#### International Centre for Diffraction Data TECHNICAL COMMITTEE MEETING MINUTES

Thursday, 17 March 2016 9:00 a.m.-12:30 p.m. Matteo Leoni, Chairman

- 1. Call to Order and Opening Remarks Matteo Leoni
- 2. Roll Call and Attendance
- 3. Additions and/or Deletions to the Agenda Matteo Leoni
- 4. Approval of the 2015 Minutes Matteo Leoni
  - **Motion 1:** Wallace moved to approve the 2015 Technical Committee Meeting minutes. *Moton passed unanimously.*
- 5. Reports/Presentations of Technical Regional Co-Chairs and International Guests
  - A. China Xiaolong Chen
  - B. Eastern Pacific Rim Takashi Ida
  - C. European Community Matteo Leoni
  - D. India T.N. Guru Row
  - E. Indian Ocean Rim Vanessa Peterson
  - F. Newly Independent States Evgeny Antipov
  - G. North America John Anzelmo

Break: 10:35

- H. South America Miguel Delgado
- I. United Kingdom and Ireland David Rendle
- 6. Subcommittee Reports and Motions
  - A. Materials
    - 1) Ceramics Winnie Wong-Ng No motions.
    - 2) Metals and Alloys Pete Wallace
  - **Motion 2:** The Metals and Alloys Subcommittee recommends to the Technical Committee that the M&A mission statement be changed as follows:

The Metals and Alloys Subcommittee shall be responsible for (1) assuring that the metals and alloys subfile meets present and future needs of metallurgists and materials scientists, (2) developing and updating the metals and alloys subfile, (3) editing metals and alloys data and products to ensure a high standard of quality, (4) extending the coverage and usefulness of the metals and alloys subfile, and (5) maintaining a web page on the ICDD site to communicate with members and other materials scientists.

Wallace moved. - Motion passesd unanimously.

**Motion 3:** The Metals & Alloys Subcommittee recommends to the Technical Committee that the Board of Directors implement BoD Motion 315-17E(2)(b) in the 2017 product.

The text of the *prior motion* and the *response* follow:

**BoD 315-17E(2)(b)** 7: Leoni recommended to the Board of Directors that the *M&A Standard empirical formula, space group, Z, Wyckoff sequence* be made available to PDF4+ users.

Note: M&A Standards are based upon the accepted Linus Pauling File (LPF) prototype structure for each material.

**Response:** Database Department - Access to these items are available to the M&A task groups today. For the general PDF-4 user, we would need to build specialty tables for this

information and make them available for display using special "Preferences" options. We have questions in deciding the priority of putting these tables in the PDF-4 database. Wallace moved. – **Motion passed unanimously.** 

3) Micro and Meso - Sue Quick – No motions.

Quick commented that headquarters' staff wants to be provided a good definition of MOFs and other porous materials; this is separate from the zeolite definitions. Speakman would like to put together a task group to review and evaluate the patterns of the meso porous materials and MOFs. Please contact Speakman if anyone would like to join the task group.

4) Minerals - Andy Roberts - No motions.

There was a motion within the subcommittee, however this request has already been implemented by headquarters and will be available in the 2016 database.

*The motion was:* 

The Minerals Subcommittee recommends to the Technical Committee that within the Mineral Name field, the first letter of all mineral names in all databases be capitalized. Presently, it is a mixture of uppercase and lowercase mineral names.

Note: All mineral names within the 00 (experimental) are capitalized. This would provide consistency across all databases that contain a Mineral Name field.

5) Organic and Pharmaceutical - Fred Wireko - No motions. Wireko discussed the following action items:

Action item #1 – Headquarters to further explore a way to transform current ICDD organic data format into the International Chemical Identifier (InChI) format, and recruited Wong-Ng to help with this endeavor.

Action item #2 – Supply list of excipients. The list is extensive now, from a pharmaceutical side, but headquarters does not necessarily have those materials of powder patterns for all of them. There will be an FTP website with a full excipient list, and it is requested that data, references, and samples (legal and/or non-toxic) that are missing, be added to the list.

Action item #3 – There has been a subclass of narcotics and psychotropic materials that headquarters has been populating. We need more people in the organic field to continue populating that subclass.

Action item #4 - Rendle and Dann have completed their list on inorganic materials, and it has been sent to Kabekkodu.

6) Polymers - Lizhi Liu – No motions.

There was discussion that despite polymers being a fast growing area for the database, there is concern we are losing contact with key members of the polymer community because companies don't want their top polymer scientists sharing information. There is a need to figure out a way to achieve better involvement from scientists working in the polymer field.

#### B. Characterization Methods and Tools

1) Electron Diffraction - Bryan Wheaton - No motions.

Action item: Electron diffraction continues to be the most downloaded tutorials, and Fawcett showed statistics that we aren't reaching even half of the people that we could be. Perhaps put together a group of power users from EBSD & TM Electron Diffraction, and meet with ICDD staff to show what's currently capable, and also educate the staff on how would they use our database.

2) Non-Ambient Diffraction - Andrew Payzant — No motions.

Payzant discussed that ideas should be explored for DXC meeting/workshop on best practices to collect high temperature data. Communication needs to be enhanced between the subcommittee and ICDD. First telecom meeting coming in September. With non-ambient being a fast growing field, the ICDD Grant-in-Aid program should strategically target

specific grantees working in non-ambient fields to acquire new patterns.

3) Synchrotron & Neutron Scattering Methods - Pamela Whitfield – No motions. There were two motions, but they have already been completed by headquarters.

Whitfield discussed that there is a need on how authors can submit TOF data as opposed to D-I lists. TOF data being added to database will make users happy.

- 4) X-ray Diffraction Methods Chris Gilmore
- Motion 4: The X-ray Diffraction Methods Subcommittee recommends to the Technical Committee that Gilmore be given a license for the PDF-4+ database so that he can work with the Metals and Alloys Task Group to implement cluster analysis with a report to be presented at the March 2017 meeting.

  Faber moved. 31 Yes, 0 No. 1 Abstain (Gilmore by name) Motion passed.
- **Motion 5:** The X-ray Diffraction Methods Subcommittee recommends to the Technical Committee that user-definable equations and robust regression be implemented in PDF-4 products. Gilmore moved. 35 Yes, 0 No, 1 Abstain (Fawcett by name) Motion passed.
  - 5) X-ray Fluorescence Mark Rodriguez
- **Motion 6:** The XRF Subcommittee recommends to the Technical Committee to develop a figure of merit algorithm for XRF data to be used for phase identification. Rodriguez moved. *Motion passed unanimously.*
- Motion 7: The XRF Subcommittee recommends to the Technical committee that a Fundamental Parameters (FP) database for XRF analysis be established using the currently existing "Elam FP database." This newly created database would serve as a baseline repository to archive and incrementally enhance FP data for the purposes of improving quantification for XRF users, equipment manufacturers, and future ICDD projects requiring accurate FP tabulations. Rodriguez moved. *Motion passed unanimously*.

TBlanton asked if Elam has the rights to name the database, or give us the database, as he created it during his employment. The issue needs to be explored further by the subcommittee.

#### C. ICDD Activities

1) Education - Carlo Segre - No motions.

Segre stated Maguire reported the number of registrants was down for last year's DXC compared to meeting the year before, despite that it was a joint conference with the TXF. This year's DXC, being held in Chicago, has over 100 more abstracts submitted than in the past.

Kottenhahn reported on web presence; that more tutorials will be placed on the website and YouTube. We encourage headquarters to post more tutorials.

- 2) PDF Editorial Staff Soorya Kabekkodu
- Motion 8: The PDF Editorial Staff recommends to the Technical Committee that the Star (\*) and Rietveld (R) quality marks are merged into Star (\*) quality mark. Kabekkodu moved. *Motion passed unanimously*.
- 7. New Business Matteo Leoni
- 8. Adjournment

## Regional Report from China

## Xiaolong Chen

Beijing National Laboratory for Condensed Mater Physics And Institute of Physics, Chinese Academy of Sciences

17 March 2016, Philadelaphia

## **Contents**

- Regional activities in China
- New advanced x-ray facility in China

## Regional Activities in China

## 12th National conference on powder diffraction and ICDD workshop



>300 attendees

Mianyang, Sichuan Prov., Oct. 26<sup>th</sup>-Oct.29<sup>th</sup>, 2015



## **Snapshots of ICDD Workshop**



27th Oct. 2015











#### ONE DAY PXRD SCHOOL, 26th Oct. 2015





#### **Organizer & Instructors:**

Prof. Cong Wang, Beihang University, China

Prof. Quanlin Liu, The University of Science and Technology Beijing, China

Prof. Meng He, The National Center for Nanoscience and Technology, China

Prof. Zhenhong Mai, Institute of physics, CAS, China

Prof. Yandong Wang, The University of Science and Technology Beijing, China

Prof. Pengcheng Zhang, Chinese academy of engineering physics, China





Local ICDD member meeting was held at the Changhong Hotel, Mianyang, China in 28<sup>th</sup> Oct. 2015.



#### ICDD Awards, 29th Oct. 2015







3 Best presentation awards.5 Best poster awards.







## Additional Activities in 2015 Technical Committee Meeting 2015



285 attendees
142 abstracts

18th National conference on residual stresses and workshop on X-ray stress determination

Chengdu, Sichuan Prov., Oct. 28-Nov.2, 2015

## **Forthcoming Events**

# 6<sup>th</sup> National Conference of Chinese Crystal Society

Place: Guangzhou, China

Time: November, 2016

## New Advanced X-ray Facility in China

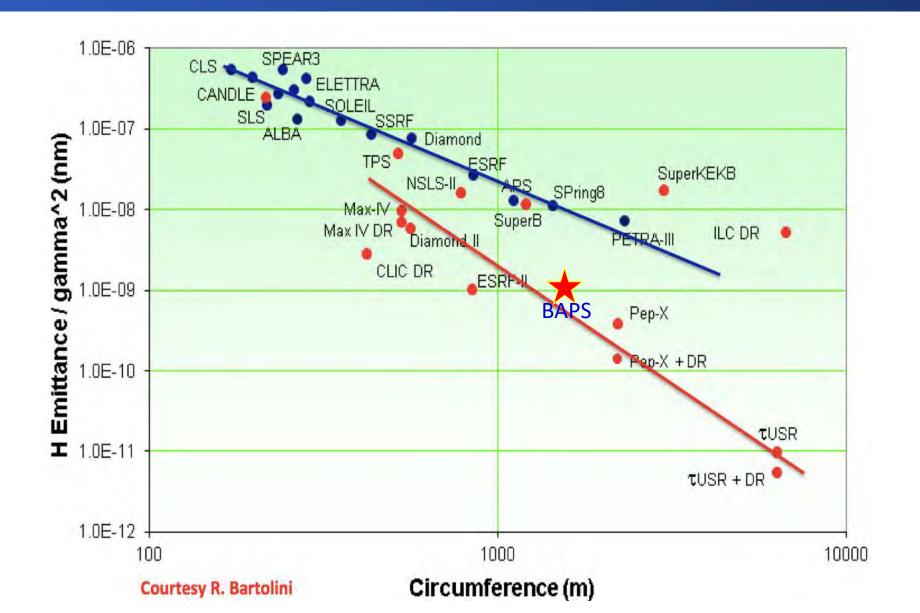
# New Facility: Beijing Advanced Photon Source (BAPS)

- High energy X-ray (50-300 keV)
- nm focus beam
- ps time resolution
- meV energy resolution

- 6GeV 1300m-length storage ring
- 250MeV LINAC
- 300m-length booster
- MBA (7) lattice



