9

Working desktop GUI



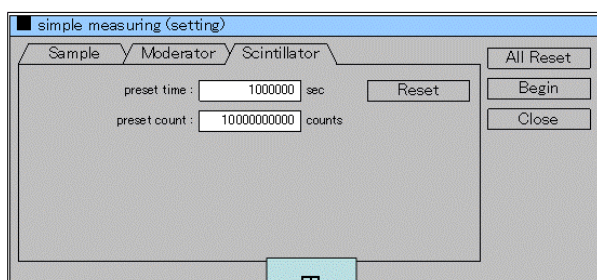
ex. TAKUMI 10

Measurement setup

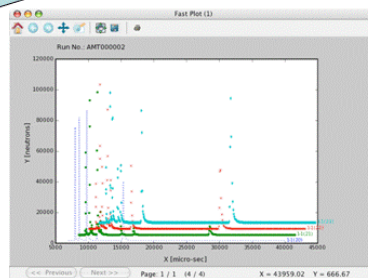
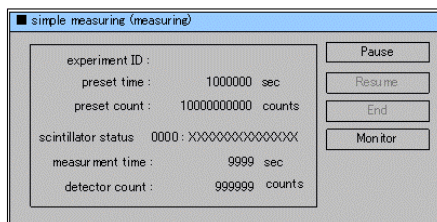


ex. AMATERAS 11

Measurement

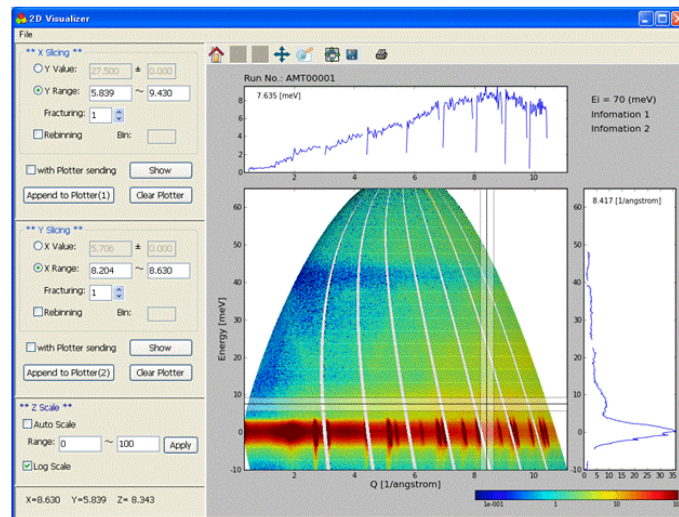


ex. TAKUMI



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Visualization



ex. AMATERAS

13

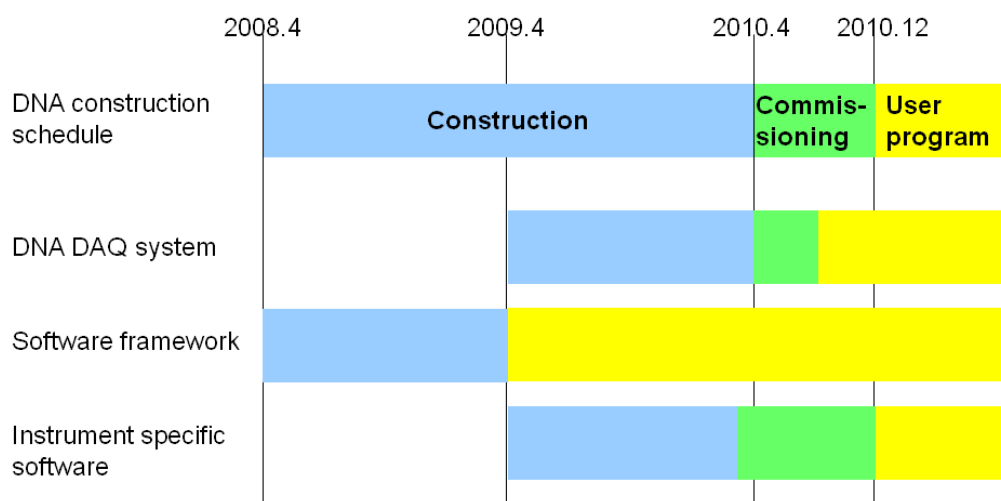
International collaboration

- KAERI-JAEA chopper software collaboration from July, 2007
- Chopper software meeting in 10-12 December, 2007



