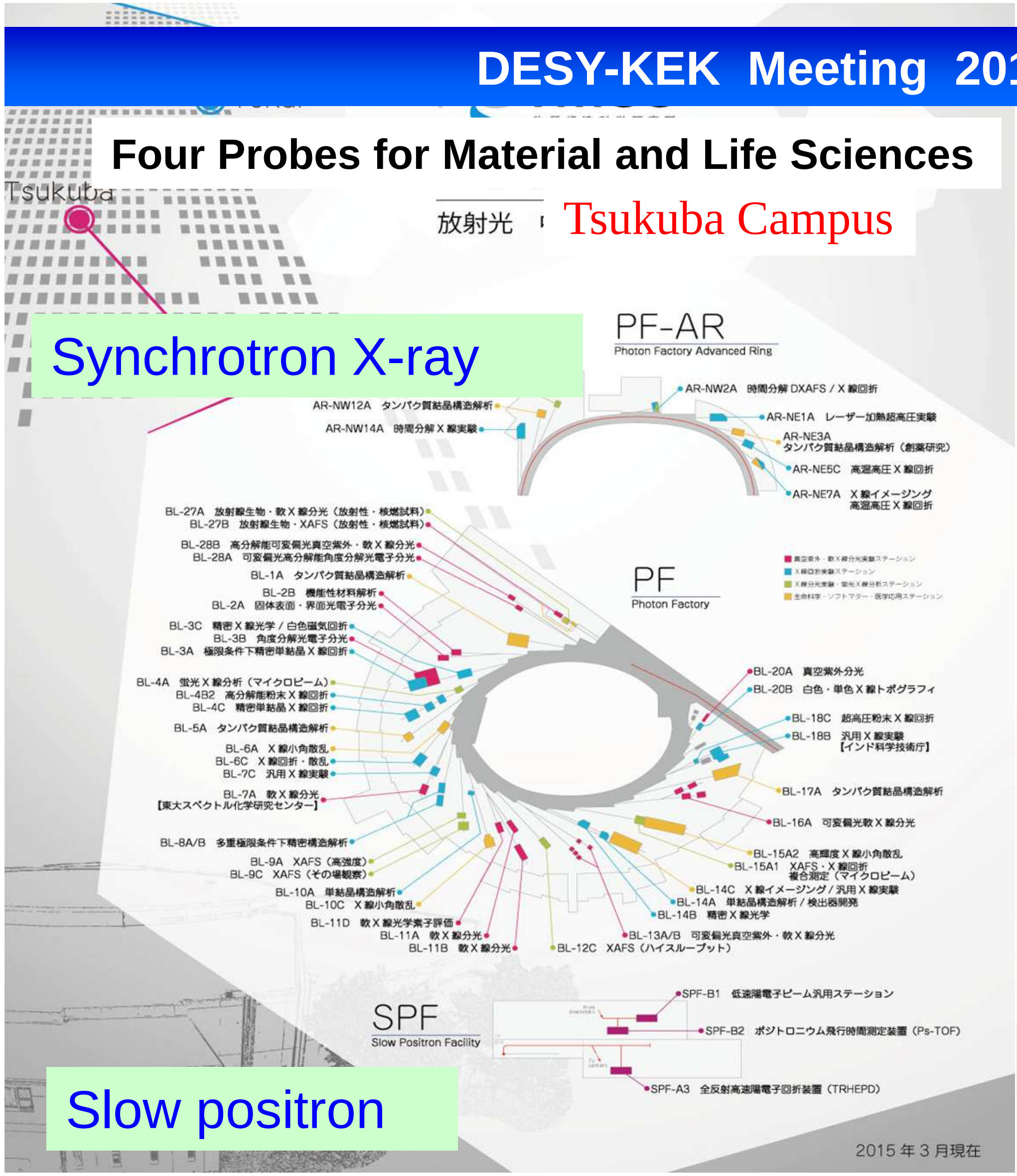
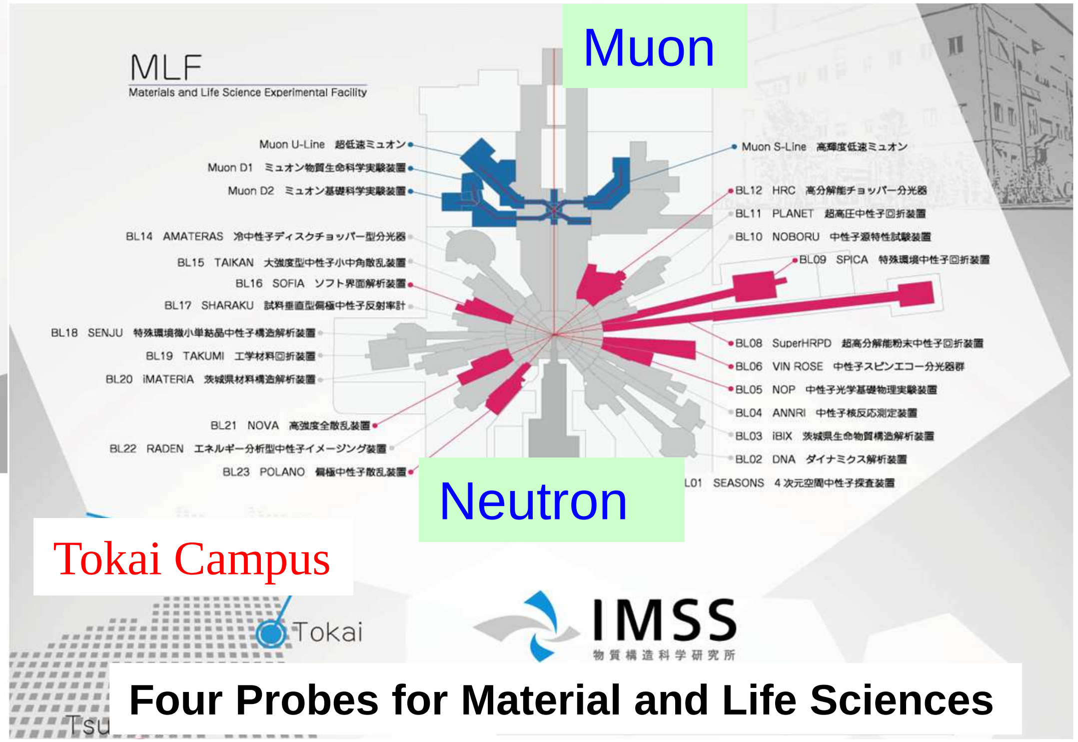


Activity of material and life Sciences in KEK

Institute of Materials Structure Science (IMSS)

Kazuyoshi Yamada



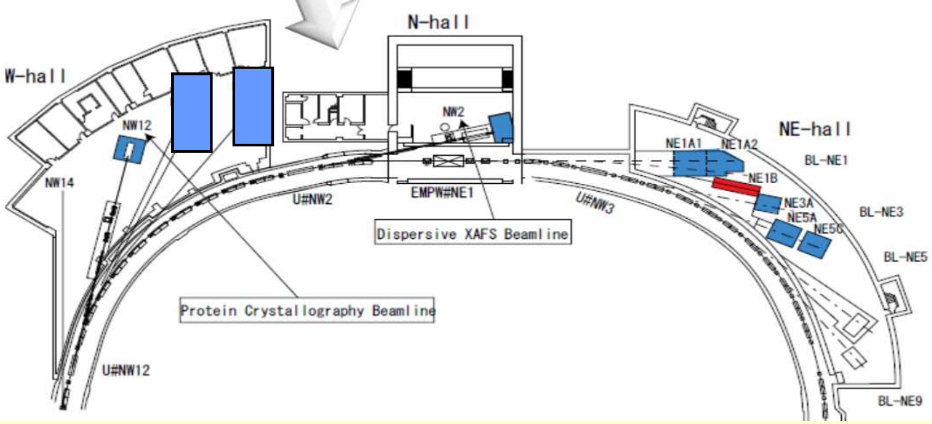
~60 beam lines

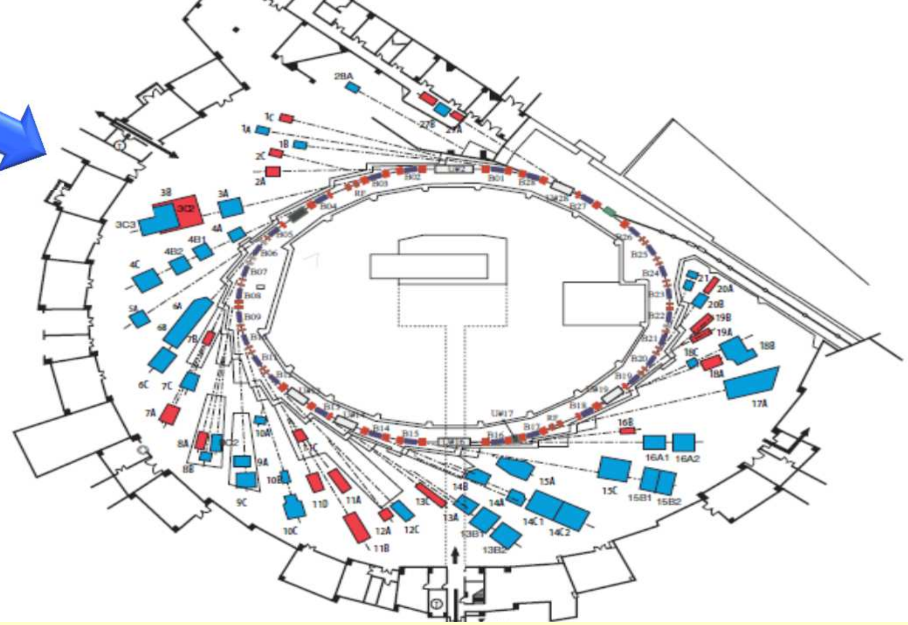
More than 3200 users/year

The Present Status of Photon Factory

User program has been running since 1983, 33 years old !

Still active, the 2nd biggest synchrotron facility in Japan
(~3,000 users/year, ~600 papers/year)





PF-AR (6.5 GeV, 60mA, SB, 8 stations, 377m)

- Operation start in 1987
- Operate always in **single-bunch mode** to produce pulsed hard x-ray

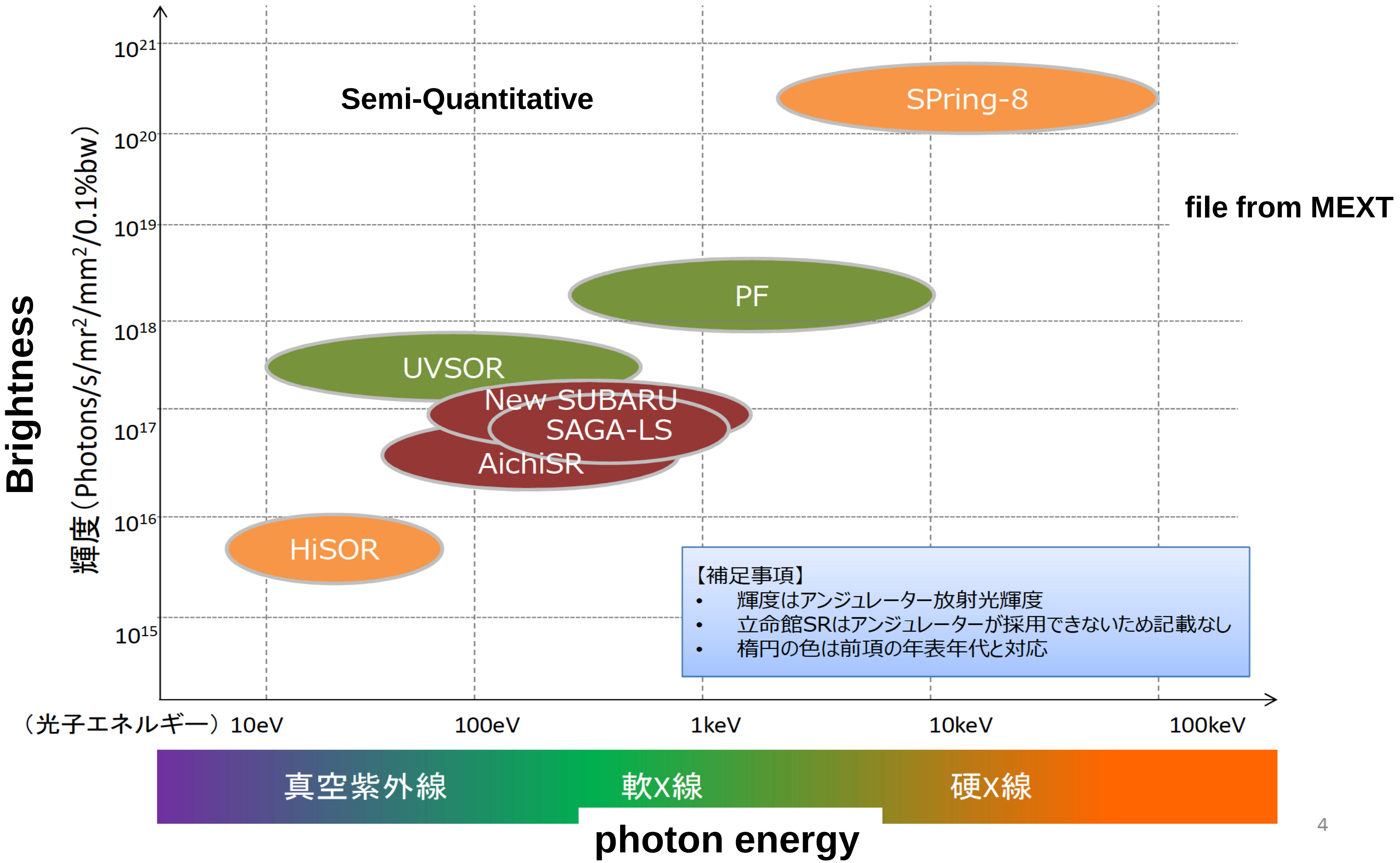
PF (2.5 GeV, 450 mA, MB, 39 stations, 187m)