## Emittance vs circumference



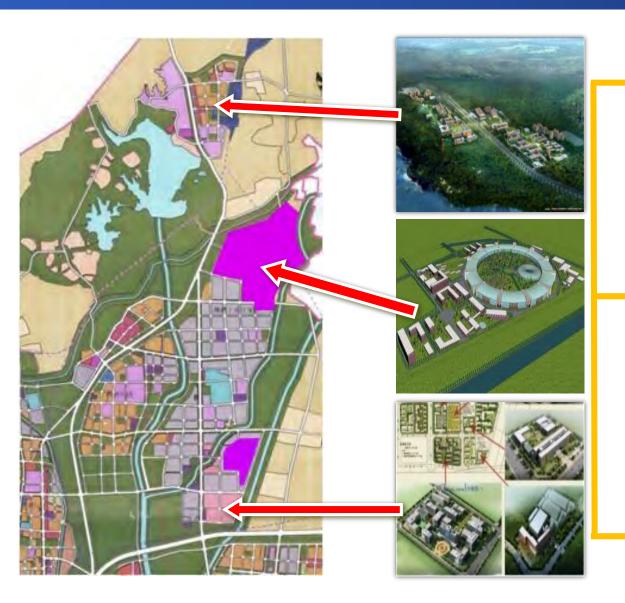
## BAPS construction plan

- ➤ Two-step construction
  - >2016-2018, R&D and testing facility (300M RMB)
  - ≥2018-2023, real facility (~4B RMB)
- > Future possibilities: ERL & FEL

### Location of BASIC (Huairou District, 65 km from IOP, 50 km from BJA)



## Presence of CAS in Huairou District



CAS University (215 acres)

"BASIC" campus (555 acres)

Tech-transfer campus (217 acres)

## BASIC floor plan (first draften lical Committee Meeting Page 20 of 144

变电站

次入口

北部边界

以高压线中心线向南退25m

以距离最近的

高压线中心线

向西退25m

次入口

东部边界

(110KV变电站

新丰村拆迁

安置选址

次入口

牤牛河中心线

#### 方案

#### **总平面图 规划用地范围 3373亩** 🚉 🚾 🚾

#### A-高能所·同步光源

A1-X射线光学实验室

A2-光束线运行实验室(二期) A3-计算中心(二期)

A4-低温超导技术及超导高频 腔技术实验室

A5-磁铁、电源实验楼

A6-束测控制实验楼

A7-超高真空及精密机械实验楼

A8-高功率实验室

A9-精密机械加工车间

A10-HEPS运行维护管理大楼 A11-BAPS运行维护管理大楼

#### B-物理所·综合极端条件实验

B1-物性表征楼 B2-STM楼 B3-超快TEM楼 B4-量子调控楼

B5a-超快激光楼 B5b-超快激光楼 B6-技术楼 B7-公共实验楼 B8-低温中心 B9-用户楼

B10-地下车库及 人防(独立)

#### 系统数值模拟器

C2-高性能计算机房

C3-用户楼

C4-地下车库及人防 (整体开挖)

C5-预留建筑

#### D-生态环境研究中心·大气环境模拟系统

#### E-生物物理研究所·国家生物医学中心

F1-清洁能源材料研发与测试(交叉研究平台)

F2-材料基因组(交叉研究平台)

F3-生物成像(交叉研究平台)

F4-环境污染控制研究(交叉研究平台)

F5-加速器 (交叉研究平台)

F6-科技服务网络中心

F7-科研综合体

F8-科研配套服务设施

F9-研究生公寓

G1-会议中心

G2-食堂

G3-学生宿舍



C-大气所·地球

C1-数据分析中心

中期预留





G4-用户楼

中国院·城市规划设计研究中心

## New synchrotron facilities in the world

Name	Country	Main parameters	Time	Notes
NSLS-II	US	3.0GeV/1000pm·rad 792m, DBA	2009 started 2014 finished	new
MAX IV	Sweden	3.0GeV/330pm·rad 528m, 7BA	2010 started 2016 finish	new
APS-U	US	6.0GeV/147pm·rad ~1100m,7BA	2014 R&D 2016 CD1	rebuild
ESRF-U II	EU	6.0GeV/130pm·rad 860m, 7BA	2015 phase I	upgrade
SPring-8- II	Japan	6.0GeV/149pm·rad ~1400m,6BA	2022-23	upgrade
ALS-U	US	2.0GeV/50-100pm·rad ~200m, 9BA	2023-24	rebuild

## Design II: ESRF-type 7BA, 6 GeV, ~1.3 km, ~50 pm

parameters	value	Units
Beam energy E <sub>0</sub>	6	GeV
Beam current I <sub>0</sub>	200	mA
Bunch number n <sub>B</sub>	2000	
Circumference	1296.14	m
Horizontal damping partition number $J_x/J_y/J_z$	2.05/1./0.95	
Natural emittance	48.3	pm
Working point (x/y/z)	113,14/41.18/0.003	
Natural chromaticity (x/y)	-143.6/-167.4	
Number of 7BA achromats	48	
Number of low-beta 6-m ID sections	48	
Beta functions in low-beta straight section (x/y)	7.9/2.8	m
Damping times $(x/y/z)$	15.9/26.6.0/21.7	ms
Energy loss per turn, U <sub>0</sub>	1.95	MeV
Energy spread $\sigma_8$	0.00091	
Momentum compaction	3.8×10 <sup>-5</sup>	
RF voltage, Vet	4.5	MV
RF frequency, f <sub>rf</sub>	499.6	MHz
Harmonic number	2160	
Natural bunch length o,	2.4	mm

## Design I: MAXIV-type lattice, 6 GeV, ~1.3 km, Page 90 4 pm

parameters	value	Units
Beam energy E <sub>0</sub>	6	GeV
Beam current I <sub>0</sub>	200	mA
Bunch number n <sub>B</sub>	2000	
Circumference	1294.2	m
Horizontal damping partition number $J_x/J_y/J_z$	2.05/1./0.95	
Natural emittance	88 (61)	pm
Working point (x/y/z)	93.14/49.40/0.0058	
Natural chromaticity (x/y)	-112/-107	
Number of 7BA achromats	44	
Number of high-beta 10-m injection sections	2	
Beta functions in high-beta injection section (x/y)	90/30	m
Number of low-beta 5-m ID sections	42	
Beta functions in low-beta straight section (x/y)	10/3	m
Damping times (x/y/z)	11.2/23.0/24.3	ms
Energy loss per turn, U <sub>0</sub>	2.25	MeV
Energy spread $\sigma_{\delta}$	0.001	
Momentum compaction	5.9×10-5	
RF voltage, Va	10	MY
RF frequency, f <sub>rf</sub>	500.36	MHz
Harmonic number	2160	
Natural bunch length o,	2,2	mm

## Selected Research Activities

## What we do

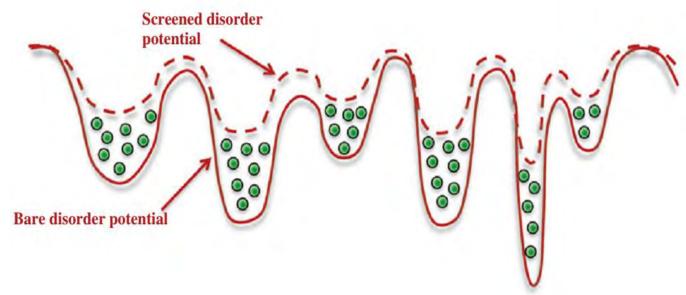
#### **Basic research**

# New compounds, new structure and new physics x-ray, neutron diffractions, Superconductors, Strong-correlated systems topological insulators

#### **Applied research**

- 1. SiC crystal growth
- 2. AlN crystal growth

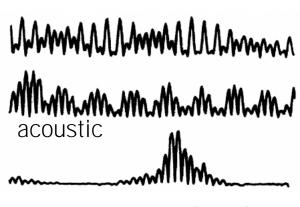
## Concept of Anderson localization 144





Nobel Prize in Physics 1977 P. W. Anderson, Sir N. F. Mott, J. H. van Vleck

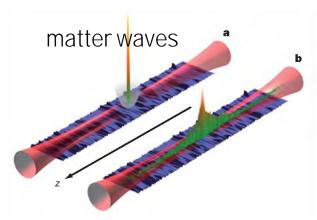
## Anderson localization of quasiparticles



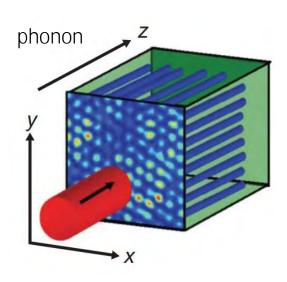
PRL 57, 3171 (1986)



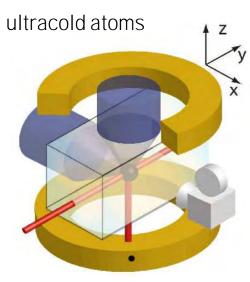
Nat. Phys. 4, 945 (2008)



Nature 453, 891 (2008)

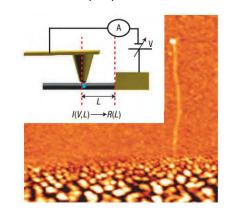


Nature 404, 850-853 (2000) Nature 446, 52-55 (2007)



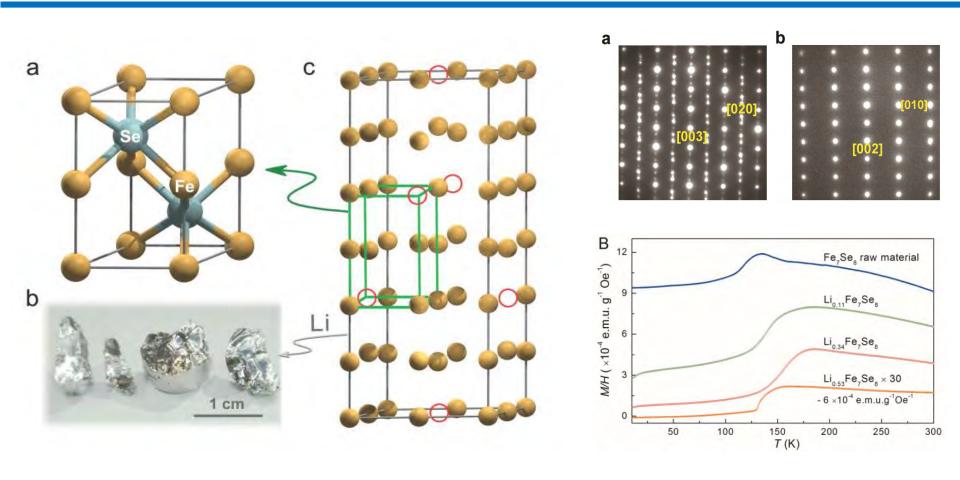
Science 334, 66-68 (2011) Nat. Phys. 8, 398-403 (2012)

electron (1D)



Nature 418, 955-959 (2002) Nat. Mater. 4, 534-539 (2005) Science 310, 289-291 (2005)

# Anderson localization of electrons of single crystals - LixFe<sub>7</sub>Se<sub>8</sub>

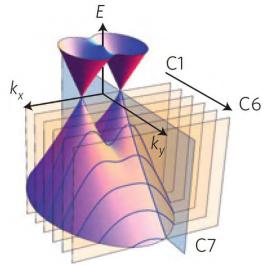


Crystal structure of  $Fe_7Se_8$ ,  $Li_xFe_7Se_8$ , and optical photograph of single crystals. The randomness due to Fe sites occupation is verified to exist.

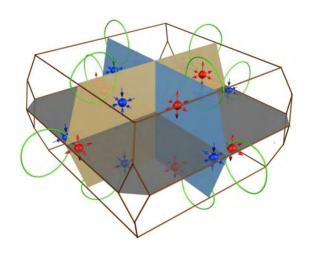
# Single crystal growth of Weyl Page 29 of 144 semimetal TaAs



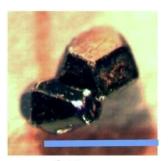
Discovery of semimetal TaAs has been listed as Breakthrough of the year.



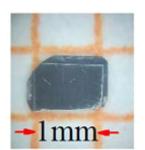
Lv, B. Q. et. al. Nat. Phys. 2015, 11, 724.



Weng, H. et. al. Phys. Rev. X 2015, 5, 011029.