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Schedule



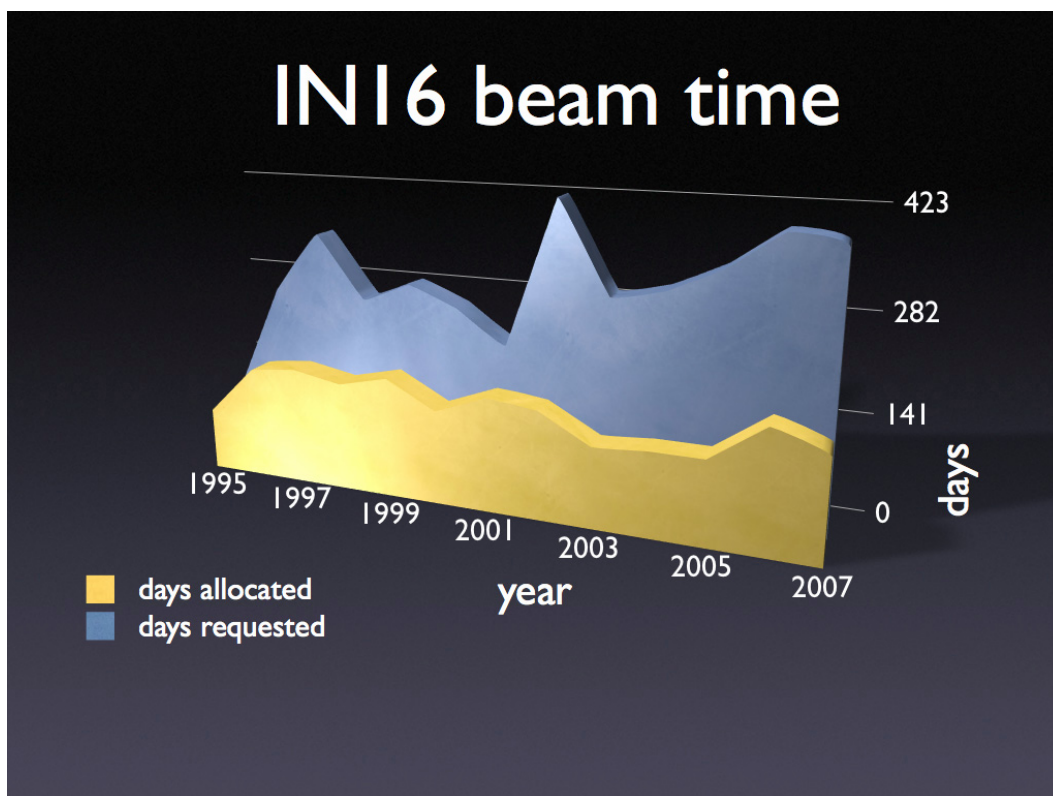
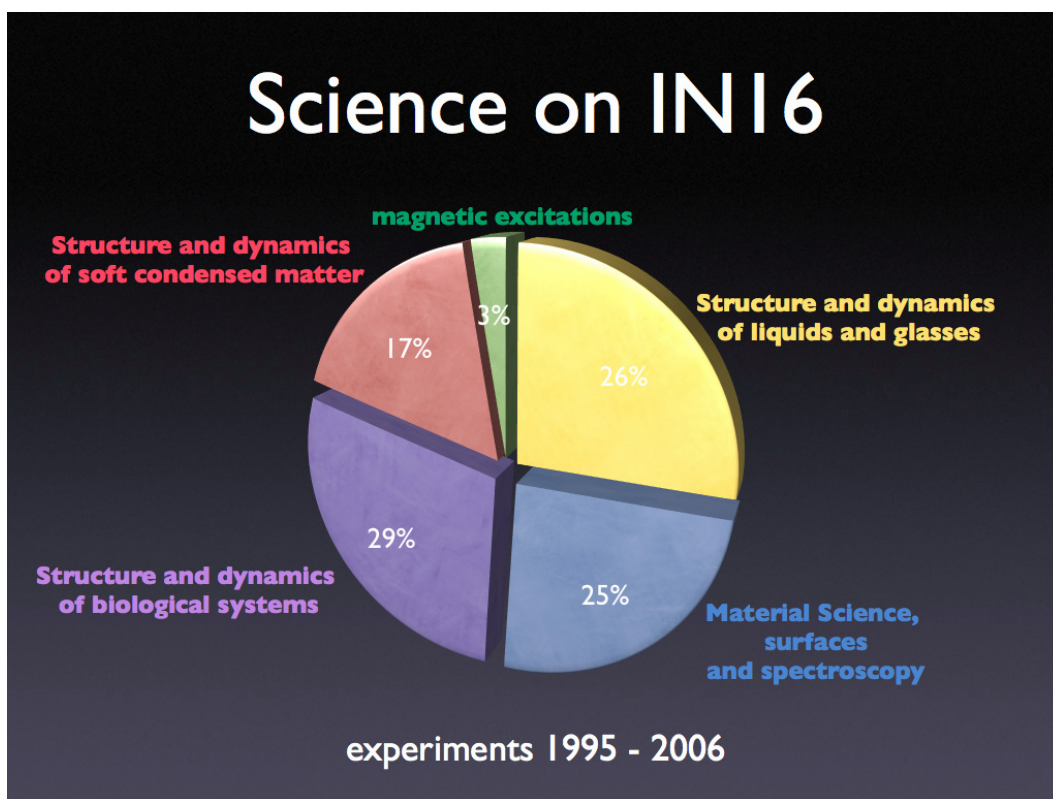
15