- Operation start in 1982
- Twice **large upgrades in 1996 and 2005**

Emittance was reduced from 130 to 36 nmrad

Characteristic photon energy and brightness of each facilities in Japan

各放射光施設の得意とするエネルギー領域

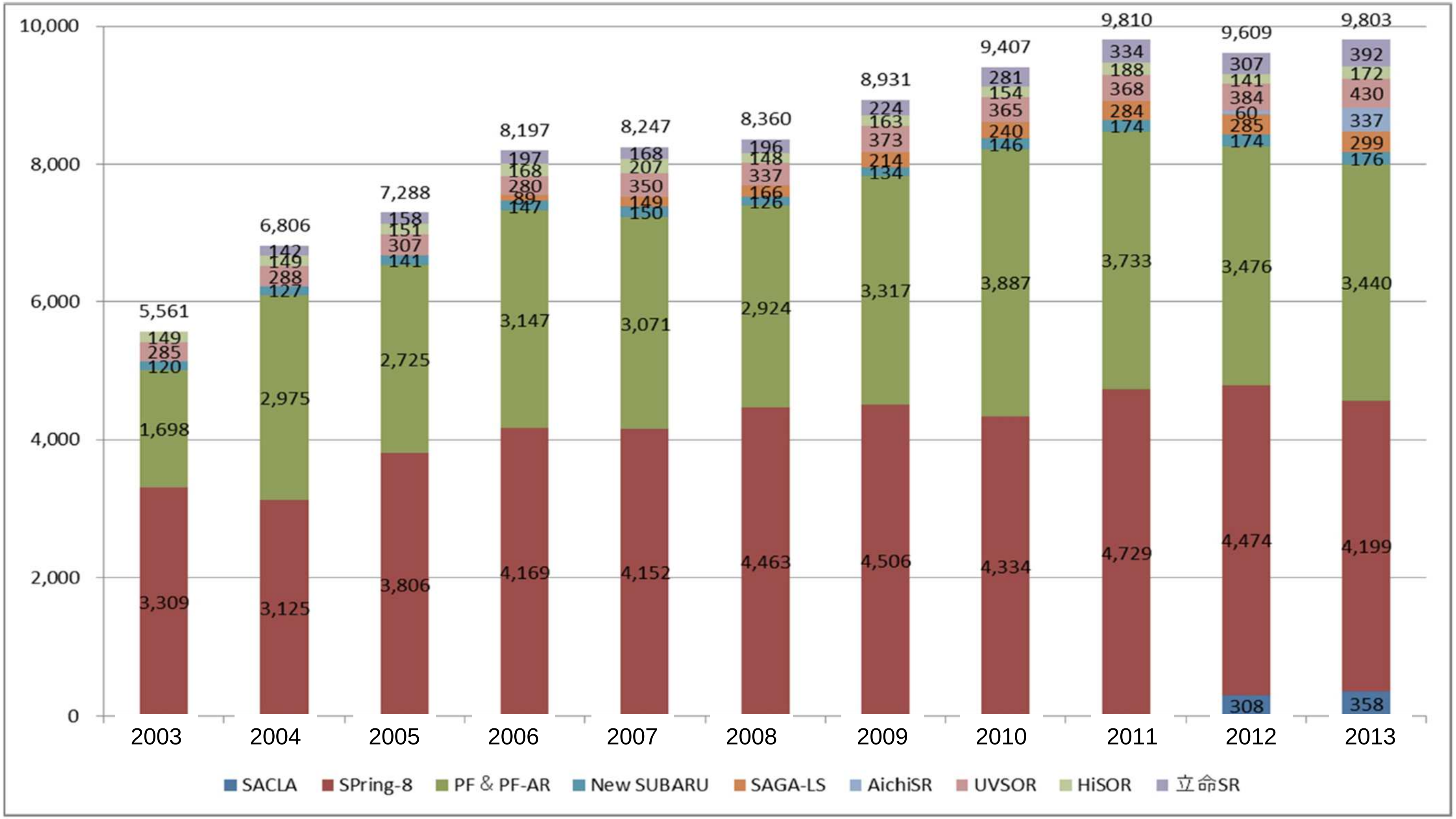


Number of unique user of each facility in Japan

file from MEXT

我が国の放射光施設のアクティビティ③

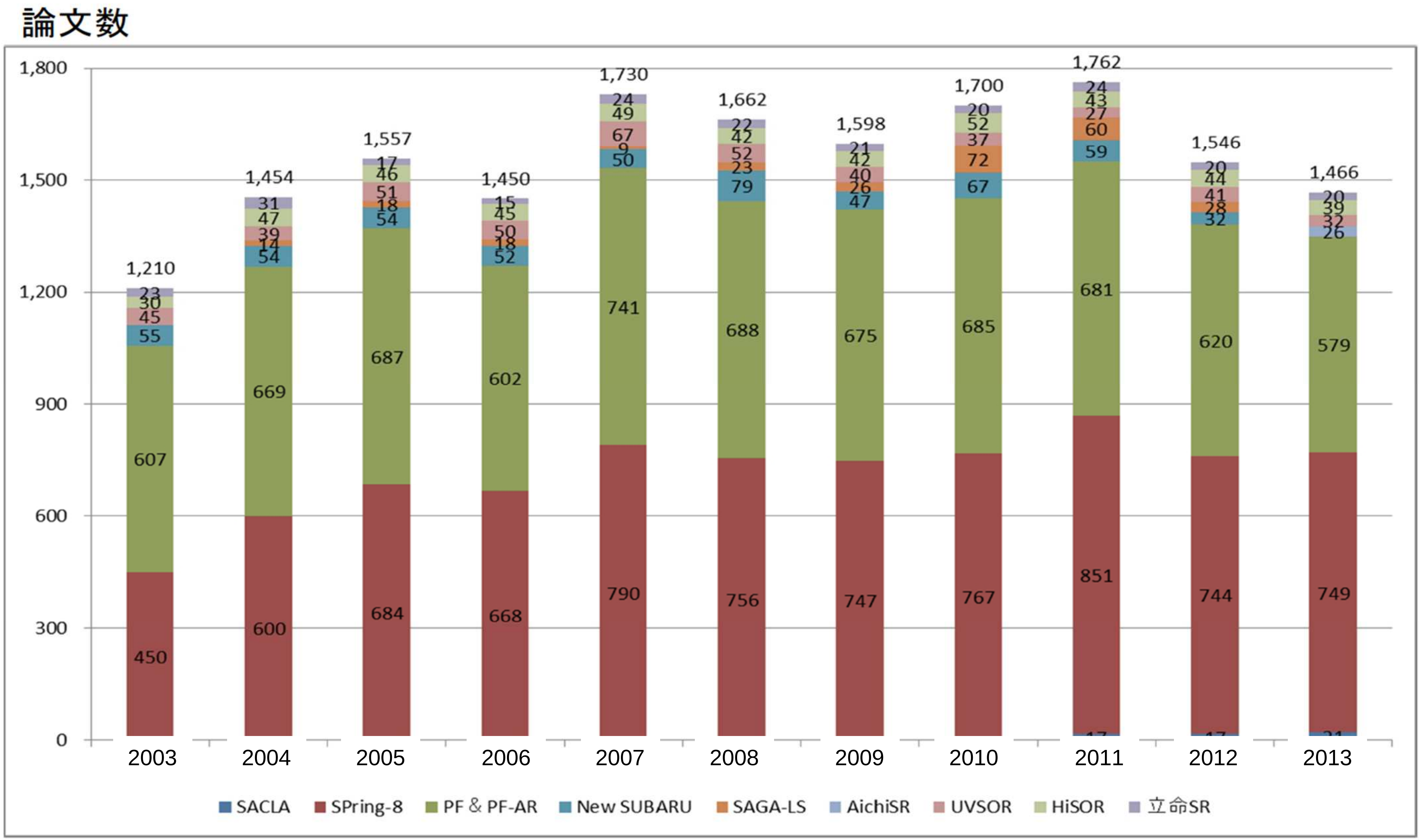
利用者数（ユニーク数）



Number of published papers used each facility in Japan

我が国の放射光施設のアクティビティ①

file from MEXT



Why PF is still active?

(1) Continuous and timely upgrade of facilities
(accelerator, beam lines, instruments)

(2) Introduce new types of experiment suited for the beam

=> Mainly focus on Flux-based experiment
rather than Luminosity-based experiment
which should be done in 3rd. generation facilities

(3) Keep power users and grow good in-house scientists

(4) Grow new users in various fields of science and technology

However, we need a new light source as soon as possible !!

Future Plan : KEK Light Source (by Sakai, Yamaguchi in detail)

The special committee under the steering committee of IMSS chose a storage ring-type light source for the 1st stage

1st Stage

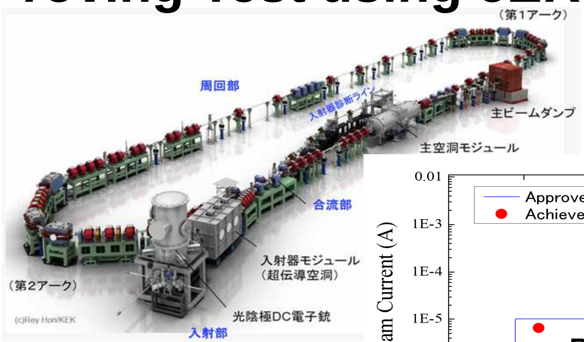
Ring-type LS
Enegy~3GeV

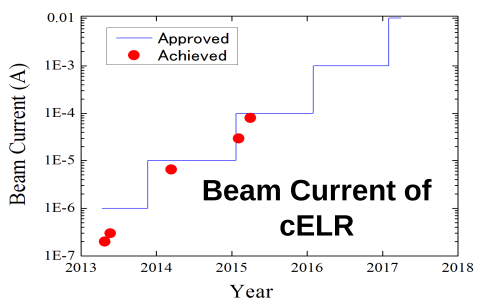
Preliminary Design	Detailed Design Preparation	Construction	Installation	Experiment

2015 2016 2017 2018 2019 2020 2021 2022 2023 2024 2025 ・・・・

Ring-type　　　　Linac-type(?)

Proving Test using cERL

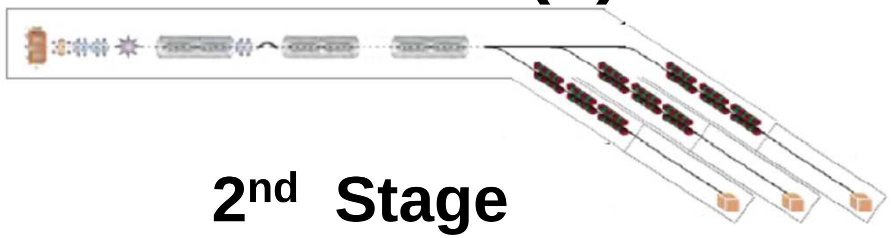




R&D

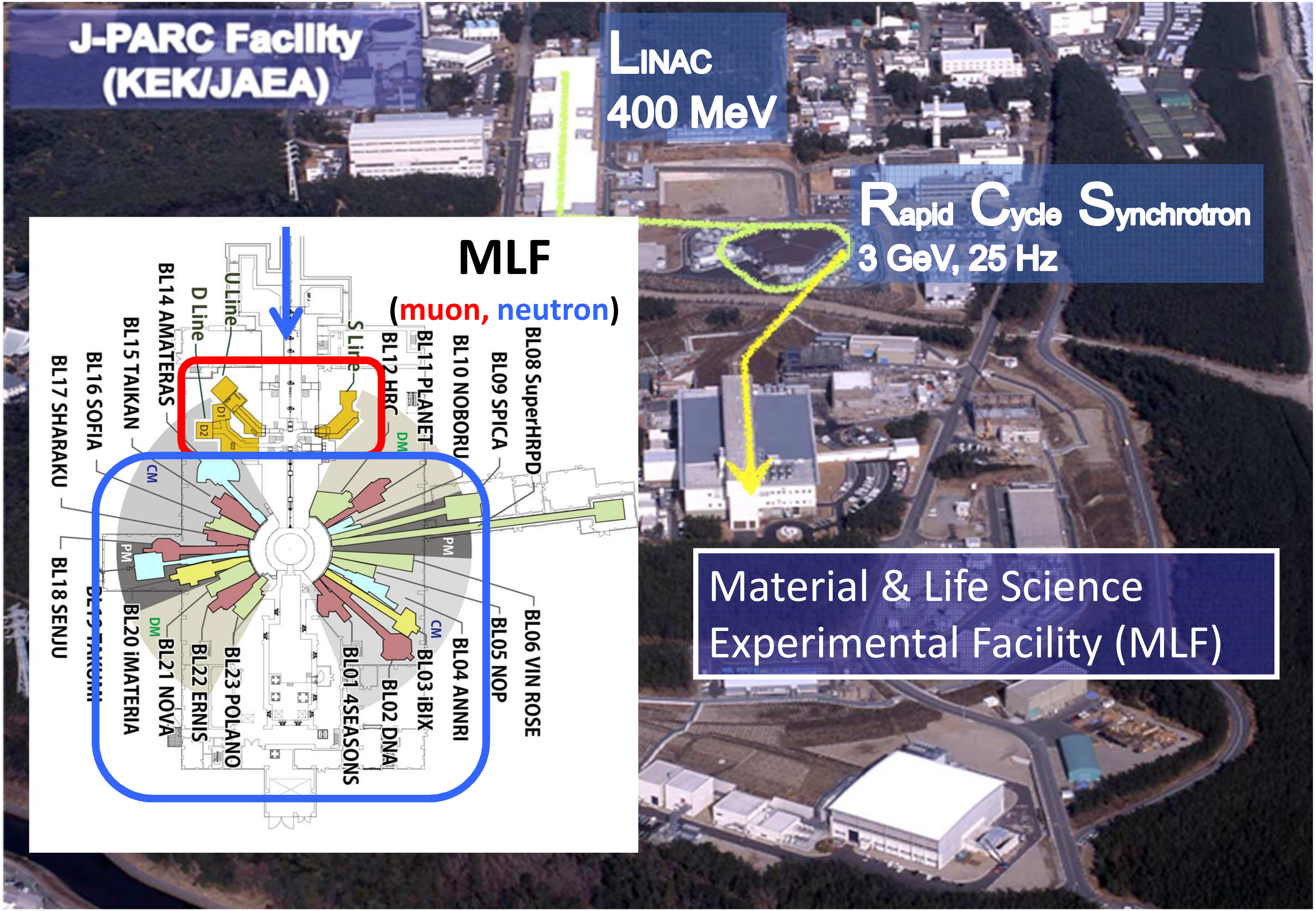
EUV-FEL

cw-XFEL(?)