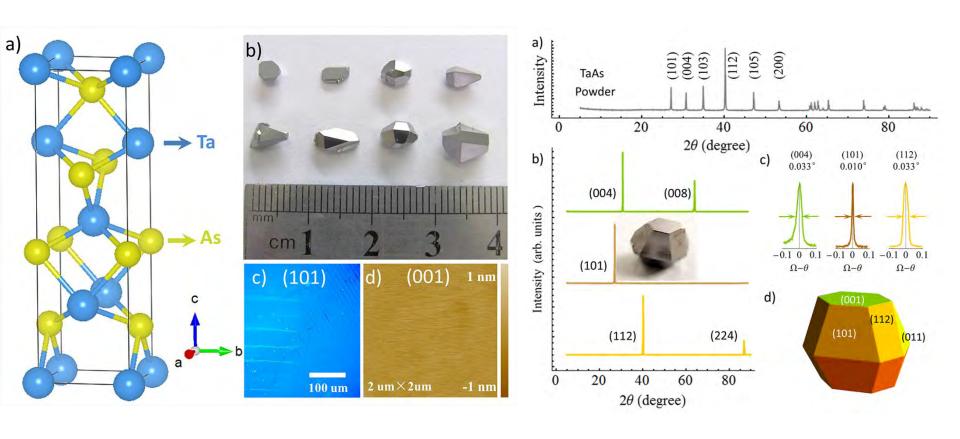
0.5 mm



Huang, S. M. et. al. Nat. Commun. **2015**, 6, 7373.

Huang, X. et. al. Phys. Rev. X 2015, 5, 031023.

# Single crystal growth of Wey Page 30 of 144 semimetal TaAs



**Crystal structure and single crystals of TaAs** 

Powder diffraction and rocking curves of TaAs

# That Its

## Overview of our research

#### Research team

Staffs: 7

**Students: 26** 



Xiaolong Chen



Jingkui liang



Liwei Guo



Yanping Xu



Wenjun Wang



**Gang Wang** 

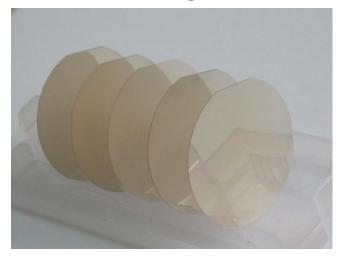


**Shifeng Jin** 

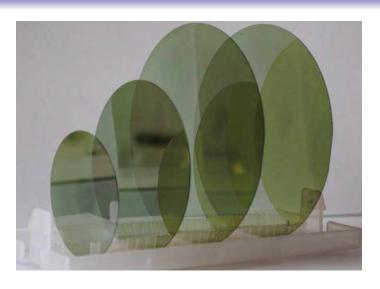
## SiC Crystal Mass Production Page 33 of 144



**Conducting 6H-SiC** 



**Semi-insulating 6H-SiC** 

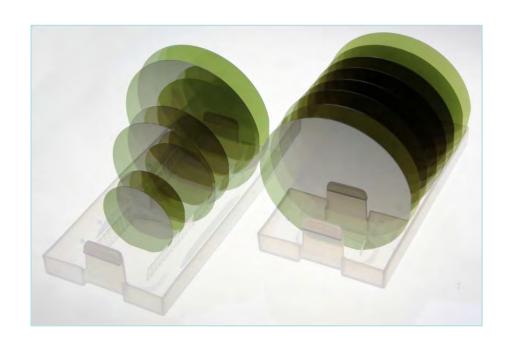


**Conducting 4H-SiC** 



**SiC ingots** 

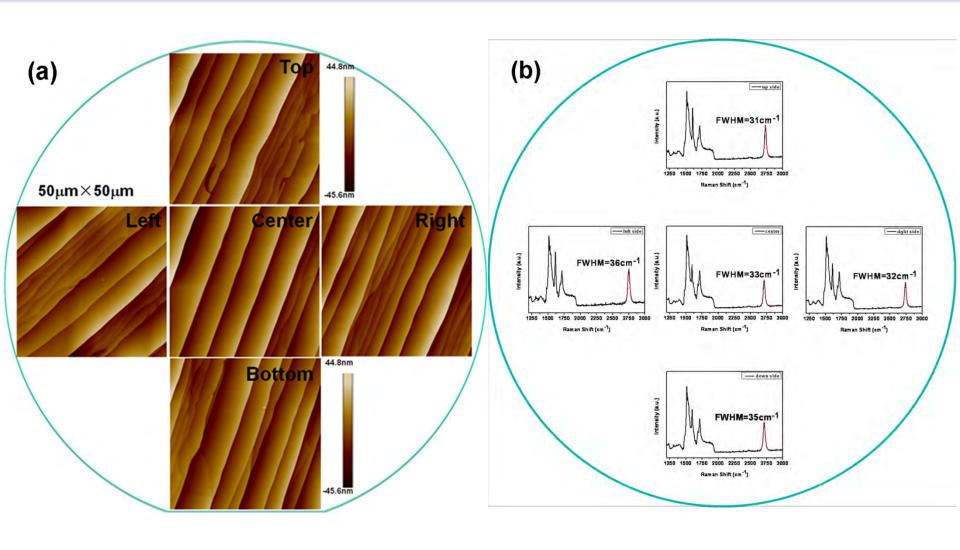
## **Latest Progress**





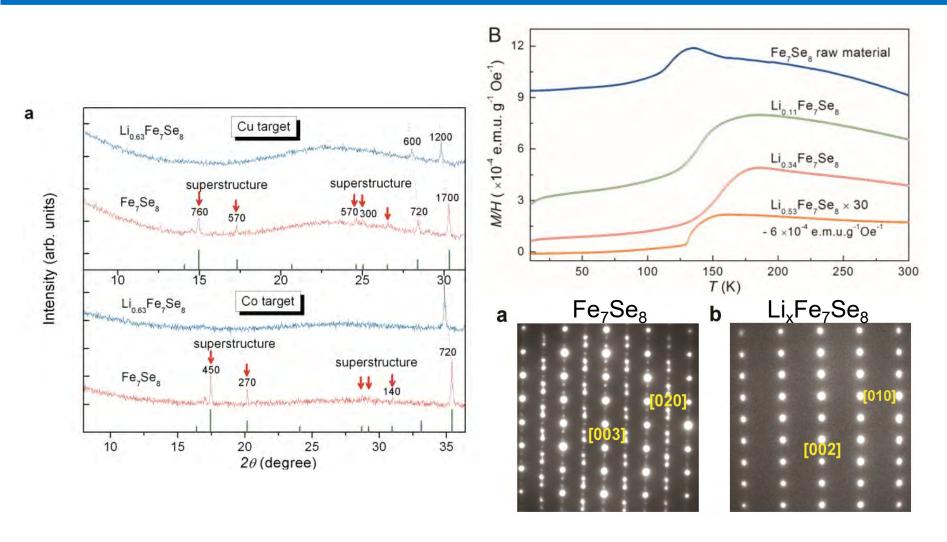
4 inches SiC crystal with Micropipe density < 1/cm<sup>-2</sup>, mass production. Developed the 6 inches SiC crystals.

## High quality Graphene on SiC water 144



Graphene: 2-3 layers; Mean step width: 10 μm

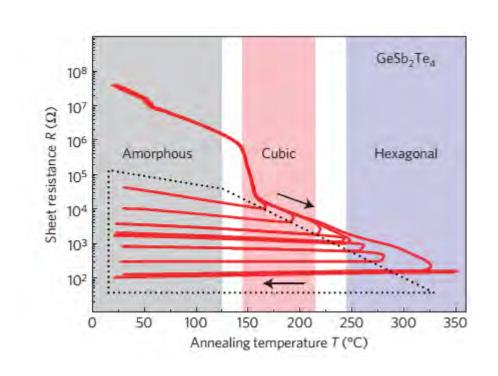
## Structure & magnetization Page 36 of 144



The randomness due to Fe sites occupation is verified to exist

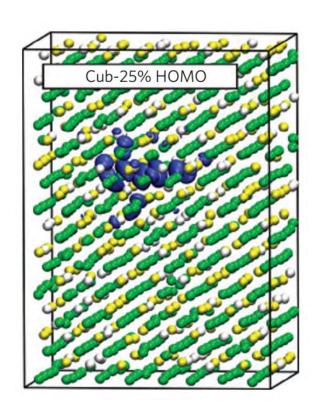
Science Adv., 2016 2(2), e1501283

# Breakthrough in 3D electron system—GeSbage 31 oct 4



**Experiments** 

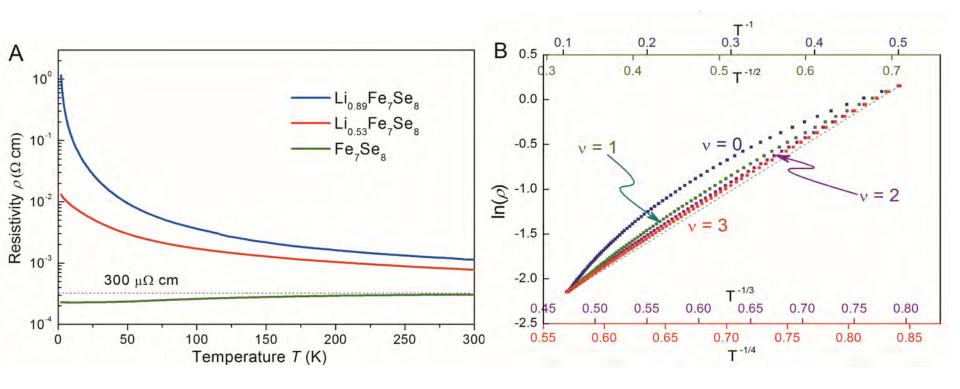
Nat. Mater. 10, 202-208 (2011)



**DFT** calculations

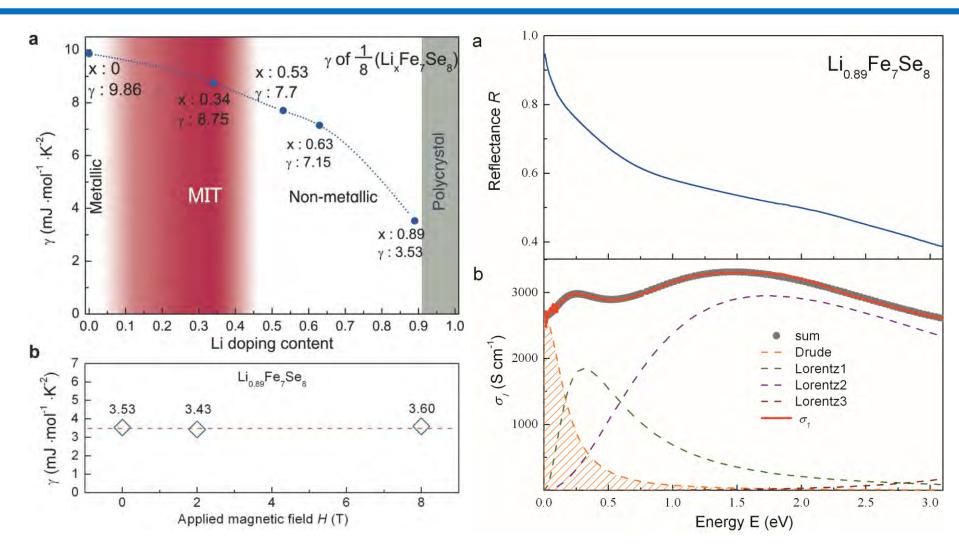
Nat. Mater. 11, 952-956 (2012)

#### Transport measurements Page 38 of 144



- Variable range hopping
- Metal insulator transition (different from doped semiconductor)
- No Efros-Shklovskii gap (Coulomb repulsion can be neglected)

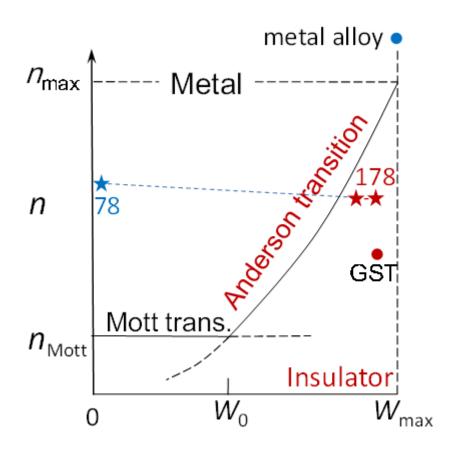
### Specific heat & Optical measurements



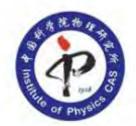
'The absence of an energy gap at the Fermi energy is a distinctive feature of Anderson localization.'