Summary

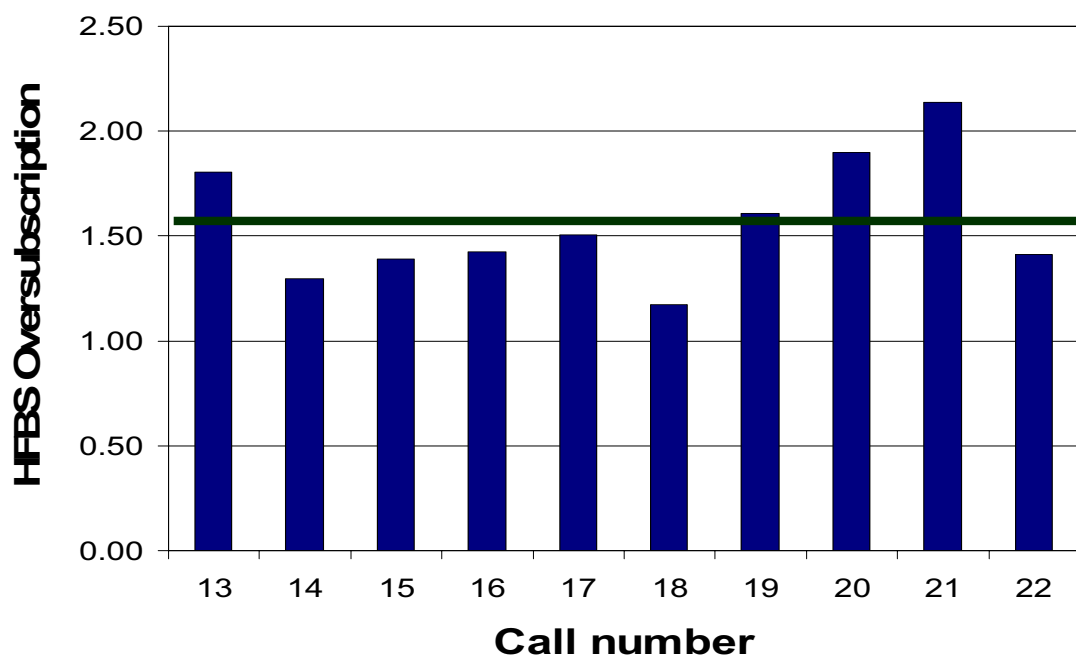
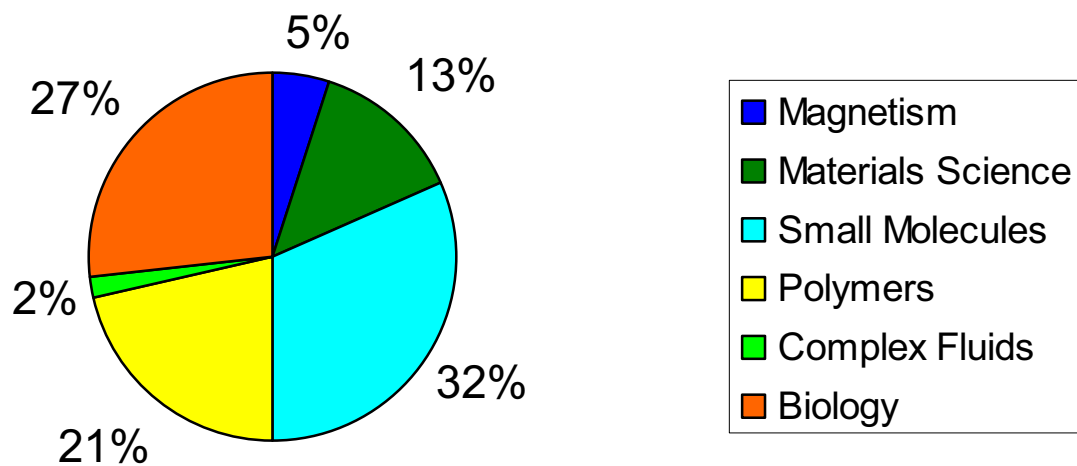
- The DAQ electronics “NEUNET” are attached the DAQ specified **Ethernet** interface called “SiTCP”.
- The functions of DAQ, Analysis, etc. are implemented as **Python** commands.
- The exchange of **XML** message between the user interface and the sub-systems (DAQ, Analysis, etc.) is **HTTP**.
- Because the sub-systems are distributed processing environment, the systems are flexible and scalable. Therefore, we can easily extend the capacity of the systems to keep in step with the increase in the proton intensity of J-PARC.

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Appendix A - IN16 data



Appendix B - NIST backscattering data



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	立方メートル	m ³
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
質量体積（比体積）	立法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
（物質量の）濃度	モル毎立方メートル	mol/m ³