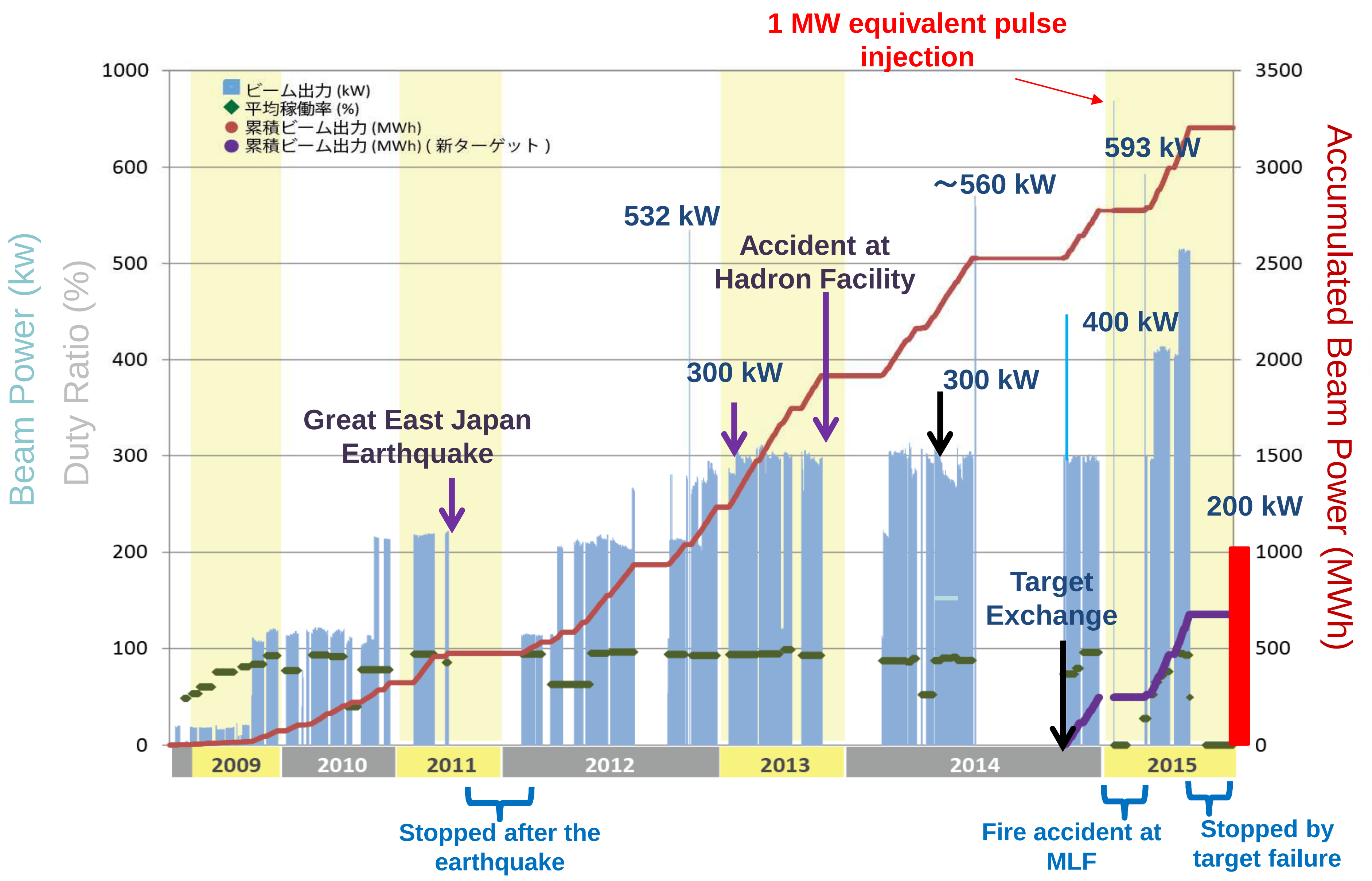
2nd Stage

Linac-type LS(?)

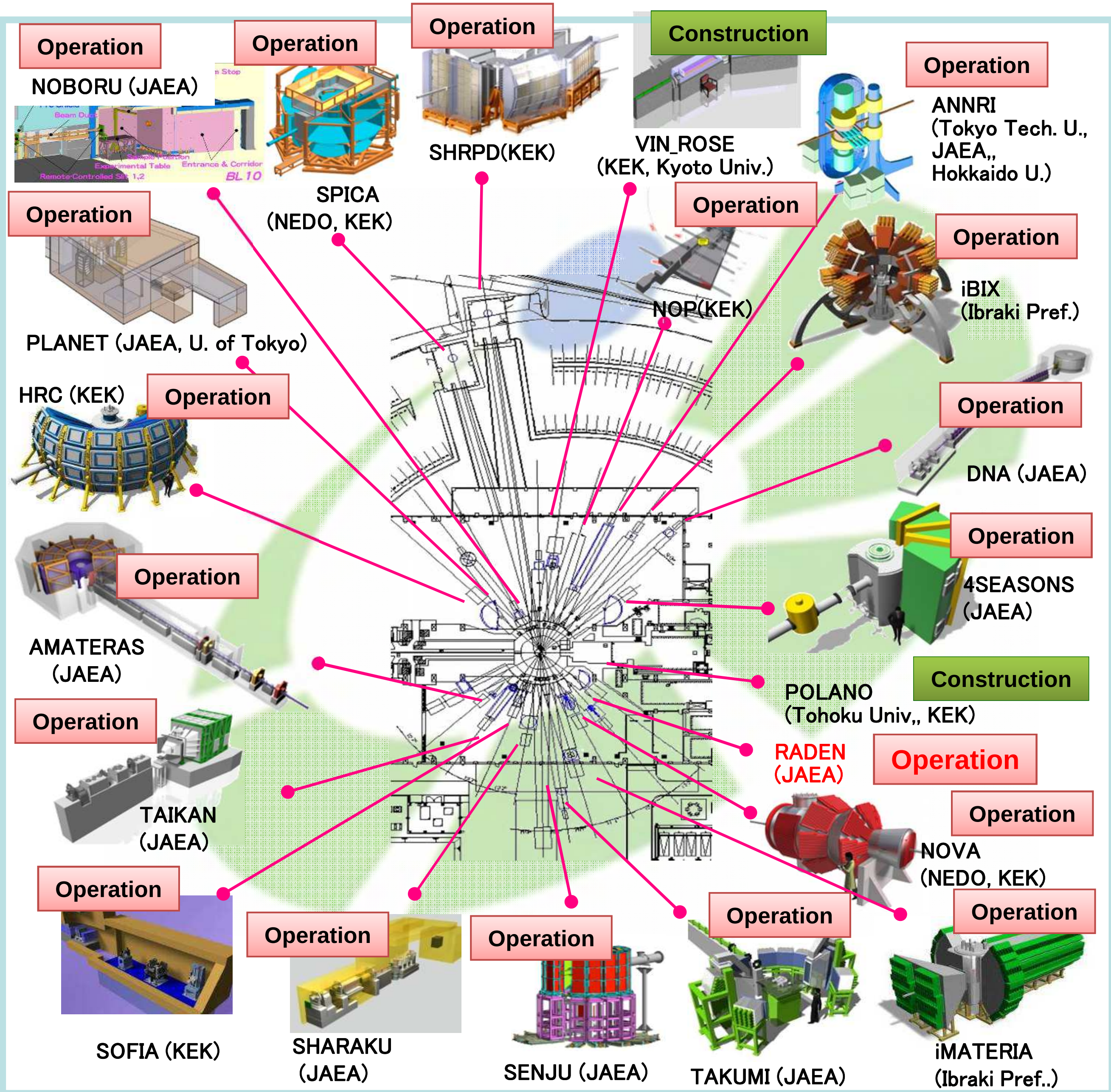


J-PARC Facility
(KEK/JAEA)
LINAC
400 MeV
Rapid Cycle Synchrotron
3 GeV, 25 Hz
MLF
(muon, neutron)
U Line
D Line
S Line
D1
D2
BL14 AMATERAS
BL15 TAIKAN
BL16 SOFIA
BL17 SHARAKU
BL18 SENJU
BL20 iMATERIA
BL21 NOVA
BL22 ERNIS
BL23 POLANO
BL01 4SEASONS
BL02 DNA
BL03 iBIX
BL04 ANNRI
BL05 NOP
BL06 VIN ROSE
BL08 SuperHRPD
BL09 SPICA
BL10 NOBORU
BL11 PLANET
BL12 HRC
CM
PM
DM
Material & Life Science
Experimental Facility (MLF)

Beam history of MLF

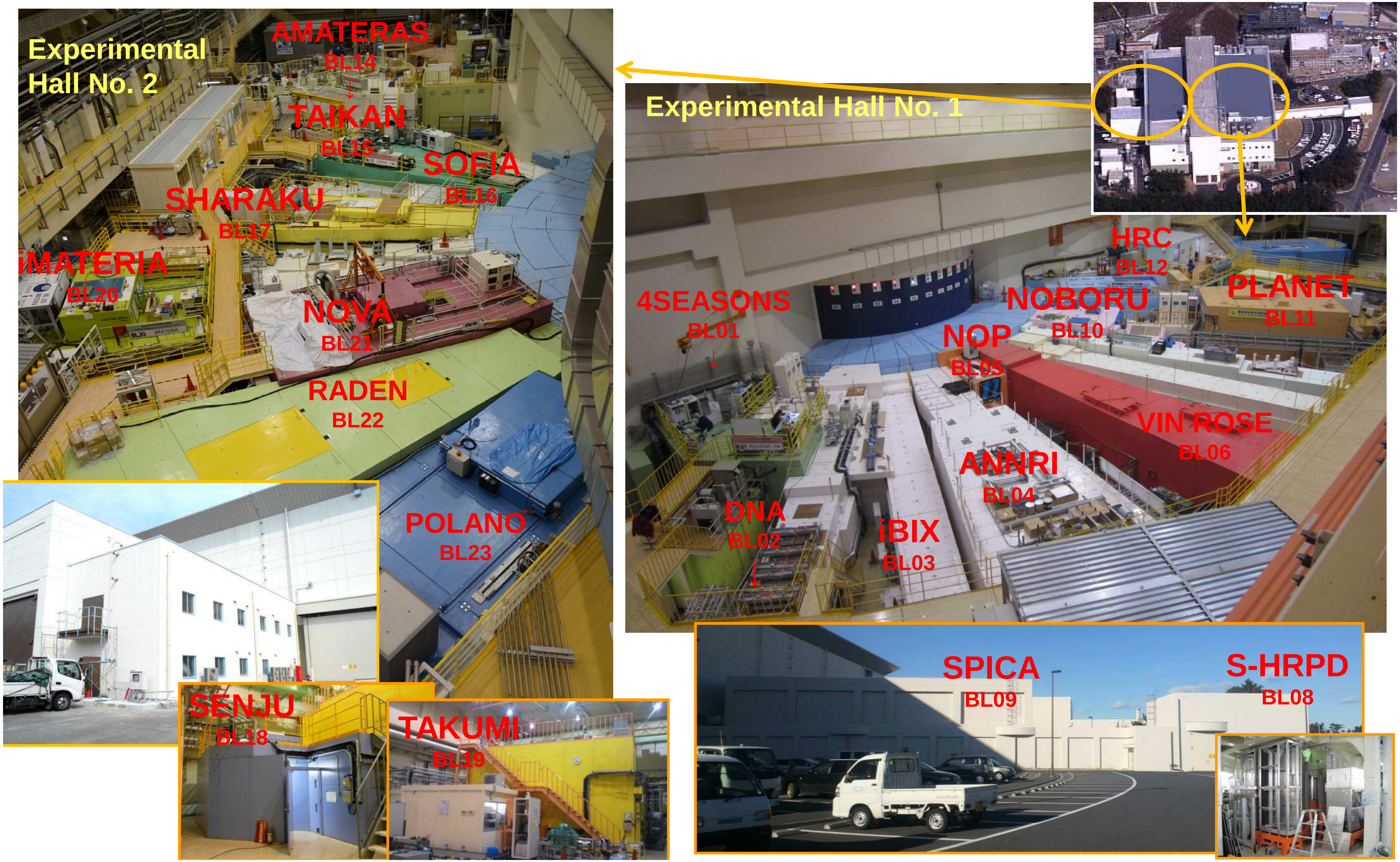


Neutron Instruments at MLF

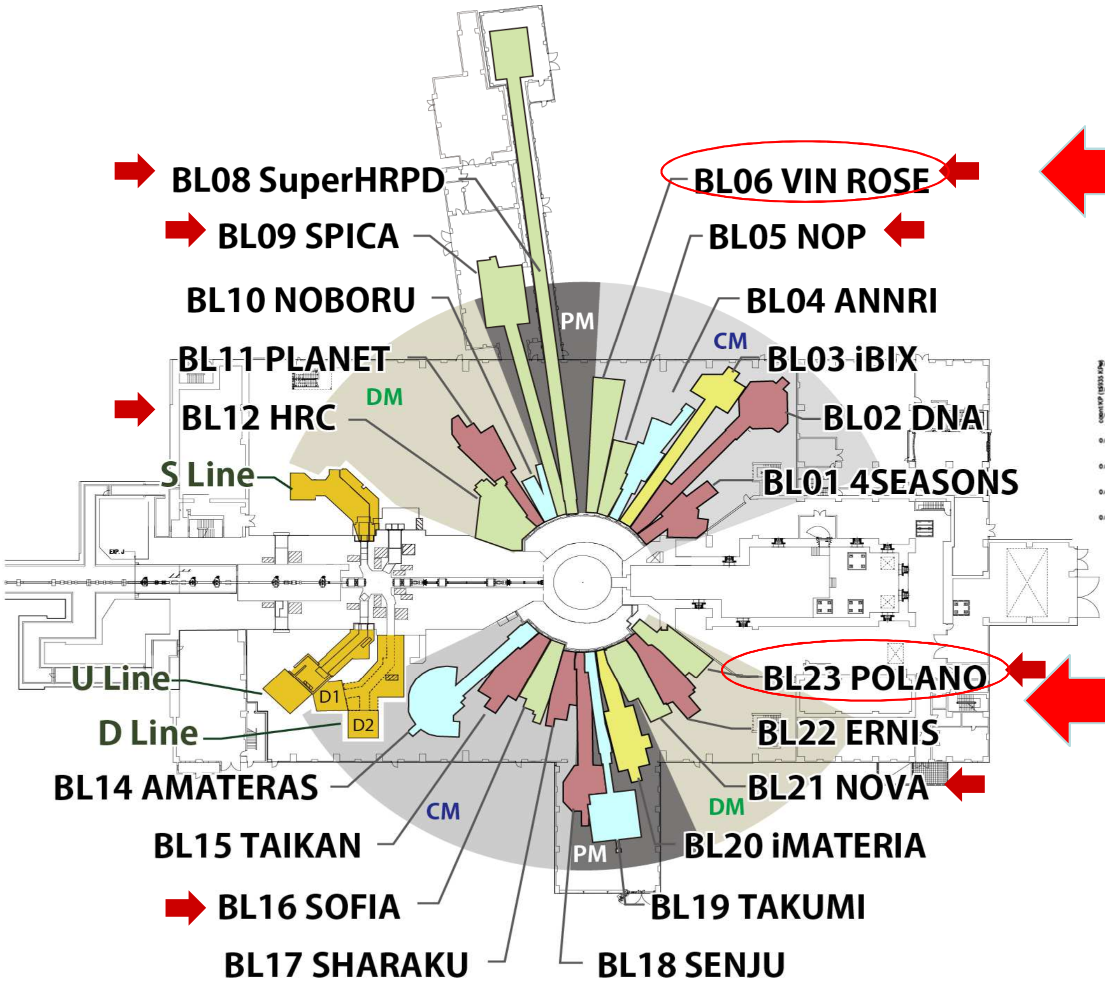


- The first neutron in May, 2008
- 23 Neutron Beam Ports
- From Fundamental Physics to Industrial Uses
- Operation: 19 (Apr., 2015)
  Construction/Commissioning:2
- Constructed by
  - ･KEK
  - ･JAEA
  - ･Ibaraki Prefecture
  - ･Universities, Institutes & Government organizations...
- Yearly Operation Days
  - ･~180
- Yearly Guest Number
  - ･731 (2014)