--D. Thouless

# A schematic diagram for finding of her potential Anderson insulators



This compound thus will serve as a rich playground for both theoretical and experimental investigations on metal-insulator transitions and disorder-induced phenomena.



# Laboratory of Advanced Materia Sof 14 & Electron Microscopy



- > 4 Academicians of CAS
- > 5 Groups
- > 32 Staffs
- > 65 Students

A01 Group: Modern analytical electron microscopy and applications

A02 Group: Exploration and crystal growth of functional crystalline materials

A04 Group: Atomic scale structure and electronic structure of functional materials

A05 Group: Nanomaterials and mesoscopic physics

A06 Group: Functional Materials electron microscopy and electron crystallography

image processing

ICDD Spring Meetings, Newtown Square, PA, 17 March 2016

# Reports of Regional Co-chair, Eastern Pacific Rim

(Japan, Korea & Philippines)

Takashi IDA, Japan

井田隆(日本)

Advanced Ceramics Research Center,



Aichi Synchrotron Radiation Center, Japan







#### **Contents**

International Scientific Meetings in Japan & Korea

2015-2016 (6 meetings)

2016-2019 (8 meetings)

Extensive Use of 2D X-ray Detector in Powder Diffraction Measurement – Combination with Synchrotron X-ray (Powder beamline BL5S2, AichiSR in Japan)

# International Meetings 2015-2016 (1/6 - 2/6)

#### I. ICCOSS XXII

The 22nd International Conference on the Chemistry of the Organic Solid State

Jul. 12 - 17, 2015, Niigata, Japan

http://www.iccoss2015.org

ICDD sponsored

130 participants including 46 students from 21 countries

Graciela Díaz de Delgado has presented ICDD Sponsored Lecture "Polymorphism in commercially important pharmaceuticals analyzed using the PDF-4 / Organics database".

2 ICDD Young Scientist Awards, 4 ICDD Poster Awards

# International Meetings 2015-2016 (2/6 - 2/6)

#### 2. IUPAC-2015

International Union of Pure and Applied Chemistry, 48th General Assembly & 45th World Chemistry Congress Aug. 6 - 14, 2015, Busan, Korea

http://www.iupac2015.org

3620 participants from 74 countries, 2611 papers presented

# International Meetings 2015-2016 (3/6 - 4/6)

#### 3. APT 2015

The 6th Asian Particle Technology Symposium

Sep. 15 - 18, 2015, Seoul, Korea

http://apt2015.org

### 4. Crystallization 2015

I Ith International Symposium on Crystallization in Glasses and Liquids

Oct. 11 - 14, 2015, Nagaoka, Japan

http://crystallization-2015.jp

# International Meetings 2015-2016 (5/6)

#### 5. **IUMRS-ICAM** 2015

14th International Union of Materials Research Societies - International Conference on Advanced Materials 2015 Oct. 25 - 29, 2015, Jeju, Korea

http://iumrs-icam2015.org

190 invited speeches, more than 2000 oral or poster presentations

## International Meetings 2015-2016 (6/6)

#### 6. AsCA-2015

The 13rd Conference of the Asian Crystallographic Association Dec. 05–08, 2015, Kolkata, India

[Indian Ocean Rim → India] <a href="http://asca2015.org">http://asca2015.org</a>

391 participants (192 India, 46 Japan, 36 Australia, 19 Bangladesh, 13 US, 13 UK, 12 Singapore, 12 Korea, 10 China, 9 Taiwan)

## International Meetings 2015-2016 (6/6)

#### 6. AsCA-2015

The 13rd Conference of the Asian Crystallographic Association Dec. 05–08, 2015, Kolkata, India

[Indian Ocean Rim → India] <a href="http://asca2015.org">http://asca2015.org</a>

391 participants (192 India, 46 Japan, 36 Australia, 19 Bangladesh, 13 US, 13 UK, 12 Singapore, 12 Korea, 10 China, 9 Taiwan)



Railway 0.08 USD / 10 miles

Tricycle, called "auto rikusha" max 5 passengers 0.3 USD / mile



# International Meetings 2016-2019 (1/8 - 2/8)

#### I. ICEP2016

2016 International Conference on Electronics Packaging

Apr. 20–22, 2016, Sapporo, Japan

http://www.jiep.or.jp/icep/index.html

Abstract deadline: Oct. 31, 2015

#### 2. ICCPS-13

13th International Conference on Ceramic Processing Science May 08–11, 2016, Nara, Japan

http://www.iccge18.jp

Abstract deadline: Dec. 20, 2015

# International Meetings 2016-2019 (3/8 - 4/8)

#### 3. MMA2016

Microwave Materials and Their Applications

Jul. 03–06, 2016, Seoul, Korea

http://encera.net

Abstract deadline: Mar. 15, 2016

#### 4. ICCGE-18

The 18th International Conference on Crystal Growth and

**Epitaxy** 

Aug. 07–12, 2016, Nagoya, Japan

http://www.iccge18.jp

Abstract deadline: Mar. 18, 2016

# International Meetings 2016-2019 (5/8 - 6/8)

#### 5. ISASC2016

4th International Symposium on New Frontier of Advanced Si-

Based Ceramics and Composites

Sep. 25–28, 2016, Busan, Korea

http://isasc2016.org/main/

Abstract deadline: Apr. 30, 2016

#### 6. AsCA2016

The 14th Conference of Asian Crystallographic Association

Dec. 04–07, 2016, Hanoi, Vietnam [Indian Ocean Rim]

http://asca.iucr.org/#meetings

# International Meetings 2016-2019 (7/8 - 8/8)

#### 7. IUCr2017

24th Congress and General Assembly of the International Union of Crystallography

Aug. 2017, Hyderabad, India [India]