輝度	カンデラ毎平方メートル	cd/m ²
屈折率（数の）	1	1

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 3．固有の名称とその独自の記号で表される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 ^(a)	rad		m・m ⁻¹ =1 ^(b)
立体角	ステラジアン ^(a)	sr ^(c)		m ² ・m ⁻² =1 ^(b)
周波数	ヘルツ	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
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	S	A/V	m ⁻² ・kg ⁻¹ ・s ³ ・A ²
磁束	ウェーバ	Wb	V・s	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
セルシウス度	セルシウス度 ^(d)	℃		K
光束度	ルーメン	lm	cd・sr ^(c)	m ² ・m ⁻² ・cd=cd
照射度	ルクス	lx	lm/m ²	m ² ・m ⁻⁴ ・cd=m ⁻² ・cd
（放射性核種の）放射能	ベクレル	Bq		s ⁻¹
吸収線量，質量エネルギー分与，カーマ線量当量，周辺線量当量，方向性線量当量，個人線量当量，組織線量当量	グレイ	Gy	J/kg	m ² ・s ⁻²
	シーベルト	Sv	J/kg	m ² ・s ⁻²

- (a) ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときいくつかの用例は表4に示されている。
- (b) 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“1”は明示されない。
- (c) 測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。
- (d) この単位は、例としてミリセルシウス度m℃のようにSI接頭語を伴って用いても良い。