Neutron Instruments at MLF

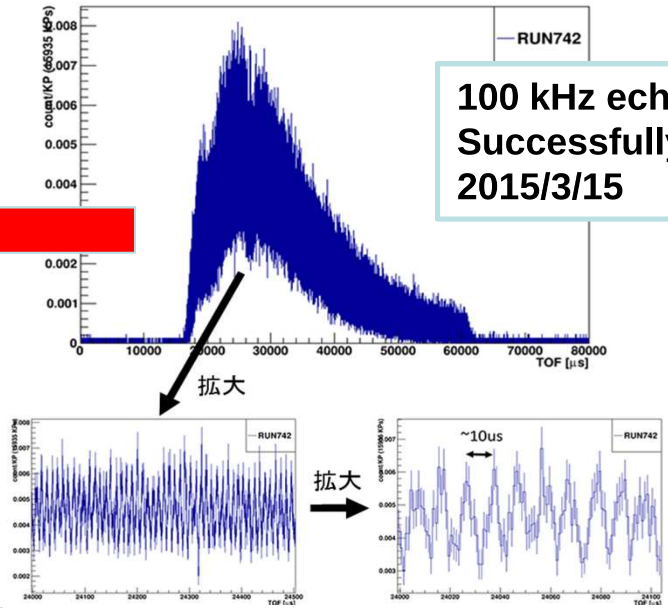


IMSS operates 8 instruments



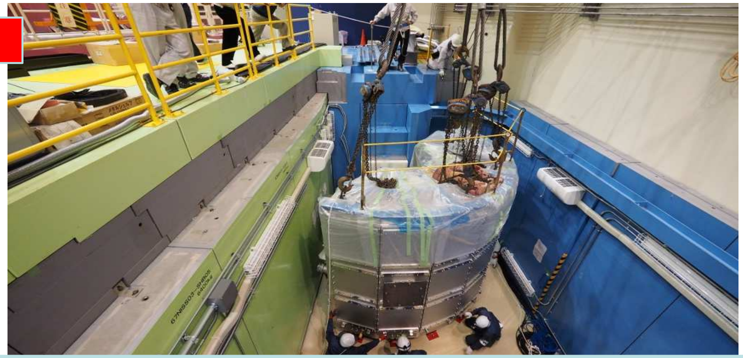
Polarization analysis of neutron spin

BL06: Spin-Echo instrument



100 kHz echo-signal Successfully observed 2015/3/15

BL23: Polarized neutron inelastic spectrometer



Main components have been installed 2015/8

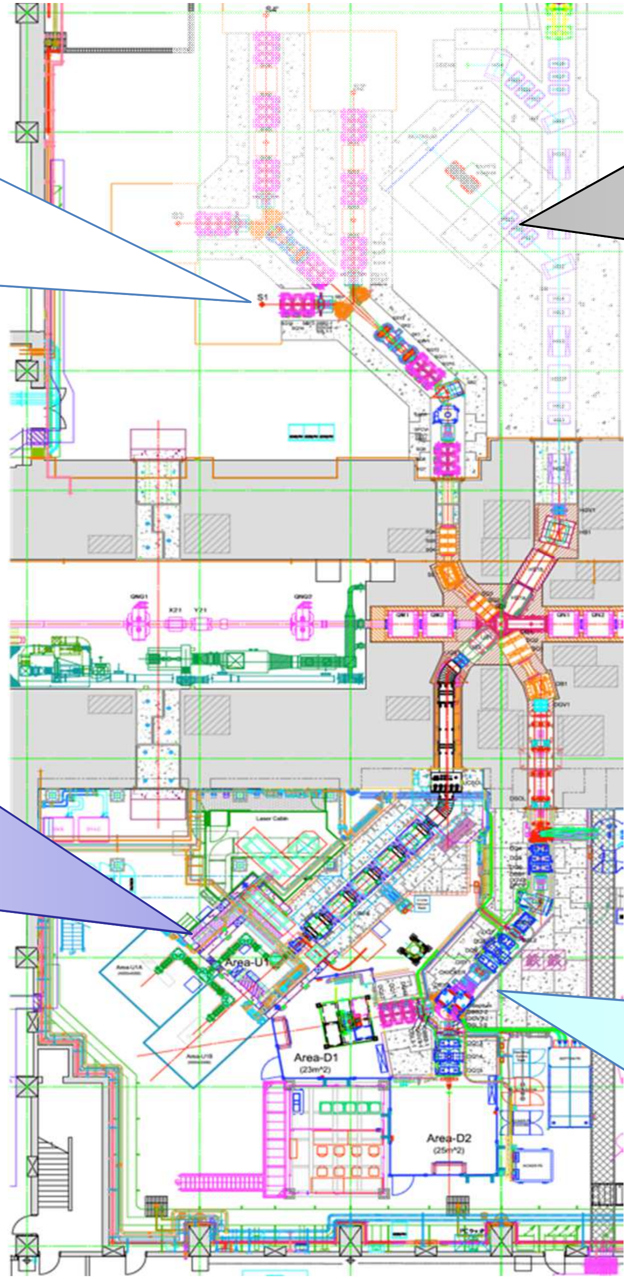
4 Muon beam lines in MLF

S-line μ^+

Slow beam（4 MeV), dedicated to bulk μSR ultralow tem-perature/high magnetic field/ pulsed excitations.
(S1:2016~)

U-line μ^+

Ultra slow beam（0.1～30 keV), near-surface, sub-micron scale condensed matter physics, chemistry, etc.

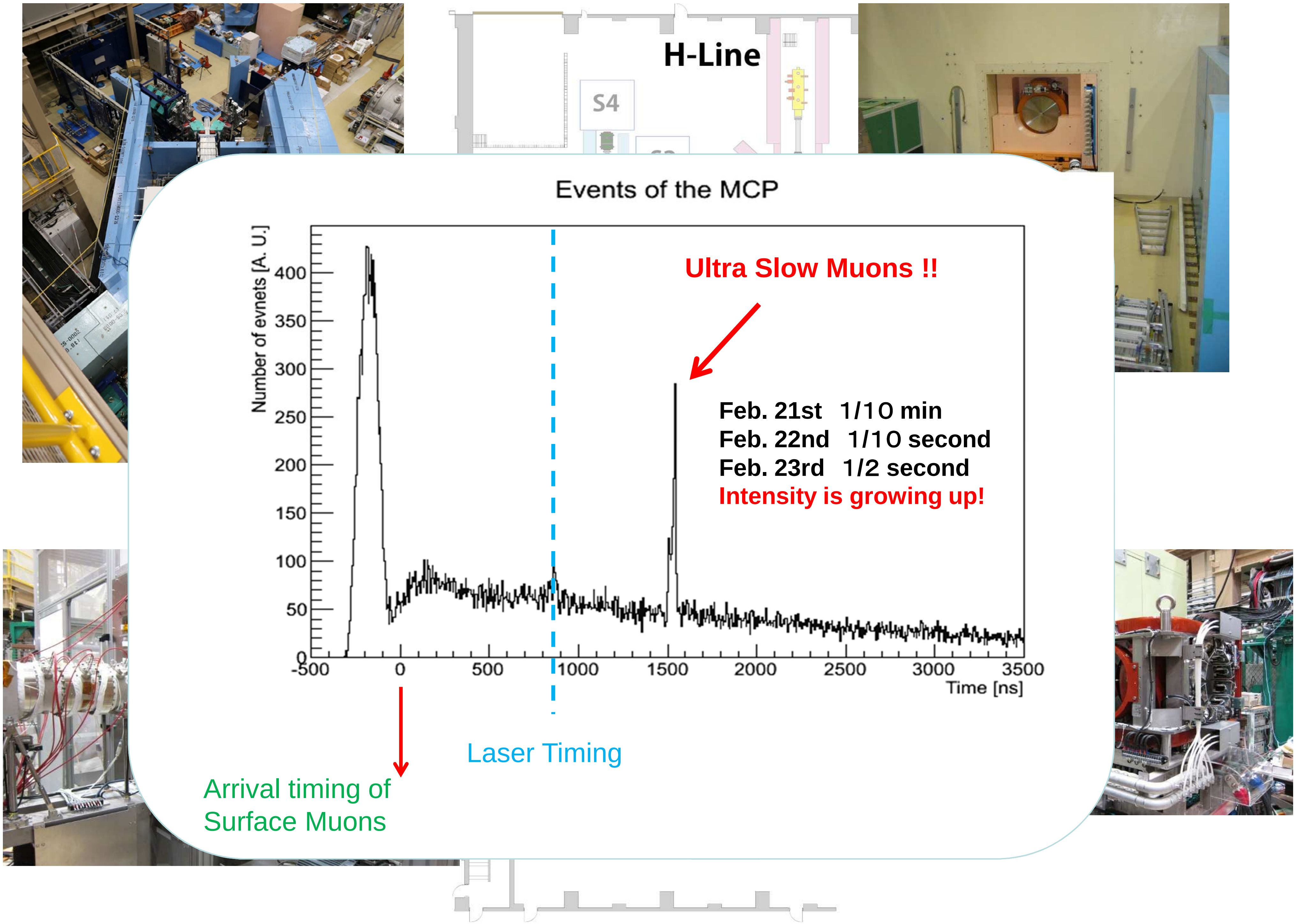


H-line $\mu^{\pm}$

Slow（4 MeV) ～fast (50 MeV) beam, for particle physics, atomic physics (“precision frontier”)

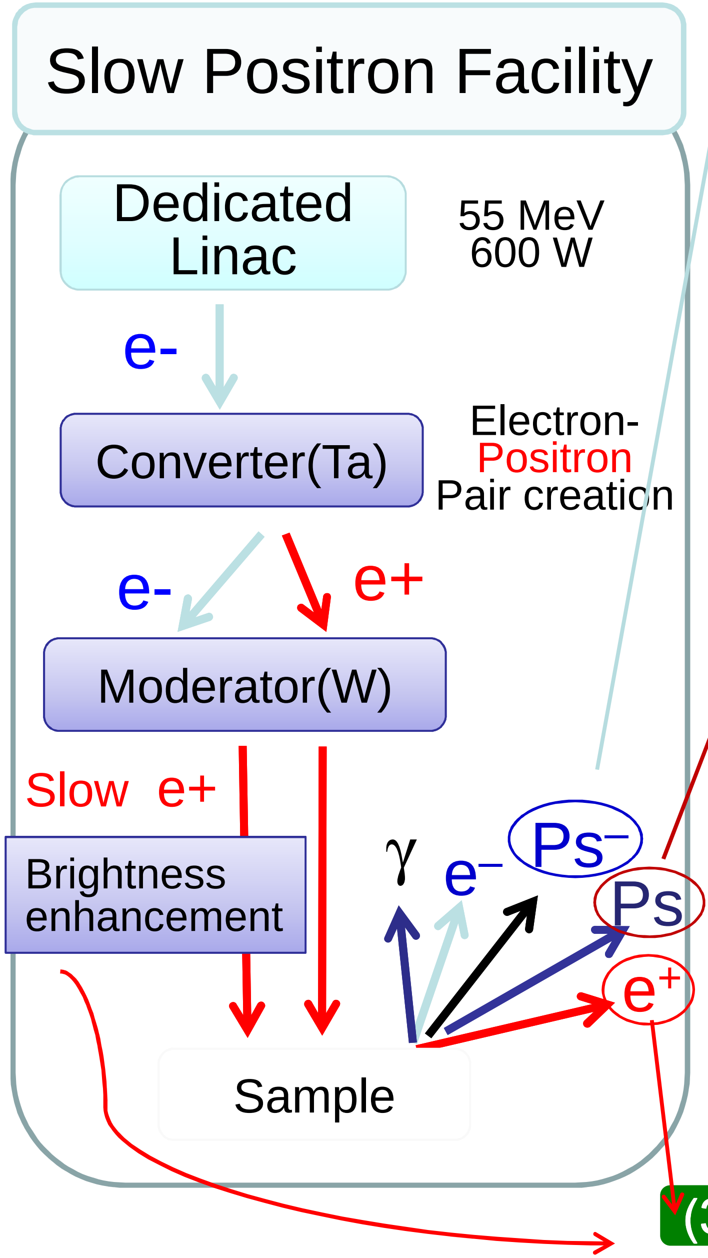
D-line $\mu^{\pm}$

Slow（4 MeV) ～fast（50 MeV), general-purpose beamine with 2 exp. areas.
(2009~)



H-Line
S4
Events of the MCP
Number of evnets [A. U.]
Time [ns]
Ultra Slow Muons !!
Feb. 21st 1/10 min
Feb. 22nd 1/10 second
Feb. 23rd 1/2 second
Intensity is growing up!
Laser Timing
Arrival timing of
Surface Muons

Three Types of Beam available in Slow Positron Facility

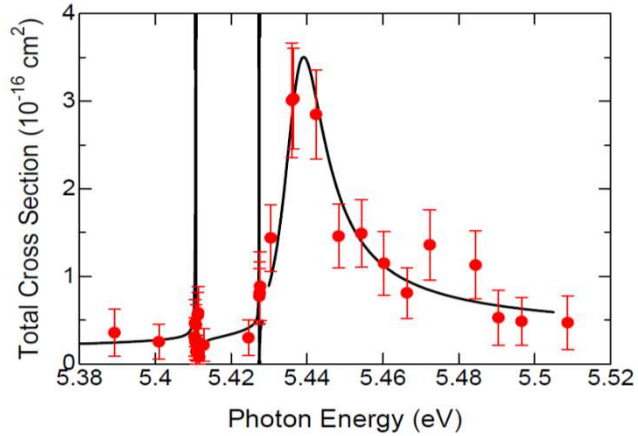


(1) Positronium negative ion, Ps^- ($e^- - e^+ - e^-$)