http://asca.iucr.org/#meetings

#### 8. PACRIMI3

The 13th Pacific Rim Conference on Ceramic and Glass

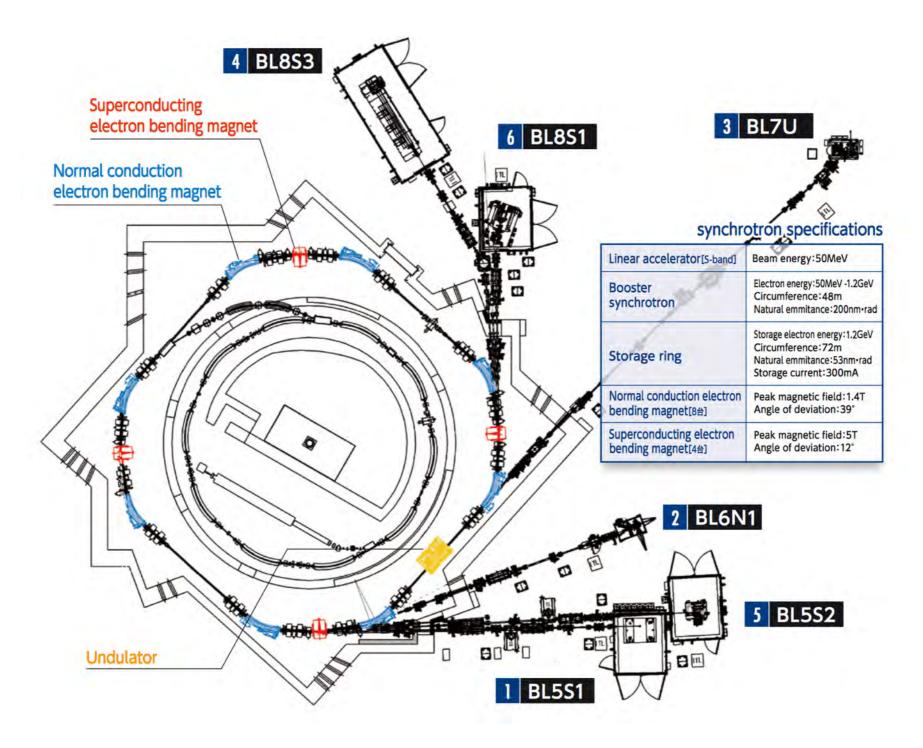
Technology

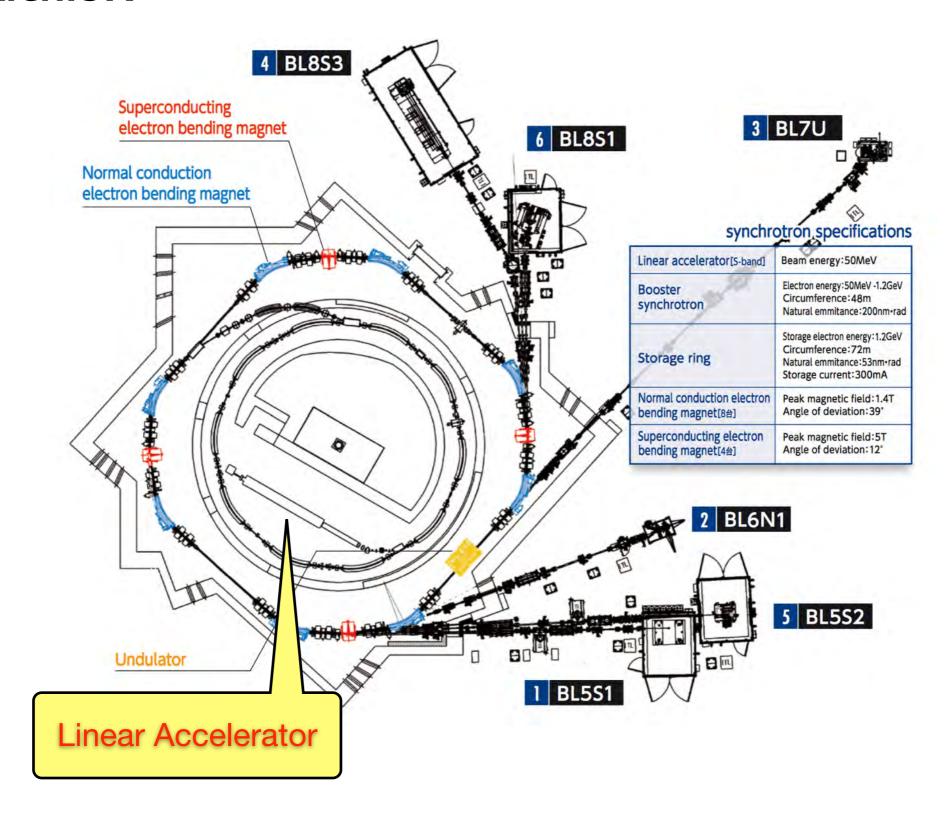
Oct. 27–31, 2019, Okinawa, Japan

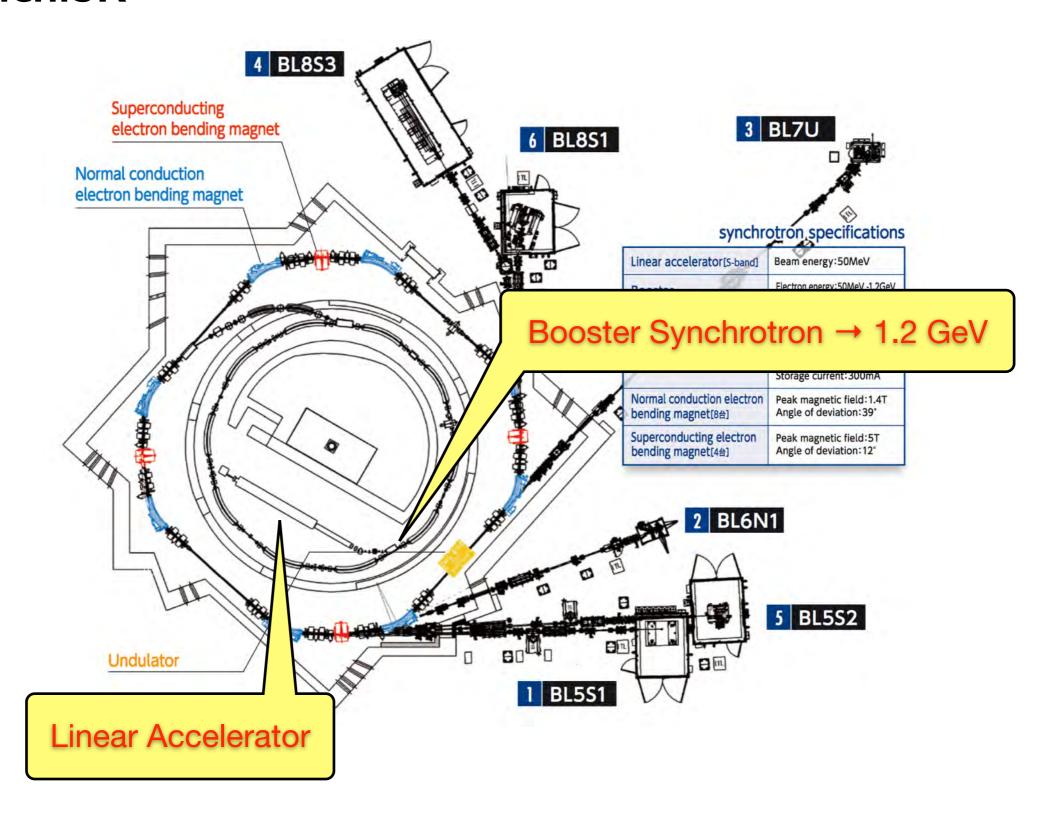
http://www.ceramic.or.jp/pacrim13/

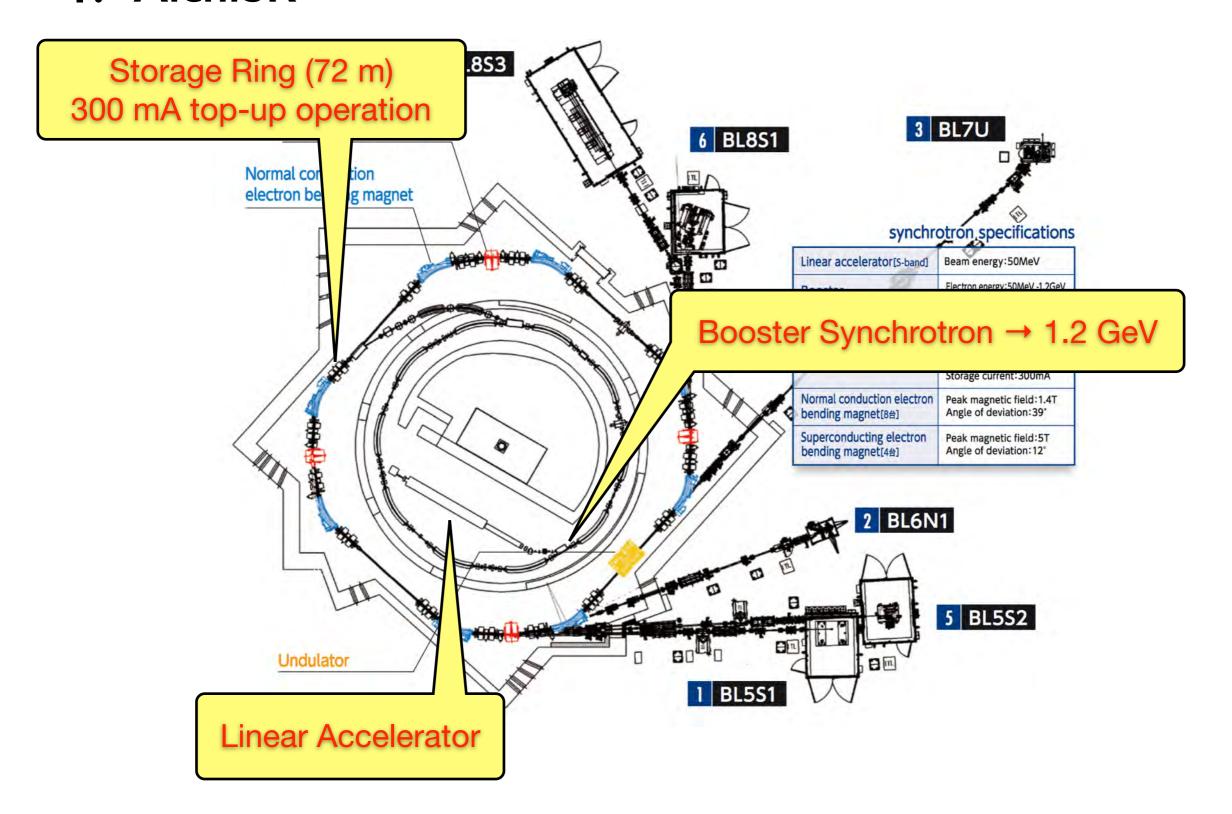
# Use of 2D X-ray Detector in Powder Diffraction Measurement – Combination with Synchrotron X-ray (Animations)

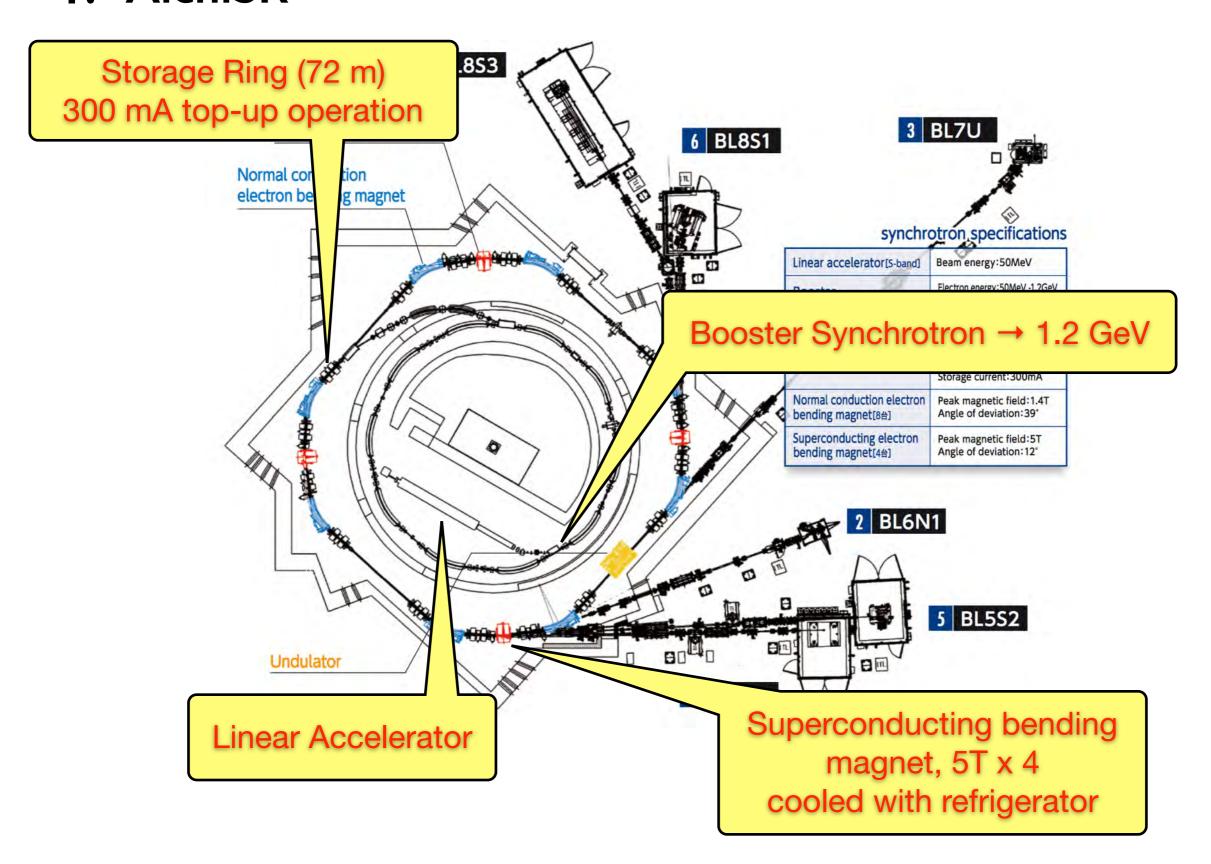
- I. AichiSR
- 2. BL5S2 beamline
- 3. High-resolution measurement
- 4. Mid-resolution measurement
- 5. Rapid measurement, in-site study