表 4．単位の中に固有の名称とその独自の記号を含む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
粘力のモーメント	パスカル秒	Pa・s	m ⁻¹ ・kg・s ⁻¹
表面張力	ニュートンメートル	N・m	m ² ・kg・s ⁻²
角速度	ニュートン毎メートル	N/m	kg・s ⁻²
角加速度	ラジアン毎秒	rad/s	m・m ⁻¹ ・s ⁻¹ =s ⁻¹
角加速度	ラジアン毎平方秒	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트로ピー	ジュール毎平方メートル	J/K	m ² ・kg・s ⁻² ・K ⁻¹
質量熱容量（比熱容量），質量エン트로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
質量エネルギー（比エネルギー）	ジュール毎キログラム	J/kg	m ² ・s ⁻² ・K ⁻¹
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
体積電荷	クーロン毎立方メートル	C/m ³	m ⁻³ ・s・A
電気変位	クーロン毎平方メートル	C/m ²	m ⁻² ・s・A
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 ² ・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트로ピー	ジュール毎モル毎ケルビン	J/(mol・K)	m ² ・kg・s ⁻² ・K ⁻¹ ・mol ⁻¹
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 ・s・A
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

表 6．国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1 h =60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	1° =(π/180) rad
分	′	1′ =(1/60)° =(π/10800) rad
秒	″	1″ =(1/60)′ =(π/648000) rad
リットル	l、L	1l=1 dm ³ =10 ⁻³ m ³
トン	t	1t=10 ³ kg
ネーパ	Np	1Np=1
ベル	B	1B=(1/2) ln10 (Np)

表 7．国際単位系と併用されこれに属さない単位で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 単位であらわされる数値
電子ボルト	eV	1eV=1.60217733(49)×10 ⁻¹⁹ J
統一原子質量単位	u	1u=1.6605402(10)×10 ⁻²⁷ kg
天文単位	ua	1ua=1.49597870691(30)×10 ¹¹ m

表 8．国際単位系に属さないが国際単位系と併用されるその他の単位

名称	記号	SI 単位であらわされる数値
海里		1 海里=1852m
ノット		1 ノット=1 海里毎時=(1852/3600)m/s
アール	a	1 a=1 dam ² =10 ² m ²
ヘクタール	ha	1 ha=1 hm ² =10 ⁴ m ²
バール	bar	1 bar=0.1MPa=100kPa=1000hPa=10 ⁵ Pa
オングストローム	Å	1 Å=0.1nm=10 ⁻¹⁰ m
バール	b	1 b=100fm ² =10 ⁻²⁸ m ²

表 9．固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	1 erg=10 ⁻⁷ J
ダイン	dyn	1 dyn=10 ⁻⁵ N
ボアズ	P	1 P=1 dyn・s/cm ² =0.1Pa・s
ストークス	St	1 St =1cm ² /s=10 ⁻⁴ m ² /s
ガウス	G	1 G ≒10 ⁴ T
エルステッド	Oe	1 Oe ≒(1000/4π) A/m
マクスウェル	Mx	1 Mx ≒10 ⁻⁸ Wb
スチルブ	sb	1 sb =1cd/cm ² =10 ⁴ cd/m ²
ホト	ph	1 ph=10 ⁴ lx
ガリ	Gal	1 Gal =1cm/s ² =10 ⁻² m/s ²

表10．国際単位に属さないその他の単位の例

名称	記号	SI 単位であらわされる数値
キュリー	Ci	1 Ci=3.7×10 ¹⁰ Bq
レントゲン	R	1 R = 2.58×10 ⁻⁴ C/kg
ラド	rad	1 rad=1cGy=10 ⁻² Gy
レム	rem	1 rem=1 cSv=10 ⁻² Sv
X線単位		1X unit=1.002×10 ⁻⁴ nm
ガンマ	γ	1γ=1 nT=10 ⁻⁹ T
ジャンスキー	Jy	1 Jy=10 ⁻²⁶ W・m ⁻² ・Hz ⁻¹
フェルミ	fm	1 fermi=1 fm=10 ⁻¹⁵ m
メートル系カラット		1 metric carat = 200 mg = 2×10 ⁻⁴ kg
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリ	cal	
マイクロン	μ	1 μ =1μm=10 ⁻⁶ m