Observation of Ps^- shape resonance in the photo-detachment reaction

$$Ps^- + h\nu \rightarrow Ps + e^-$$

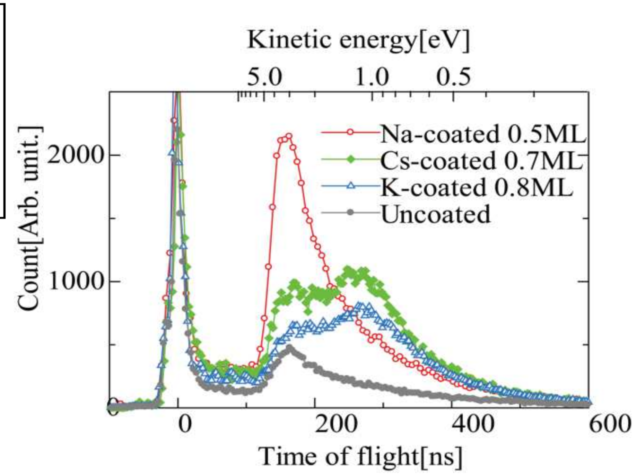
The first laser spectroscopy of Ps^-



(2) Positronium time-of-flight (Ps-TOF)

TOF spectroscopy of the Ps emitted from a sub-monolayer alkali-metal coated tungsten surface

Interaction of the positrons with a two-dimensional electron gas on the surface



(3) Positron surface diffraction (scientific topics shown later)

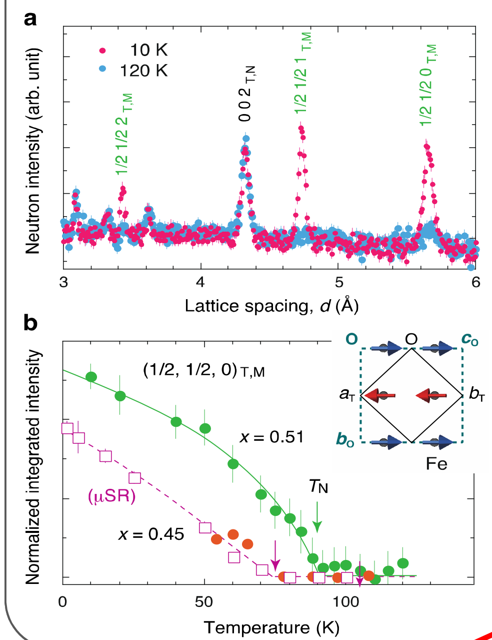
Scientific Topics

(1) "Multi-probe use" (Iron-based superconductor) (Neutron, Muon, X-ray)
(2) Hydrogen; structure and dynamics in matter (Neutron)
(3) Industrial application and new materials for innovation (X-ray)
(4) Local probe in matter (Muon)
(5) Surface structure (Slow positron)

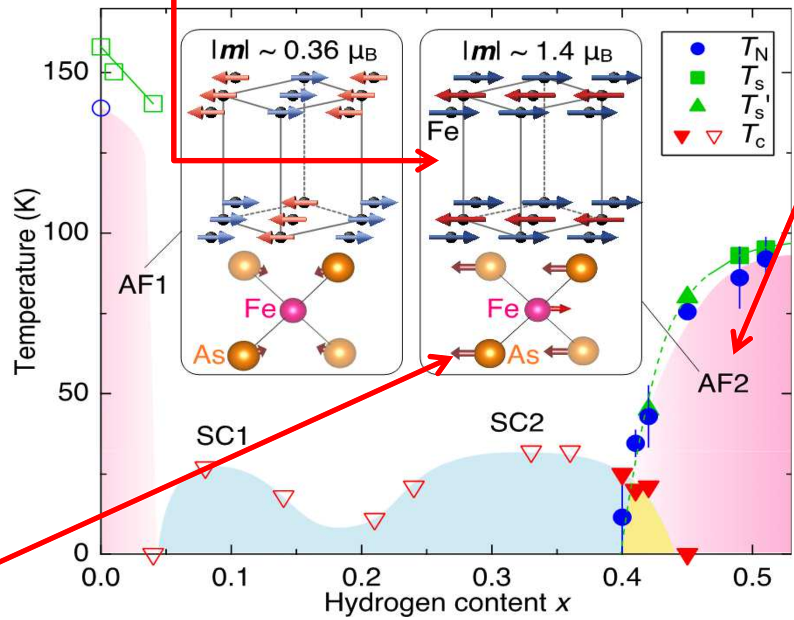
Fe-based superconducting material $LaFeAsO_{1-x}H_x$ using multi-probe analysis

Discovery of a new magnetic phase (AF2) and its contrasting properties to the original one (AF1)

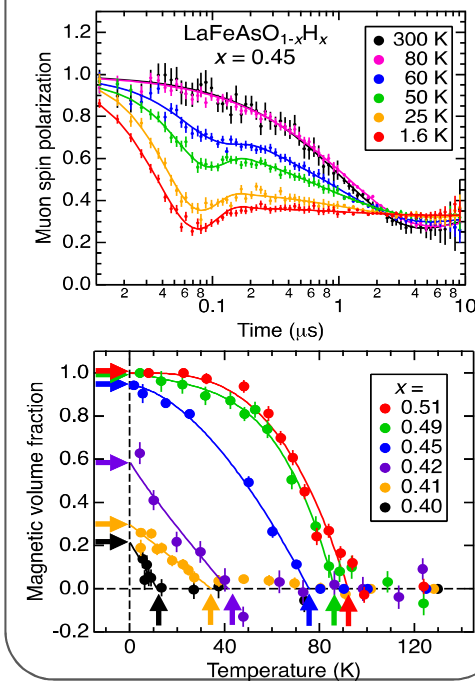
magnetic structure (neutron)



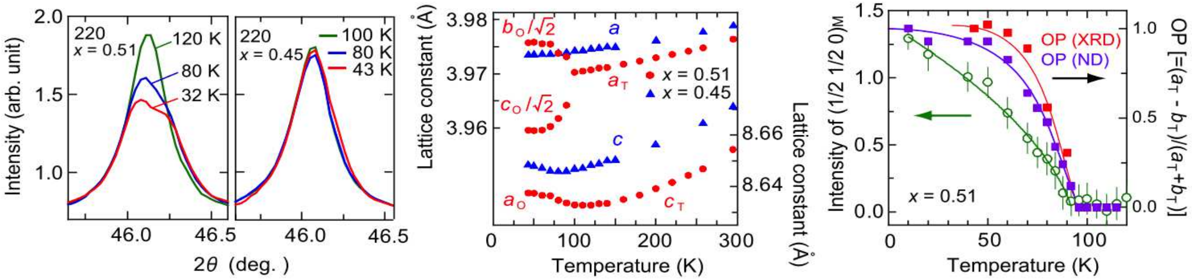
Structural and magnetic phase diagram of $LaFeAsO_{1-x}H_x$



magnetic phase diagram (muon)

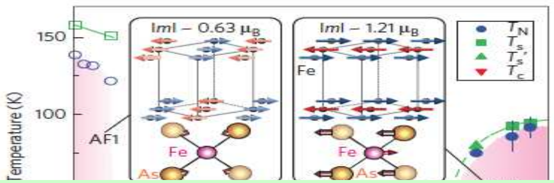


Crystal structure (X-ray)

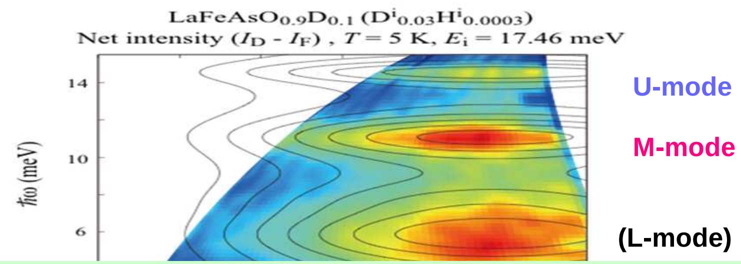


Nature Physics 10, 300 (2014).

Tunneling motion of hydrogen atom is highly influenced by conduction electrons



Tunneling excitations by neutron scattering



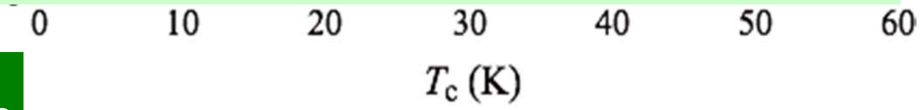
To summarize the multi-probe use in iron-based superconductor

Muon; discovered the second magnetic phase (AF2) and drew the overall mag. phase diagram

X-ray; discovered the structure phase transition above AF2 and determined atomic sifts at the transition

Neutron; determined the spin structure and superconducting gaps by the hydrogen tunneling spectra

The obtained information is very important to elucidate the relation between magnetism and superconductivity in this system



温度 T (K)

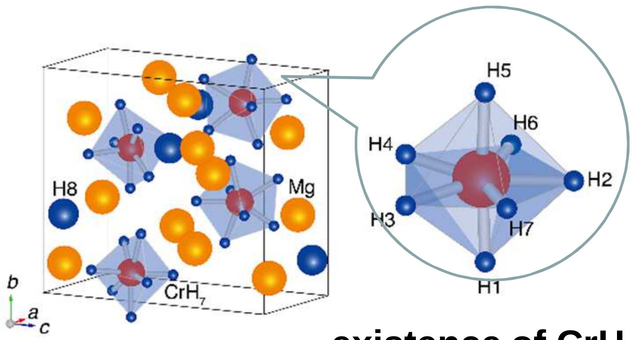
Tunneling excitation changes the spectra near the superconducting transition in the energy range close to the superconducting gaps Δ_1 and Δ_2

Neutron scattering plays a vital role to elucidate structural and vibrational state of hydrogen in matter

• Structural study for newly synthesized materials

Mg_3CrH_8

Successfully synthesized under 5 GPa at 700℃. Crystal structure determined by neutron turned out the identical one predicted by first principle calculation



existence of CrH_7 ion !

Courtesy : Orimo Gr. , Tohoku Univ.

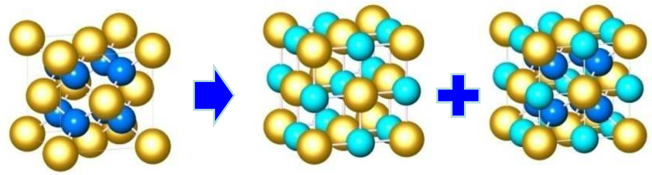
New hydrogen storage material or a candidate of new superconductor?

Collaboration ; Neutron + X-ray+ infra-red spectroscopy

S. Takagi et al., Angewandte Chemie, 54. 5650 (2015).

• Hydrogen behavior under high pressure

La-D



LaD_2 — LaD — $LaD_{2+\delta}$

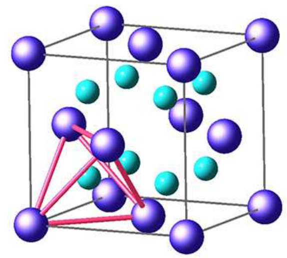
ambient pressure — beyond 11 GPa

Pressure induced phase separation into LaD and LaD_3

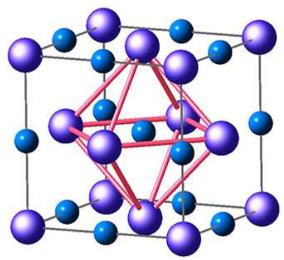
Collaboration ; Neutron + X-ray

A. Machida et al Phys. Rev. Lett., 108, 205501 (2012).

Fe-D



6.3GPa at 988 K
tetrahedral site only



7.4GPa at 300 K
octahedral site partially

Hydrogen site in Fe depends on pressure

Relation with hydrogen brittleness ?

A. Machida et al., Nat. Commun. 5, 5063 (2014).

SIP Cross-ministerial Strategic Innovation Promotion Program

Operated by the cabinet office.

Structural Materials for Innovation

SIP-SM4I Structural Materials for Innovation

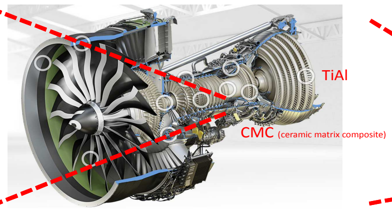
Ceramic-coated engine

Fiber Reinforced Plastics

robust against thermal shock etc.

Polymer & FRP

stress



New composite materials ; How to measure mesoscopic and macroscopic structures?