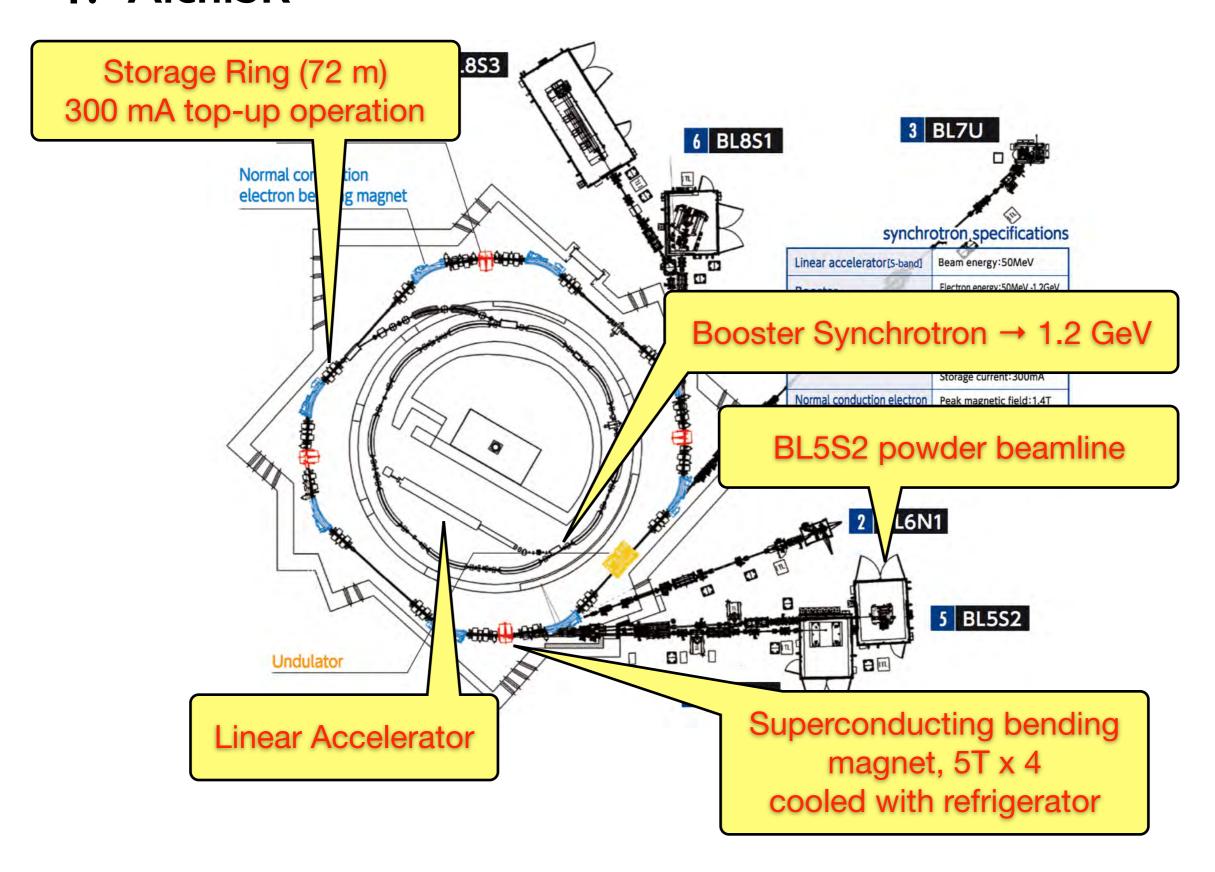






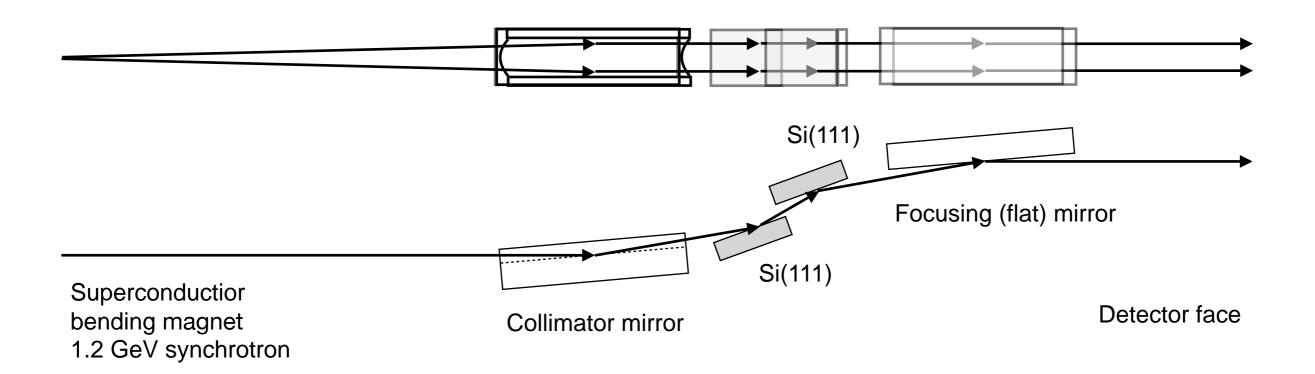


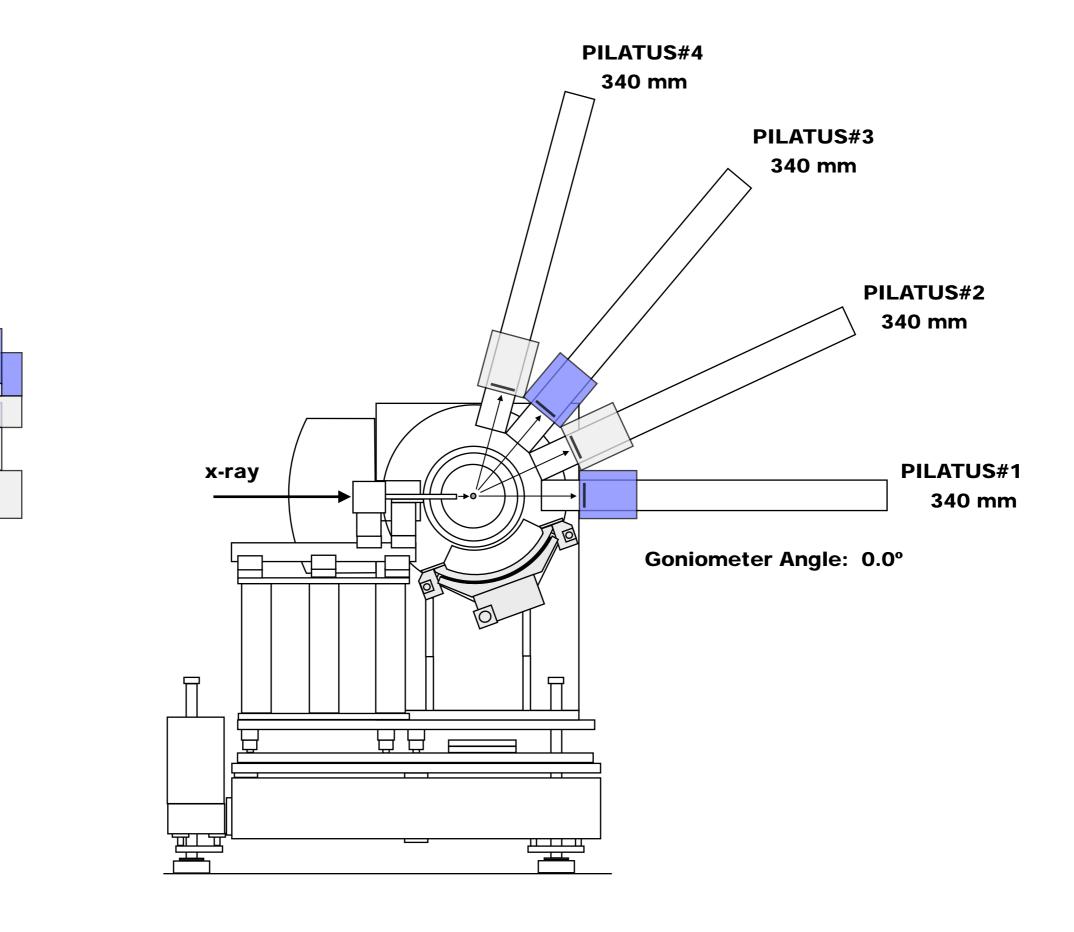


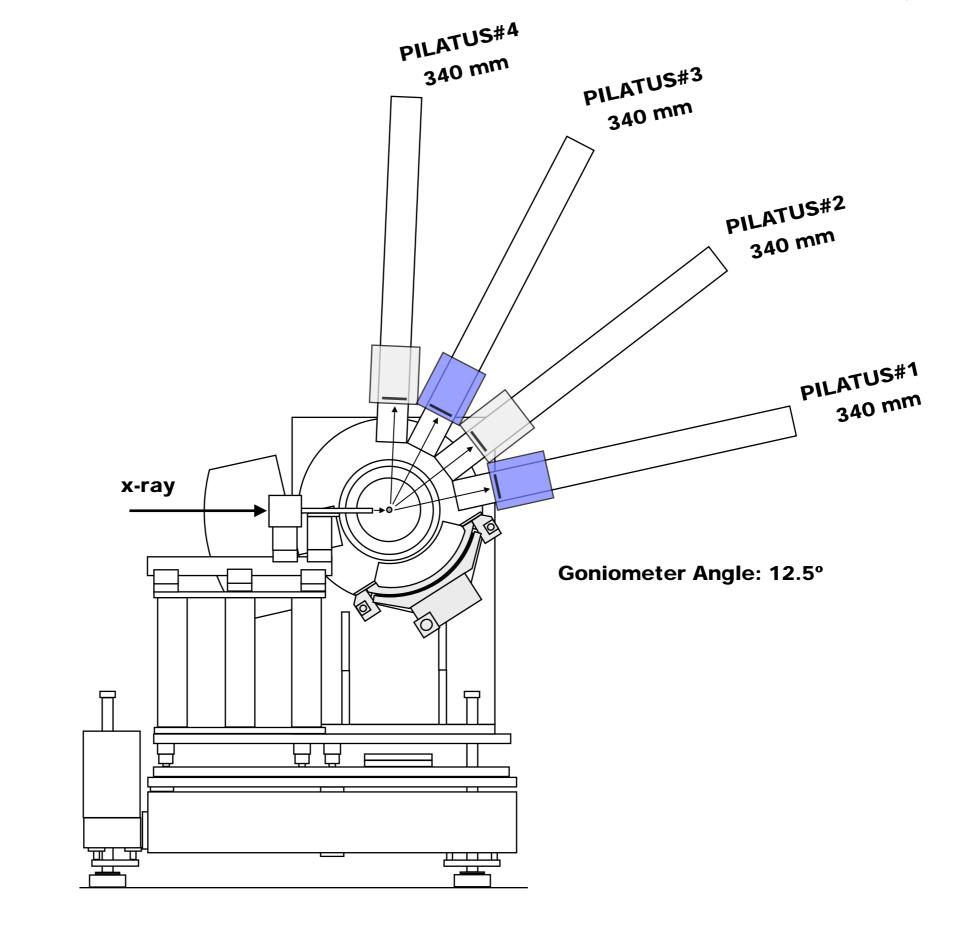


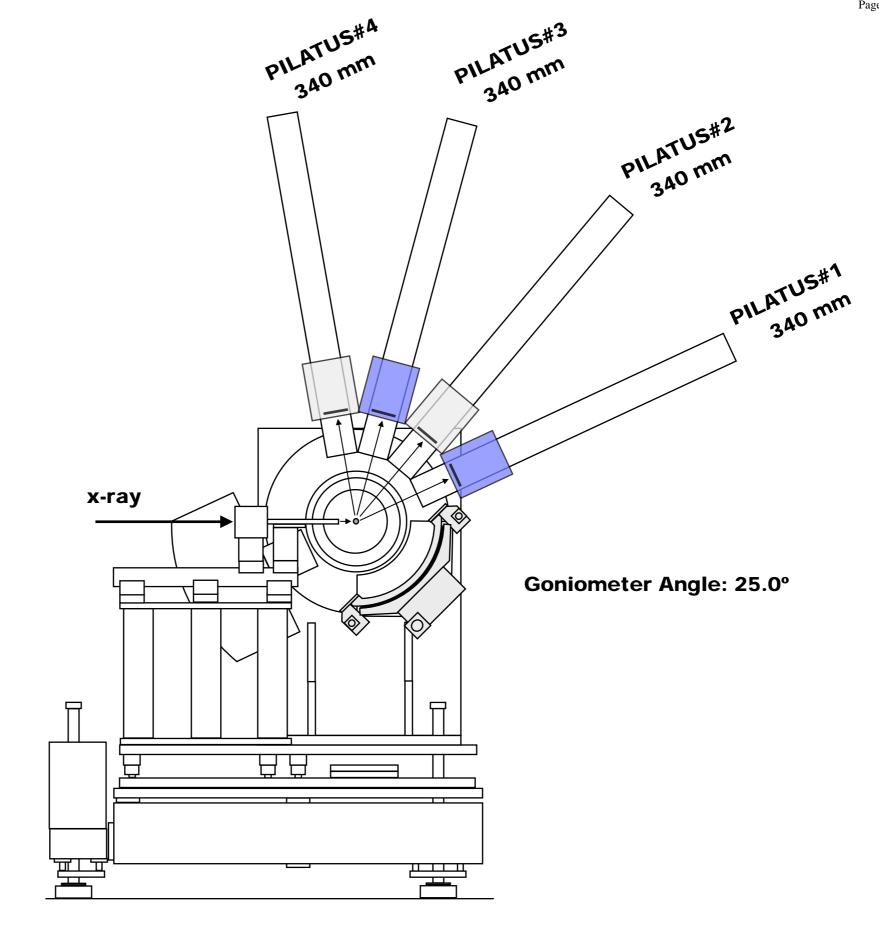
# AichiSR BL5S2 powder beam line

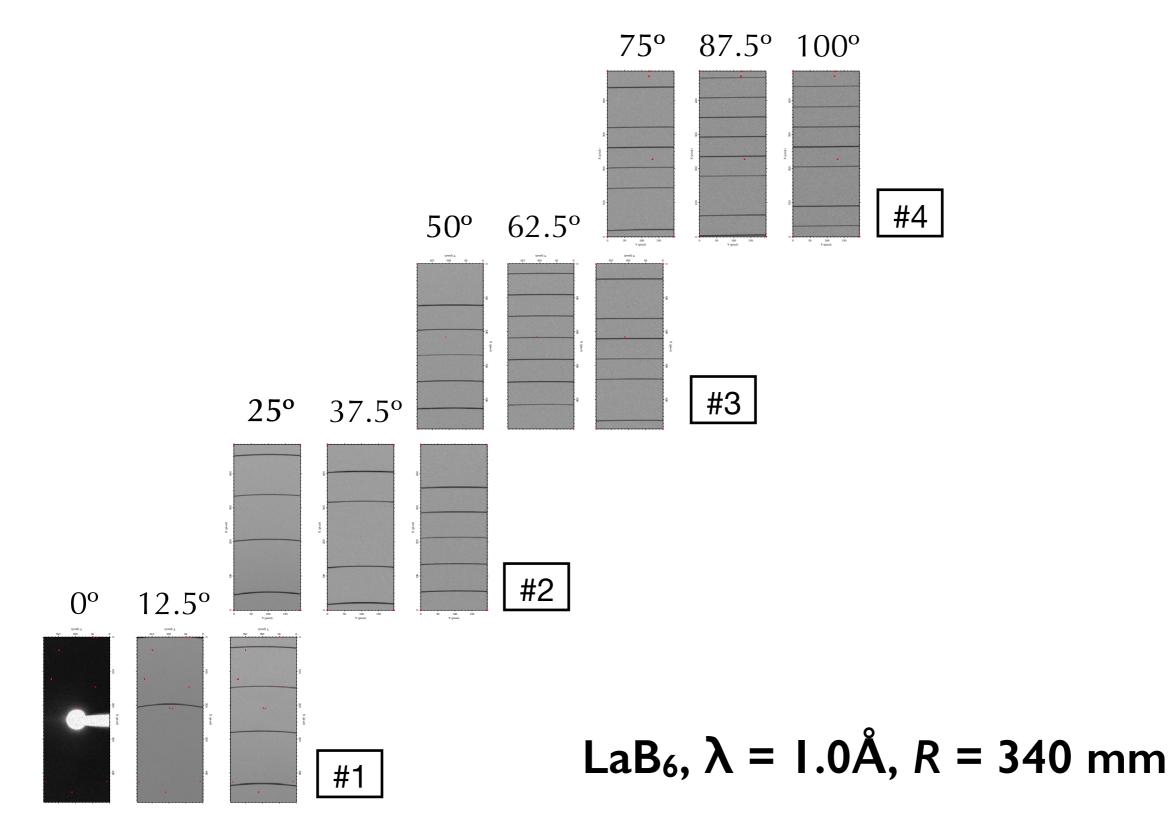
# Use of 2D X-ray detector assumed Focal geometry of beam line optics

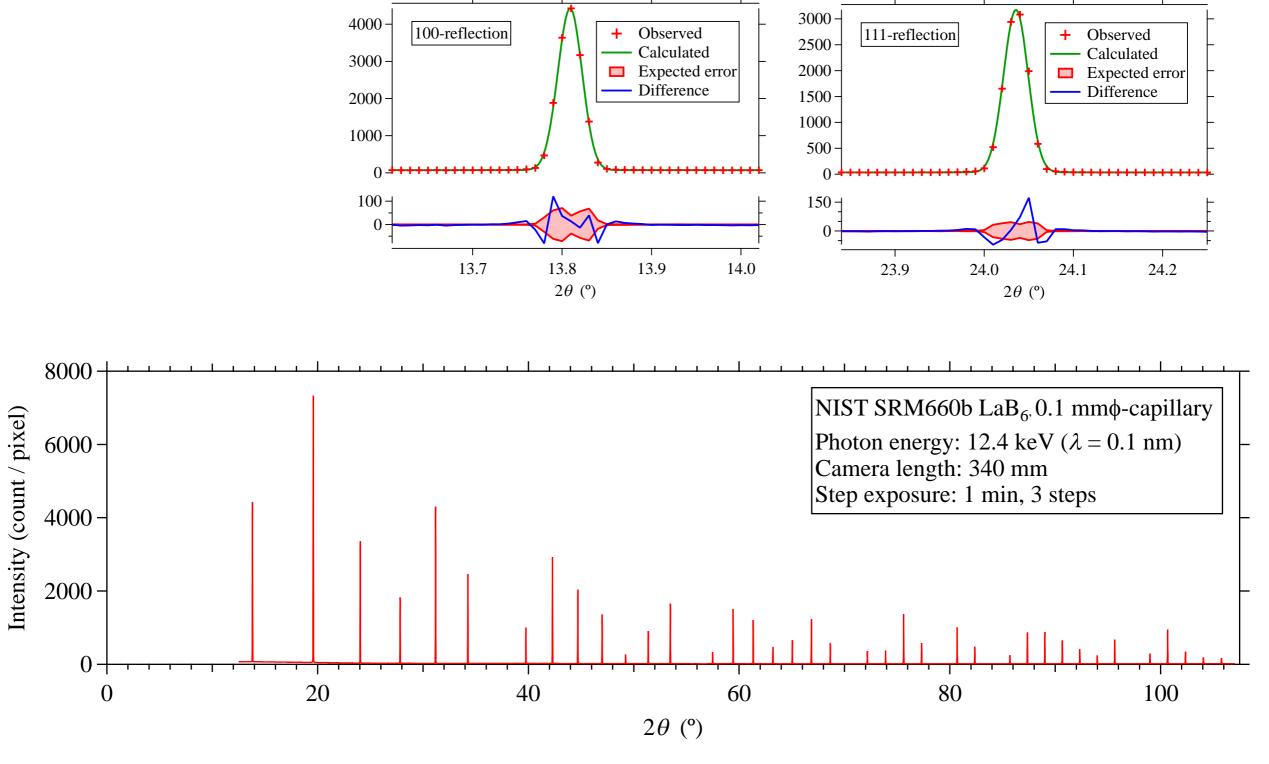