27 Japanese industries participate in this project

KEK takes a part in IMASM group of SMI(Structural Materials for Innovation)

IMASM (Innovative Measurement and Analysis for Structural Materials)

Synchrotron radiation in PF is utilized to measure target materials

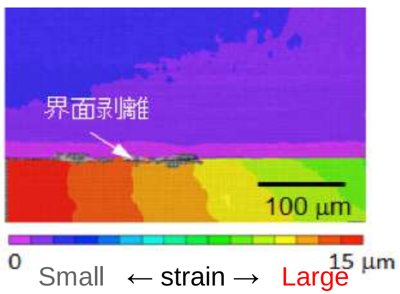
Elucidation of the failure mechanism of structure
-mechanism of crack initiation and propagation-

2D & 3D visualization of each factors by in situ measurements

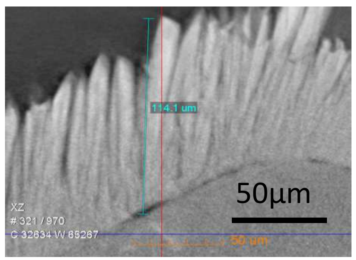
(a) Strain & Stress mapping

(b) Cracks imaging

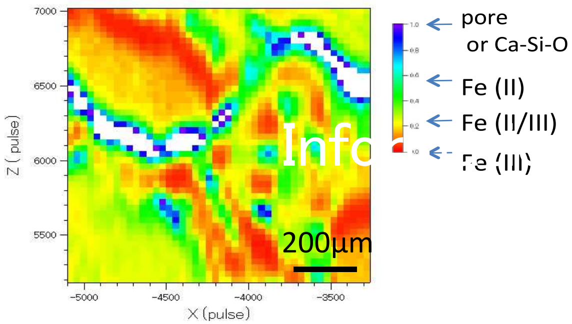
(c) Chemical-state mapping



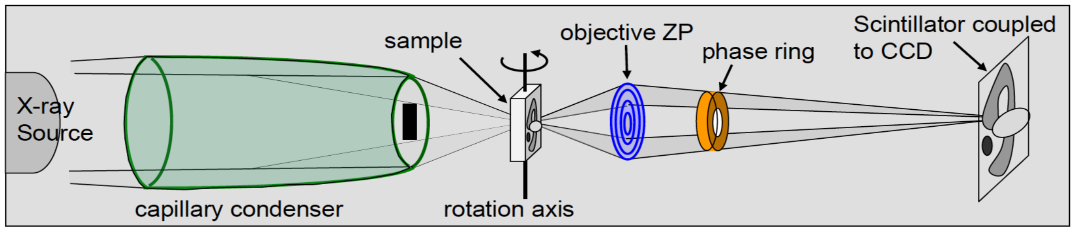
Moire method



X-CT



XAFS mapping



Construction has been started

XAFS-CT (X-ray Microscope)

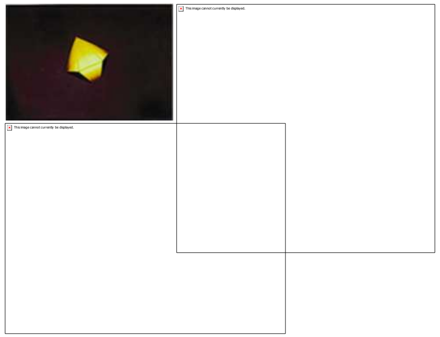
High throughput experiment on protein structure determination using a robot

—Drug discovery—

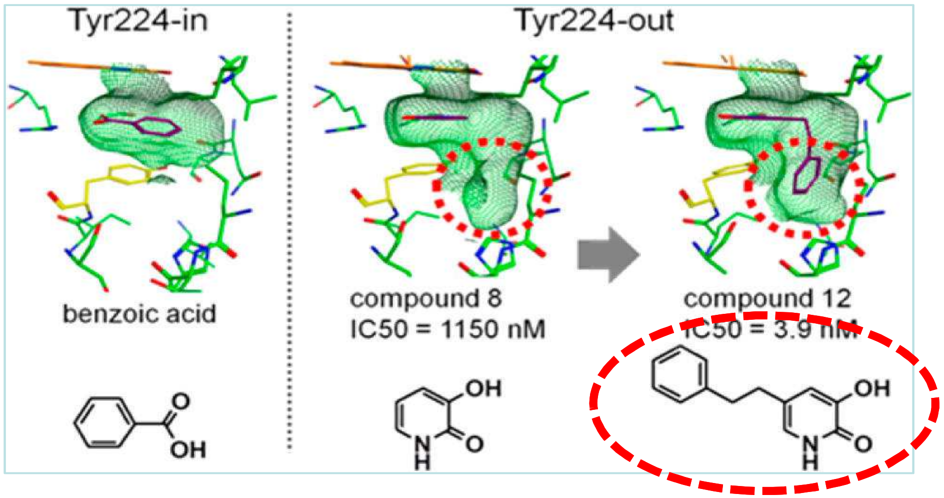
Development of a drug for schizophrenia (精神分裂病)

<Summary> Schizophrenia is a typical mental disorder, the major symptoms of which include hallucinations, delusions, autism, and apathy. IMSS established a beamline, NE3A, in PF for research funded by Astellas Pharma Inc. **Astellas Pharma Inc. has succeeded in the development of a therapeutic drug for schizophrenia by using the NE3A beamline in PF-AR.**

The high-throughput beamline NE3A constructed in PF-AR for research funded by Astellas Pharma Inc.



High-throughput measurement with an automated robot. NE3A shows one of the world's highest performance and can handle **350 data sets a day.**



A drug having a high medicinal effect was developed by modifying the structure of a molecule bound to a target protein. Modern drug discovery cannot be conducted without synchrotron radiation experiments. About 15 drug discovery companies are now using PF for advancing their drug discovery research.

<Impact on the society> The efficacy of this therapeutic drug for schizophrenia in clinical trial was demonstrated in a recently published report, and the drug has been receiving much attention. If the drug is introduced in the market, options available for drug treatment will increase, and the drug will contribute to the promotion of rehabilitation of schizophrenics.

How to make anticorrosive steel without painting

Synchrotron radiation analysis of rust on steel in the atmosphere

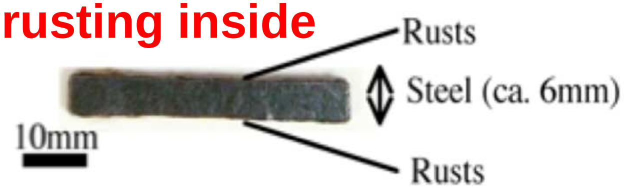
<Summary> The anticorrosive mechanism of steel materials that can be used when it has been kept unpainted for a long time under atmospheric environment was revealed by in situ observations (XAFS, XRD) with synchrotron radiation. It was discovered that the addition of a trace amount of metal elements produced *good rusts* that improve corrosion resistance. (Nippon Steel & Sumitomo Metal Corporation)

Good rust vs. bad rust (よい錆と悪い錆）

Steel left at the seashore for 9 years and sandwiched between rust layers (above and below).

Rusting mechanism of anticorrosive steel containing a trace amount of Ni (Ni-advanced weathering steel) was revealed by in situ observations with synchrotron radiation.

Good rust prevents rusting inside



Bad rust penetrates inside

Ni-advanced weathering steel: A protective layer with fine grains is formed at a surface layer, which can keep negative ions away and prevent further rust.

Conventional weathering steel: Steel materials rust because a protective layer is not formed.

<Impact on the society> The social and economic impacts of rust are not only in direct cost (approx. 3–4% of GNP) for countermeasures to deterioration and so on but also in the large indirect cost involved in breakdown, decline in efficiency, and decline in safety and reliability of infrastructure. The elucidation of a mechanism for improving the corrosion resistance of steel by this research will contribute to the reduction of such direct and indirect cost to maintain the safety and security of infrastructure.

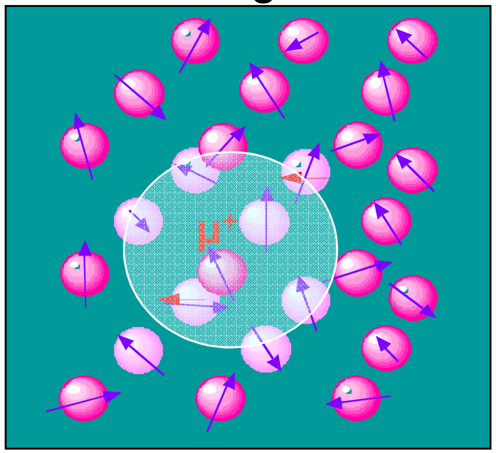
positive muon is a very sensitive probe for local magnetic field(LMF) in material

Origin of Local Magnetic Field

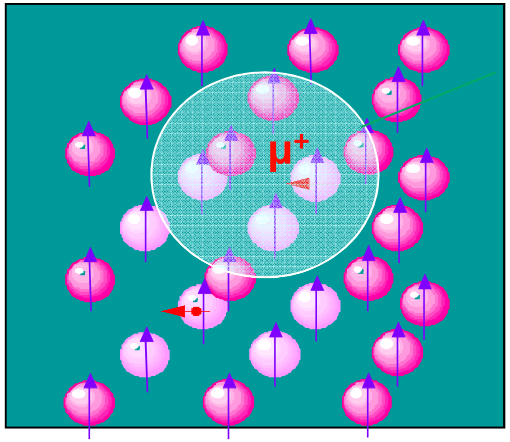
Information of LMF is detected by the time spectra and spatial distribution of emitted positron at the collapse of muon

Spins around muons in magnetic materials	Electrons around muons in materials
Study of magnetic state in materials	Study of hydrogen state in materials

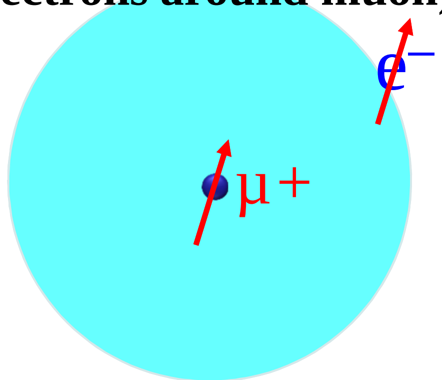
Paramagnetic



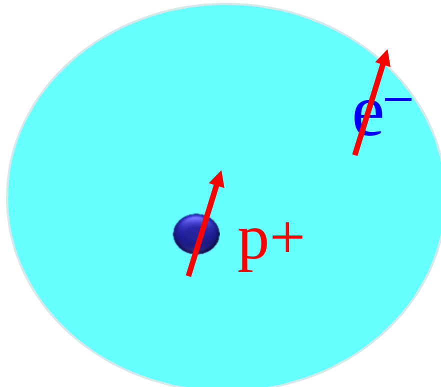
Ordered (ferromagnetic)



Muonium (Mu^0) behaves like hydrogen in materials (muon sensitively detects LMF from electrons around muon)



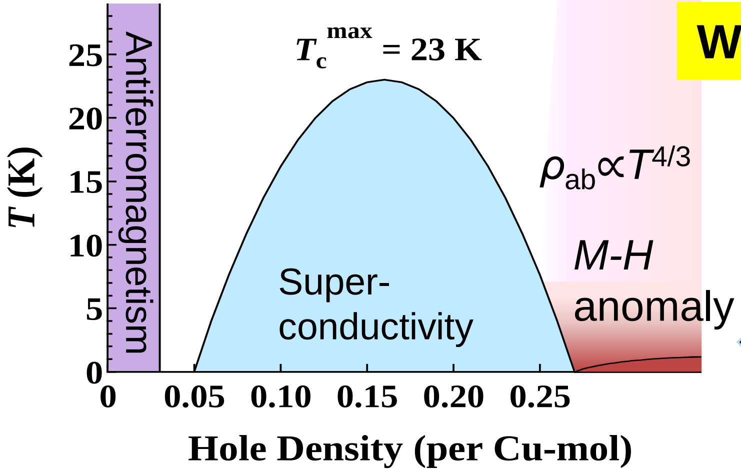
Muonium (Mu^0)



Hydrogen (H^0)

Possible ferromagnetic fluctuations in non-superconducting heavily overdoped Bi-2201 cuprate

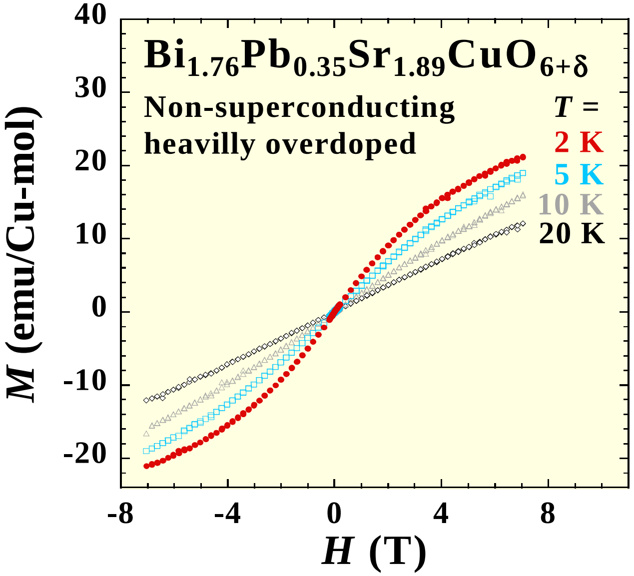
T. Adachi (Sophia U.), Y. Koike (Tohoku U.) G.

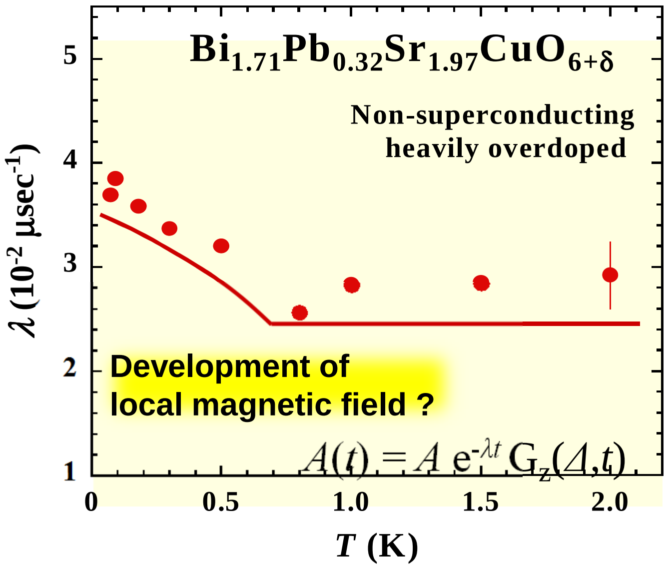


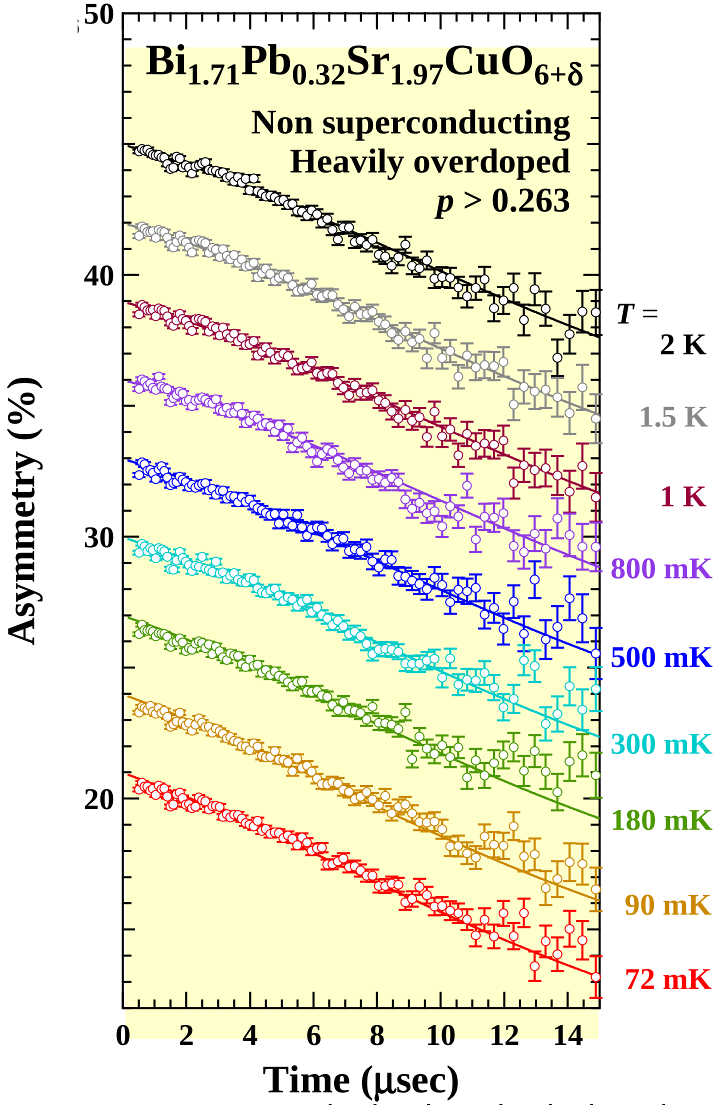
Why superconductivity disappears in overdoped region ?