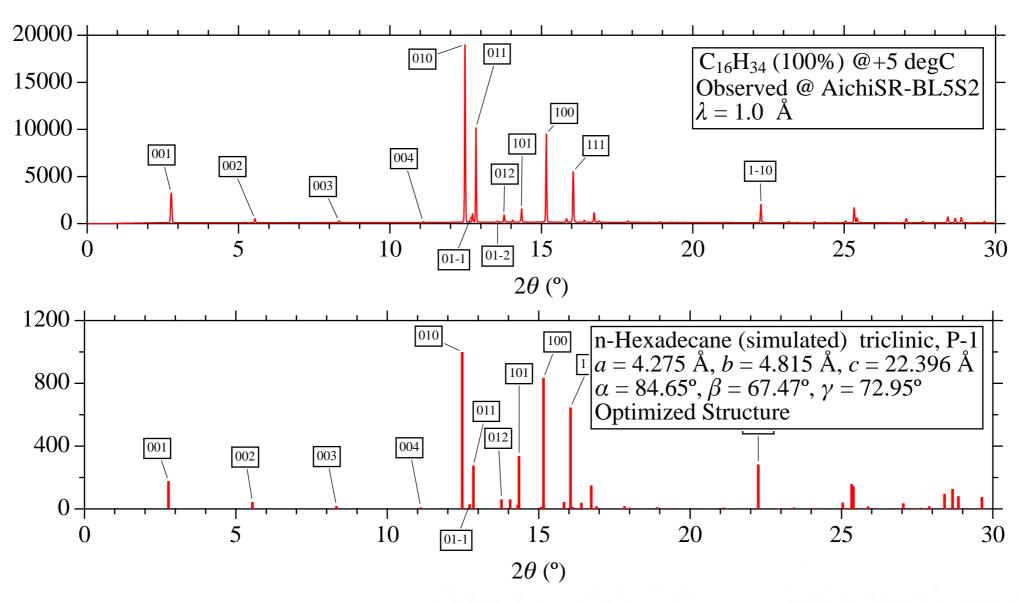




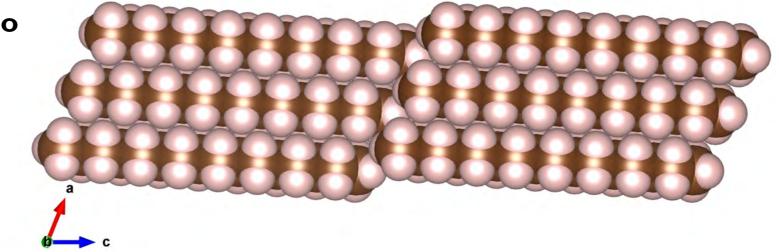


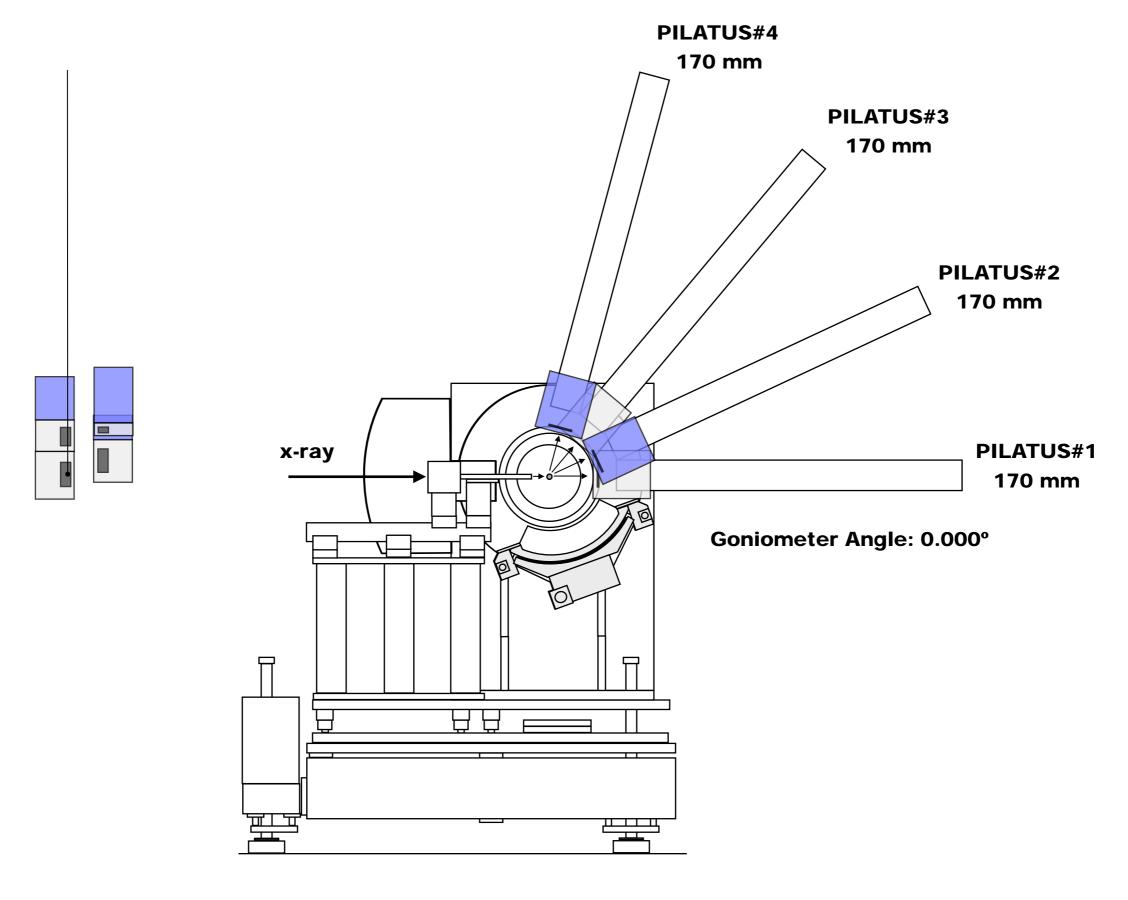


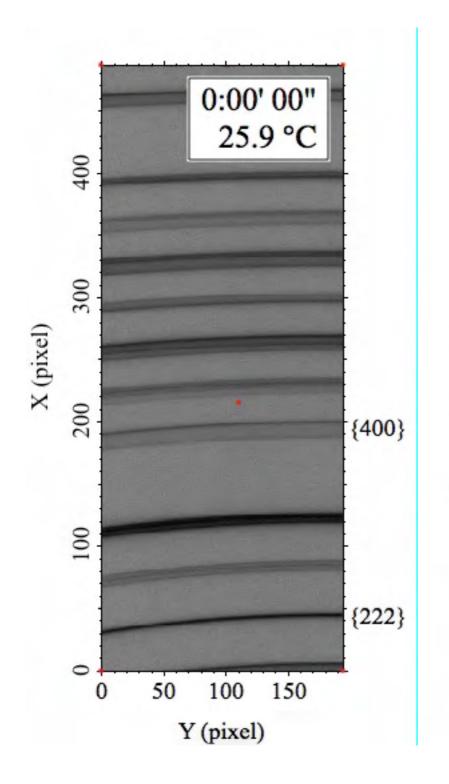
Total measurement time: 3 min



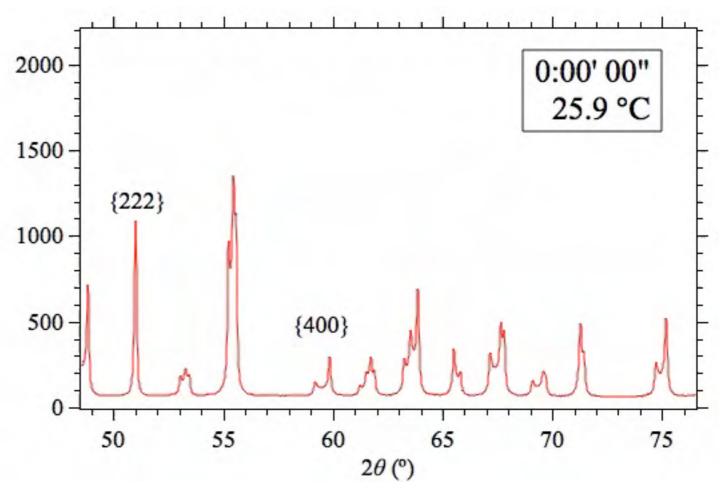
Intensity @  $2\theta = 2.5^{\circ}$  reasonable