Ferromagnetism destroys superconductivity ?
(Sonier et al)

Extreme sensitivity to local magnetic field much higher than magnetic neutron scattering







submitted to Physical Review B

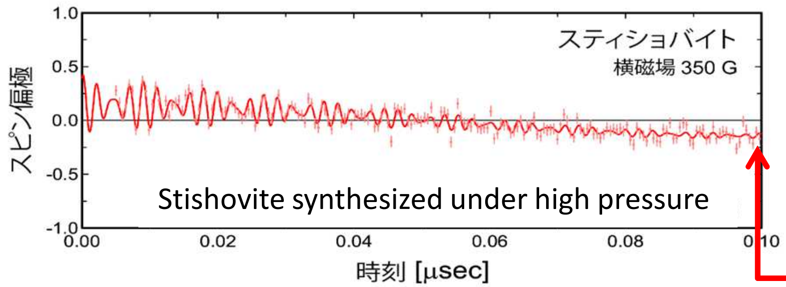
Muon can simulate hydrogen-sate in materials

Neutral Atomic Hydrogen in the Earth's Deep Mantle ?

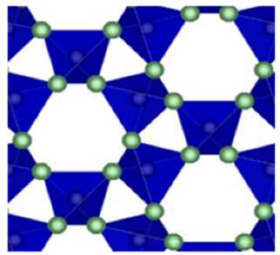
Potential impact on the model of hydrogen circulation mechanism in the Earth

◆ Implanted muon has been found to be in a neutral atomic state (“muonium”) in Stishovite (a high-pressure phase of SiO_2) that is present in the lower Mantle.

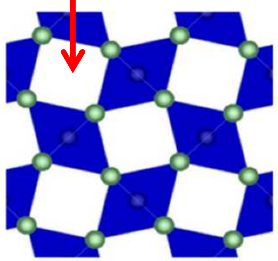
◆ Because implanted muon simulates electronic state of interstitial hydrogen in matter, the observation suggests that **hydrogen can exist as neutral atom at the interstitial sites in the lower mantle**, contrary to the current consensus that hydrogen would be present only as water (H^+ and OH^-) at substitution sites.

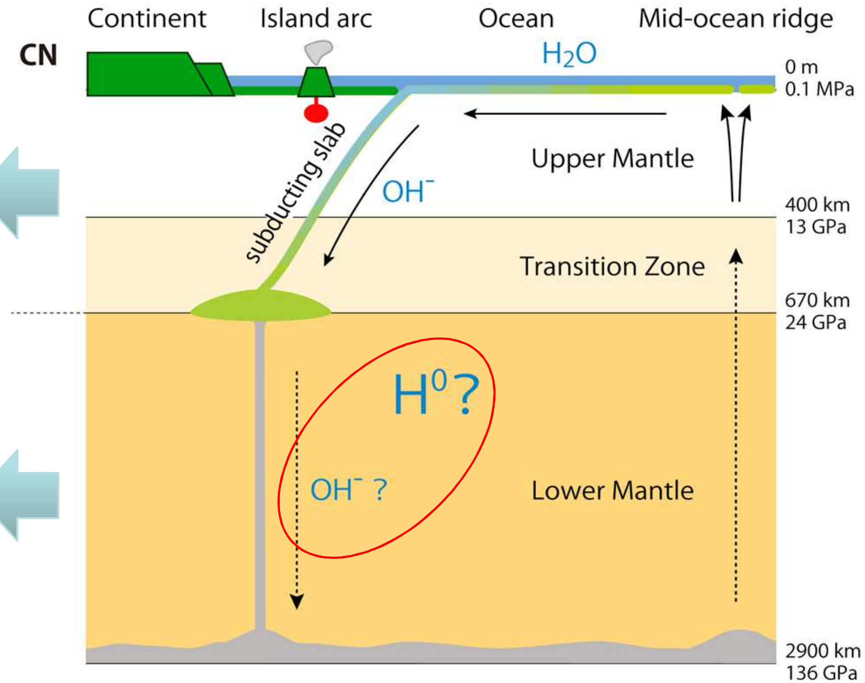


Quartz



Stishovite





SCIENTIFIC REPORTS

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Muonium in Stishovite: Implications for the Possible Existence of Neutral Atomic Hydrogen in the Earth's Deep Mantle

SUBJECT AREAS:
GEOPHYSICS
CONDENSED-MATTER PHYSICS

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Nobumasa Funamori[1], Kenji M. Kojima[2], Daisuke Wakabayashi[1], Tomoko Sato[3], Takashi Taniguchi[4], Norimasa Nishiyama[5]*, Tetsuo Irifune[5,6], Dai Tomono[7]†, Teiichiro Matsuzaki[7], Masanori Miyazaki[2], Masatoshi Hiraishi[2], Akihiro Koda[2] & Ryosuke Kadono[2]

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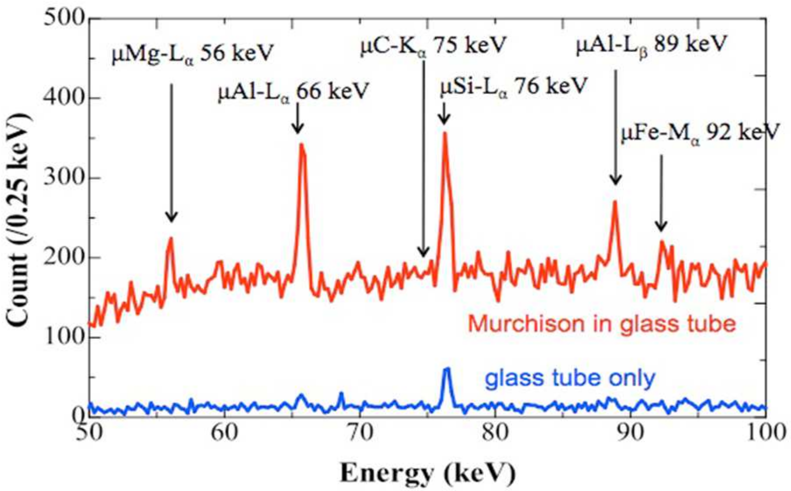
N. Funamori *et al.*, Scientific Reports **5**, 8437 (2015)

Non-destructive element analysis using muonic X-ray

Demonstration of bulk sensitive light-element-analysis on interstellar object

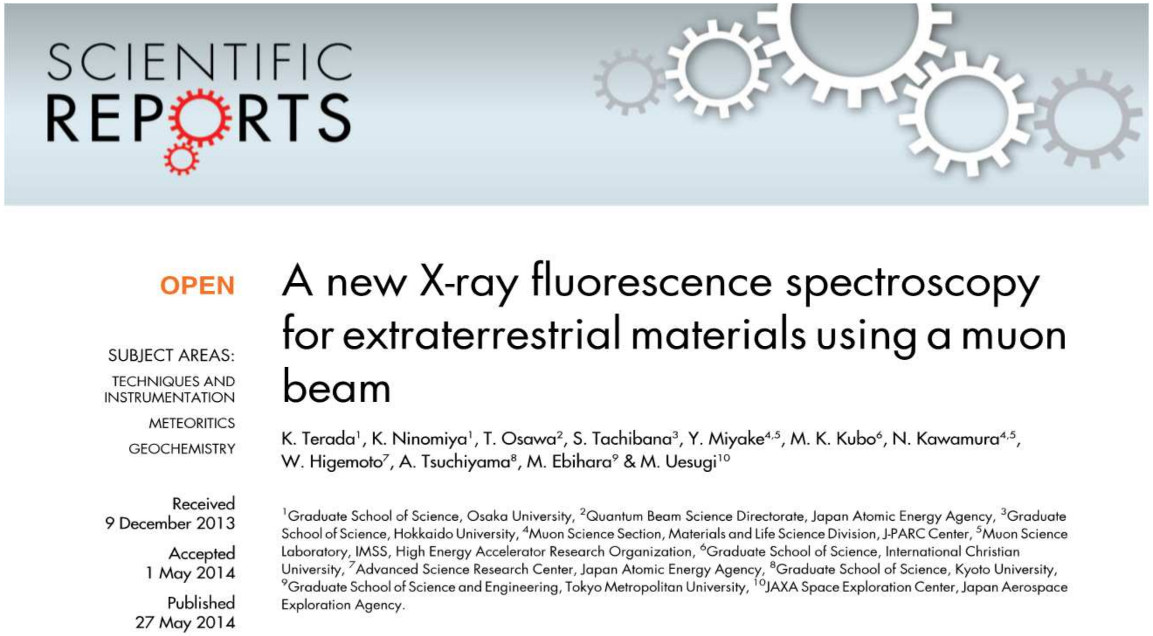


It is demonstrated on a carbon-rich meteorite that the element-specific muonic X-ray spectroscopy can provide information on the content of light elements deep within the specimen, paving a path to the application of the technique to the specimens brought back by the “Hyabusa II” mission in the future.

Because of mass difference emitted muonic X-ray from samples has much higher energies compared to electron.

↕

complementary to neutron-capture prompt γ-ray analysis



SCIENTIFIC REPORTS

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SUBJECT AREAS:
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METEORITICS
GEOCHEMISTRY

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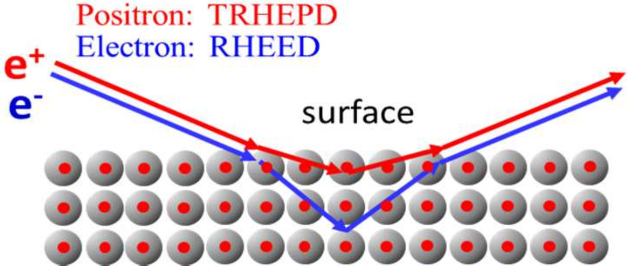
A new X-ray fluorescence spectroscopy for extraterrestrial materials using a muon beam

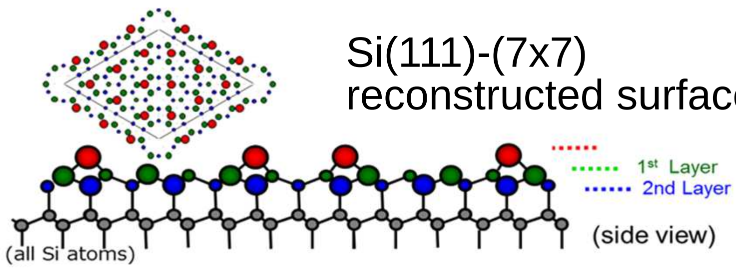
K. Terada[1], K. Ninomiya[1], T. Osawa[2], S. Tachibana[3], Y. Miyake[4,5], M. K. Kubo[6], N. Kawamura[4,5], W. Higemoto[7], A. Tsuchiyama[8], M. Ebihara[9] & M. Uesugi[10]

[1]Graduate School of Science, Osaka University, [2]Quantum Beam Science Directorate, Japan Atomic Energy Agency, [3]Graduate School of Science, Hokkaido University, [4]Muon Science Section, Materials and Life Science Division, J-PARC Center, [5]Muon Science Laboratory, IMSS, High Energy Accelerator Research Organization, [6]Graduate School of Science, International Christian University, [7]Advanced Science Research Center, Japan Atomic Energy Agency, [8]Graduate School of Science, Kyoto University, [9]Graduate School of Science and Engineering, Tokyo Metropolitan University, [10]JAXA Space Exploration Center, Japan Aerospace Exploration Agency.

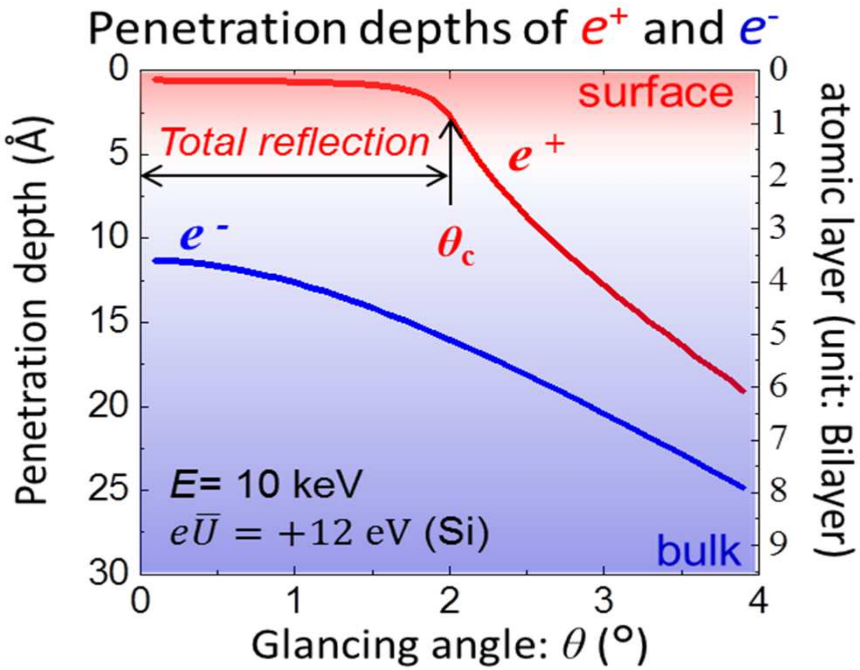
(3) Total-reflection high-energy positron diffraction (TRHEPD)

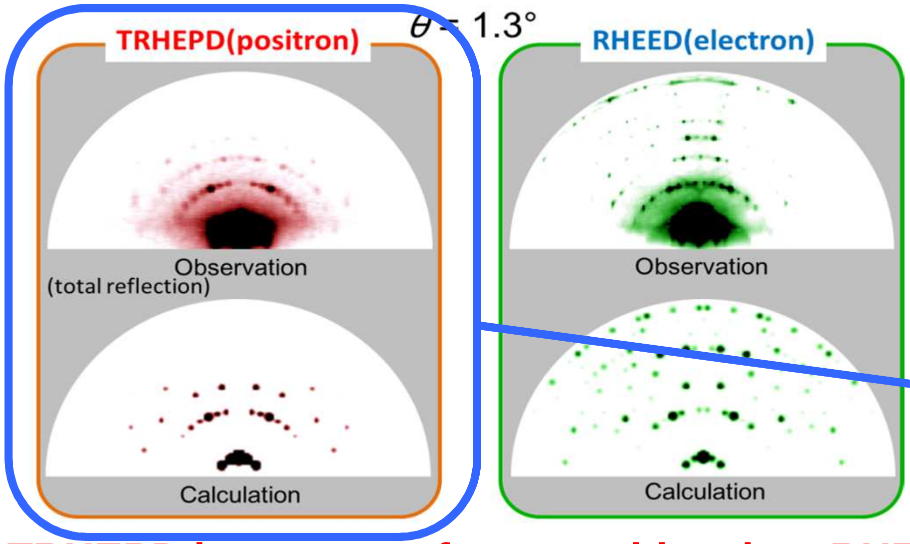
Surface sensitivity of TRHEPD



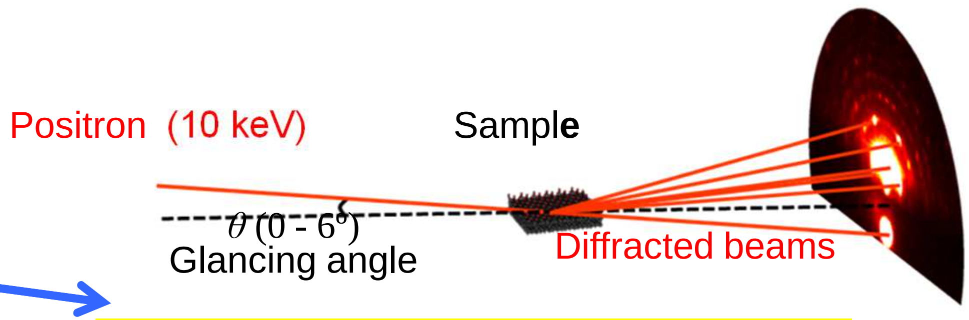


Si(111)-(7x7)
reconstructed surface





TRHEPD is more surface sensitive than RHEED.

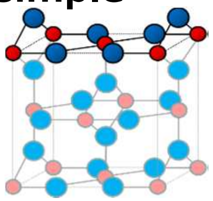


much better agreement with model calculation compared electron diffraction

Structure analysis of rutile-TiO_2(110)-(1×2) surface

Rutile-TiO_2(110)(1×1) surface is simple

● Ti ● O



already established (most stable)

annealing at ~1200K

Positron diffraction finally solved a 30 years long standing problem on the surface structure of TiO_2

Final model proposed by TRHEPD

double periodicity

double periodicity (1×2) appears

● Ti ● O

?

Many possible structures proposed.

No so far proposed structure explained TRHEPD data.

Missing-Row: 7.1 %
Ti_2O_3 4.6 %
Ti_3O_5 6.9 %
Ti_2O 5.3 %

???

Missing Row

Added Ti_2O_3

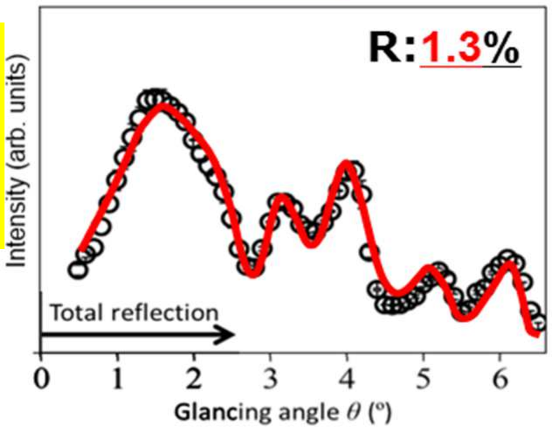
Added Row (Ti_3O_5)

Added Ti_2O

Probably, previous data taken by other method contain useless information inside the surface.

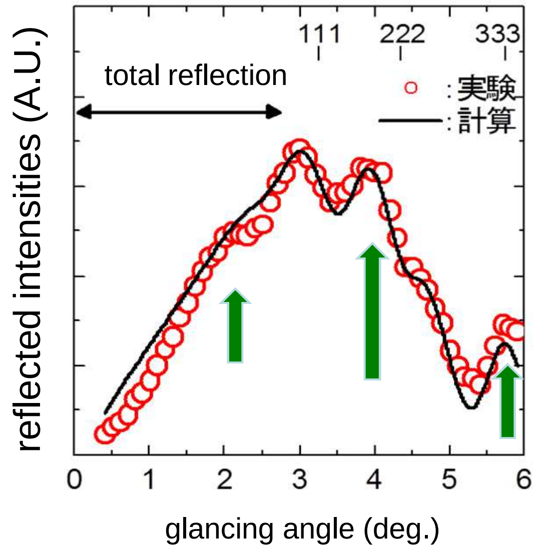
Newly proposed model reasonably reproduces the experimental data

One-beam analysis

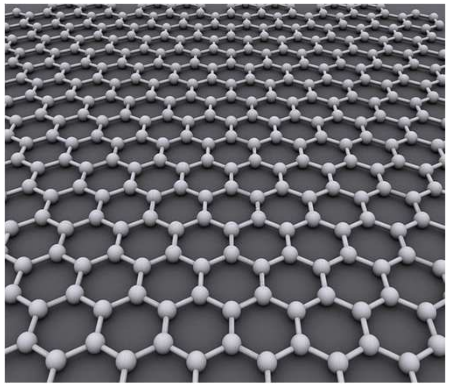


Graphene on metal substrate

graphene on Cu(111) substrate

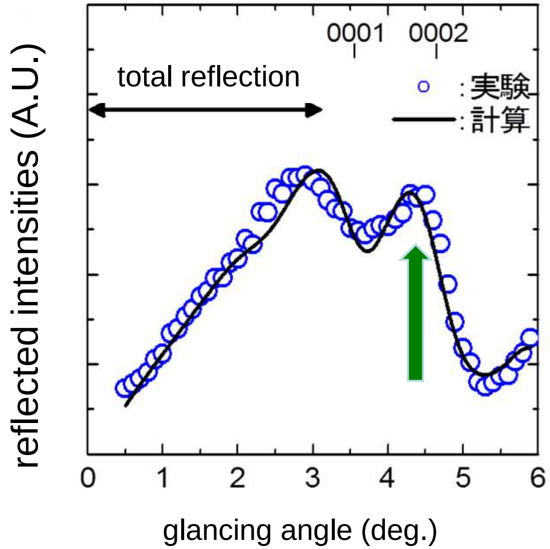


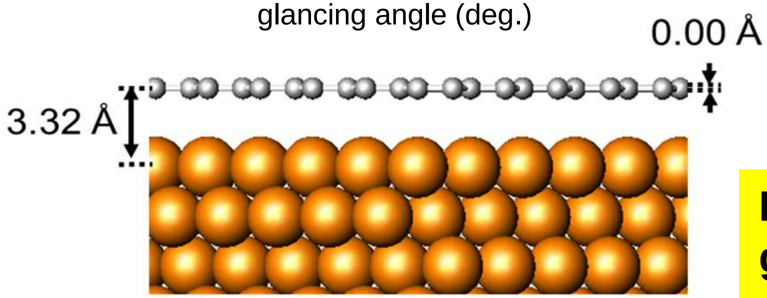
graphene



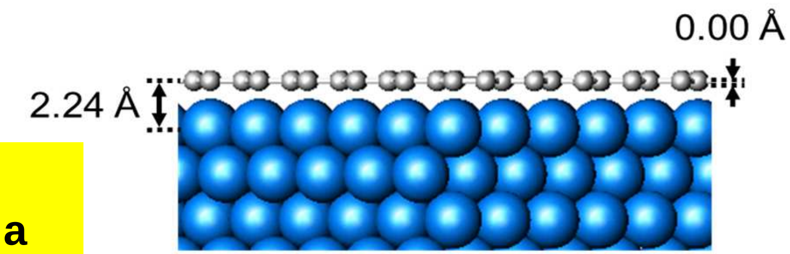
Wikipedia

graphene on Co(0001)substrate





Distance between a graphene sheet and a metal substitute can be determined by positron diffraction



Weak interaction with Cu substrate

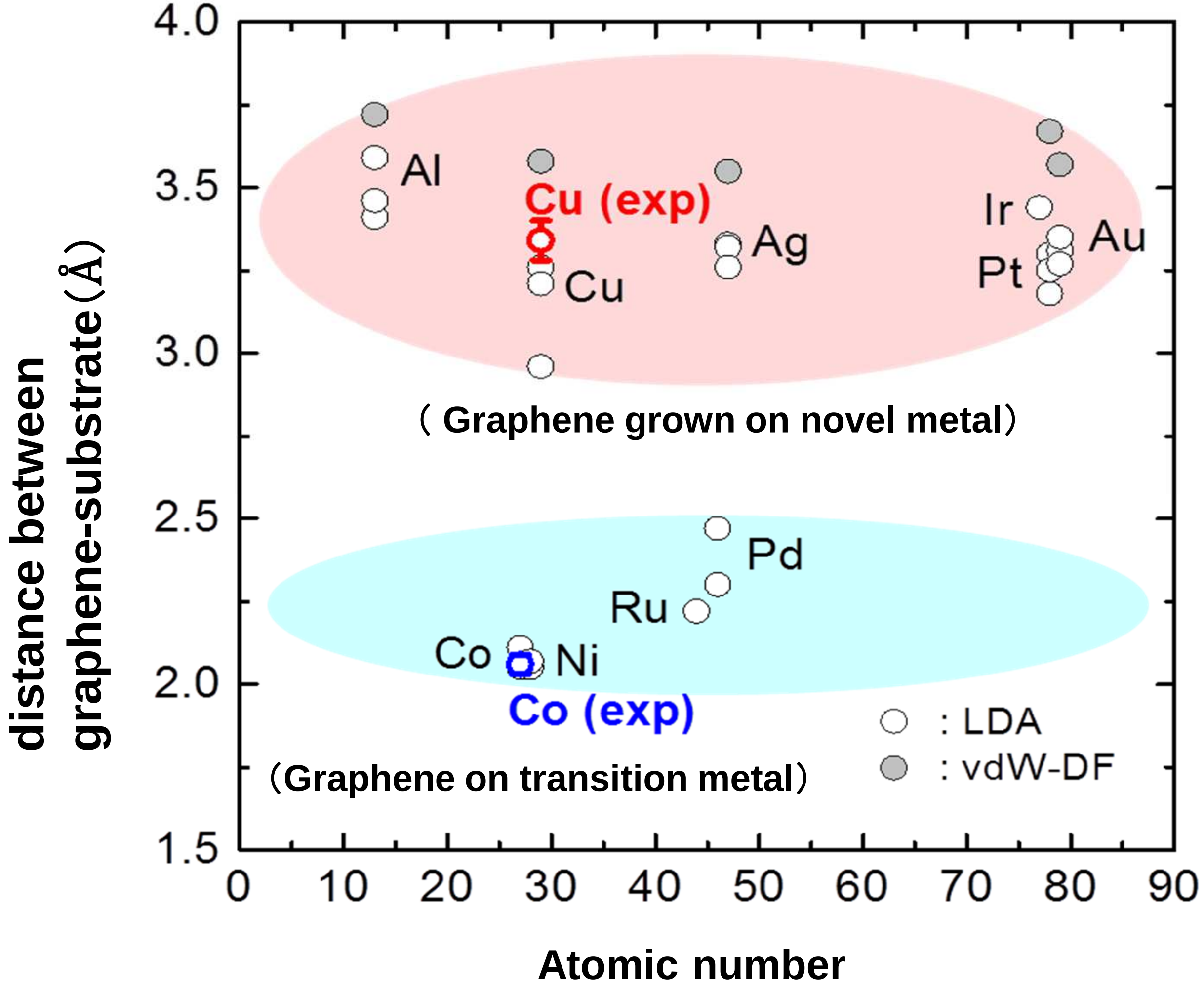
Interlayer distance of graphite is 3.35A

Strong interaction with Co substrate

Interaction exists through d-electrons

Graphene grown on metal substrate

Interlayer distance of graphite(3.35A)



Two groups depending on the interaction between carbon and metal

Nearly perfect agreement with theoretical value and experimental one

These data are important to synthesize electronic devices using graphene

Now and future of four probes (Personal prospect)

	Synchrotron	Neutron	Muon	Positron
Diffraction (static structure)	Charge scattering orbital ordering magnetic structure local structure	Nuclear and magnetic scattering	Charge scattering by re-acceleration of ultra-slow muon (Challenging) Magnetic scattering (More challenging)	Charge scattering surface structure Magnetic scattering (Challenging)
Local probe	Imaging (phase sensitive Local diffraction, spectroscopy (New facility)	Imaging Resonance absorption Local vibration Magnetic imaging	Local magnetic field Hydrogen state Element analysis by muonic X-**ray**	Positron annihilation Spin dependent positron annihilation
Inelastic scattering (dynamical structure)	Element-selective Charge excitation Magnetic excitation (New facility)	Magnetic excitation Lattice vibration Polarization analysis of pulsed beam	(Much more challenging)	Dynamics of surface structure (Much more challenging)

Summary (Material and life sciences in IMSS)

(1) IMSS has four quantum beam probes for material and life sciences, synchrotron radiation and slow positron in Tsukuba campus, neutron and muon in Tokai campus. More than 50 beam lines for these probes accept users ~3200/year.

(2) Synchrotron facilities (PF, PF-AR) are still active as the second biggest synchrotron facility in Japan with timely upgrade of beam lines and accelerator. However, in order to make a quantum jump in research as well as user program, a new facility is indispensable. A future plan for a storage ring-type synchrotron facility is considered. We have to learn a lot from PETRA project.

(3) Two beam lines of spin-echo and chopper spectrometer utilizing of polarized neutron beams will accept user program in JFY2016.

(4) First ultra cold muon beam was observed in U-line.

(5) Selected scientific outputs and outcome including multi-probe use and hydrogen and industrial application are introduced.

(6) Strategic utilization of four probes in future is summarized.

Thank you for your attention