# BaTiO<sub>3</sub>, $\lambda = 1.0$ Å, R = 170 mm





# Regional co-chair for EU report 2015-2016

Matteo Leoni
PICAM - University of Trento - Italy

Matteo.Leoni@unitn.it



# International Year of Light







## Currently weak situation



Some events in Europe in 2015 sponsored by ICDD

18-21 May 2015

Pharmaceutical Powder X-Ray Diffraction Symposium (PPXRD)
Bad Herrenalb, Germany



Some events in Europe in 2015 sponsored by ICDD

23-28 Aug 2015

**European Crystallographic Meeting (ECM)** 

Rovinj, Croatia



23 Aug 2015

ICDD Workshop @ European Crystallographic Meeting (ECM) Rovinj, Croatia



### Some events in Europe in 2015 sponsored by ICDD



21-24 Sept 2014 Size-Strain VII Oxford, UK







5-10 Jul 2015 **Euroclay 2015** 

Edinburgh, not yet independent Republic of Scotland







### Future events 2016

Some interesting events in the Euro zone in 2016

12-15 Jun 2016 **European Powder Diffraction Conference EPDIC 15**Bari, Italy

7-8 Dec 2016
8th Joint BER II and BESSY II User Meeting
Berlin, Germany

#### ICDD PDF-4 Workshop

T. N. Guru Row Indian Institute of Science, Bangalore, India ssctng@sscu.lisc.amet.in

The ICDD PDF-4 Workshop was held on June 26, 2011 as a pre-conference meeting of the 20th International Conference on the Chemistry of the Organic Solid State (ICCOSS XX), June 25-30, 2011. The conference was organized by the Solid State and Structural Chemistry Unit of the Indian Institute of Science (IISc), Bangalore, India. The details of the workshop are as follows:

Title: ICDD PDF-4
Date: June 26, 2011
Time: 9:00 a.m. to 4:00 p.m.
Venue: Faculty Hall, IISc, Bangalore

Lead Instructor: Soorya Kabekkodu, International Centre for Diffraction Data (ICDD), USA (Figure 1).

Assisted by: T. N. Gurn Row, IlSc, India, Graciela Delgado, Universidad de los Andes, Venezuela (Figure 2).

The Power Diffraction File (PDF) contains over 700 000 entries in two major databases. Release 2010 PDF-44 contains predominately inorganic materials and has 301 282 material data sets and PDF-44/Organics contains organic and pharmaceutical materials and has 436 901 material data sets. This workshop demonstrated the extensive data mining potential of the PDF-44 database using the powerful search capabilities of DDview and worked examples. The database itself can be data mined to provide insights into the materials state of materi, crystallimity, solid solution behavior, polymorph composition, and multiphase composition, and multiphase composition.



Figure 1. (Color online) Sourya Kabekkodu (lead instructor) and workshop attenders at the ICEID PDF-4 Workshop at the Indian Institute of Science, Bangalore.



Figure 2. (Color unine) Graciela Delgalo-lecturing at the (CDE) PDF-4 Workshop at the Indian Institute of Science, Barradore.

The following topics were covered at the workshop:

- Selecting search criteria for up to 53 unique search fields.
- · Viewing/analyzing search results.
- · Using history and standard formats to optimize searches.
- · Using digital patterns for data simulations and analysis.

The workshop started with brief introductory remarks by Prof. Guru Row and an example from his personal research, followed by Dr. Sootya Kebbakoda and Prof. Graciefa Delgado who covered the above topics throughout the day with hands on training, winding up with a technical discussion involving the participants.

The workshop also emphasized the use of the database for phase identification with SIFVE+ software and a range of examples to allow participants to work on materials of particular interest to them. Some registered participants brought their laptop computers to make the best use of the hands-on session and problem-solving decussions.

The participants were from various educational institutions, and also included representatives from R&D associated with the pharmaceutical and cement industries from different parts of India. Several participants were also registrans of the main meeting.

This is the first such training program on ICDD PDF-4 offered in India, and the participants benefitted greatly.





### Vanessa K. Peterson

GINSTO Australian Nuclear Science and Technology Organization vanessa.peterson@ansto.gov.au

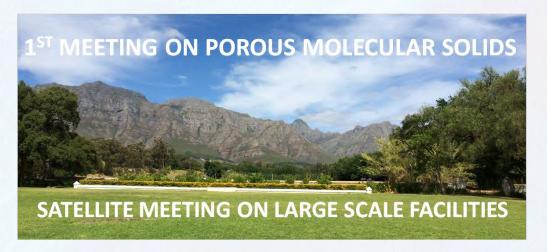
### Indian Ocean Rim



### Past activities: 2015



- 1st Meeting on Porous Molecular Solids: Stellenbosch, S. Africa 7 10 Apr
  - Large scale facilities satellite meeting



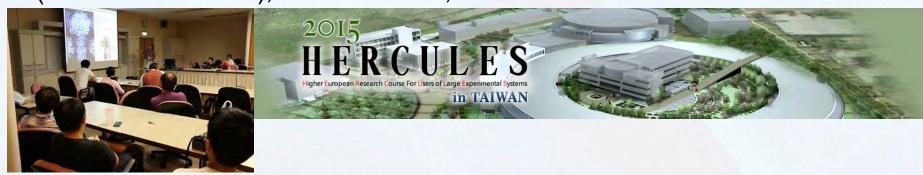
- International Workshop on Topological Structures in Ferroic Materials, Australia 19 - 21 May
- International Conference on Materials for Advanced Technologies (ICMAT 2015), Singapore, 28 June - 3 July



### Past activities: 2015



 Higher European Research Course for Users of large Experimental Systems (HERCULES 2015), Taiwan 6 – 24, Jul



- 14<sup>th</sup> Asian Oceana Neutron Scattering Assoc. (AONSA) Meeting, Aust. July
- 2<sup>nd</sup> Asia Oceana Conference on neutron scattering (AOCNS), Austr. July



9th Asia Oceania Forum for Synchrotron Radiation Research (AOFSRR) & User Meeting, Australia 25 - 27 Nov



### Past activities 2015/16



### • Judaba 8 16 - 21 Aug, 2015 S. Africa

Interdisciplinary workshops: S. African Crystallographic Society & Structural Chemistry Commission of the IUCr).
Serendipity versus prediction – functional materials and processes

Crystallisation Down Under 2016 (crystal growth, computational)
 Australia 11 - 12 Jan 2016



Australasian Crystallography School 2016, Australia 31 Jan - 5 Feb 2016

### Past activities: 2016



41st Lorne Conf. on Protein Structure & Function Australia 7 - 11 Feb



Australasian Soft Matter Scattering Workshop Australia 11 - 12 Feb



### Upcoming activities in the region



 30th Biennial Conference of the Society of Crystallographers in Australia and New Zealand (Crystal30). 29 Mar-1 Apr 2016 Australia

- International Conference on Electronic Materials (ICEM), IUCr July 2016
   Singapore
- 1st Pan African Conference on Crystallography (PCCr1), Cameroon, 6- 10 Oct 2016
- Asian Crystallographic Association meeting (AsCA 2016), Vietnam, 4-7
   Dec. Contacted ICDD regarding sponsorship.

ICCOSS 23 2017 (ICCOSS XXIII) is planned to be held in Stellenbosch, South Africa. April 3-7, 2017.



### **AXAA 2017**



AXAA-2017 workshops, conference and exhibition will be held in Melbourne, 5-9 February 2017.



## ansto

Nuclear-based science benefiting all Australians

# NIS Co-Chair report (2015 – 2016)

### 2nd Baikal Materials Science Forum



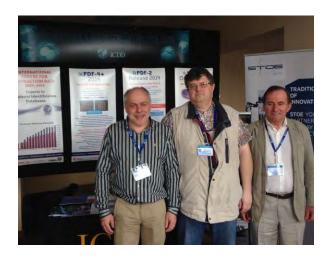
### **DEAR COLLEAGUES!**

RUSSIAN ACADEMY OF SCIENCES
Siberian Branch of RAS
Russian Foundation for Basic Research
Mendeleev Russian Chemical Society
Baikal Institute of Nature Management of SB RAS
Lomonosov Moscow State University
Buryat State University

### YOU ARE INVITED TO PARTICIPATE IN THE 2<sup>ND</sup> BAIKAL MATERIALS SCIENCE FORUM,

which will be held in the Republic of Buryatia on June 29 - July 5, 2015 (Ulan-Ude and v. Gremyachinsk, Lake Baikal)

The purposes of the all-Russian scientific conference with the international participation «The 2<sup>nd</sup> Baikal Materials Science Forum» are to discuss fundamental and applied problems of inorganic material science, to present last achievements in this area and to promote creative









### **Plans for 2016/2017**

### VIII Crystal Chemistry conference – May 30/June 3 - Suzdal



ICDD booth Session on Databases Session on powder diffraction

**FeSe based superconductors and related compounds**Professor Xialong Chen, Institute of Physics Chinese Academy of Sciences

### **Plans for 2016/2017**

- ICDD workshop in L'viv (Ukraine) Igor Zavaliy
- New members



Register now

on: 12 months, billed annually single license

out...

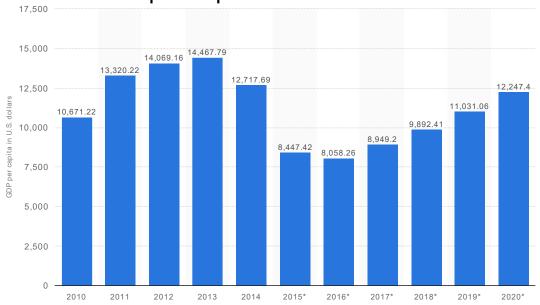
duct per capita

omestic product GDP

GDP

GDP per capita





### Report of the Technical Regional Co-Chair

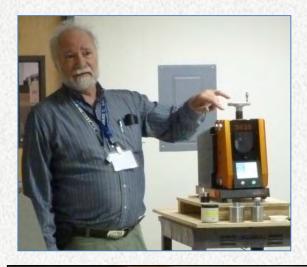
- North America -

March 2016 John Anzelmo

### ICDD Clinics - Headquarters Page 96 of 144

### Practical X-ray Fluorescence 27 April – 1 May 2015









### ICDD Clinics - Headquarter Spage 97 of 144

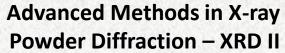


### Fundamentals of X-ray Powder Diffraction - XRD I

1 - 5 June 2015







8 - 12 June 2015



### ICDD Workshops

### Rietveld Refinement & Indexing - Basic Workshop

28 – 30 September 2015 - Headquarters

### Rietveld Refinement & Indexing - Advanced Workshop

1 - 2 October 2015 - Headquarters



PDF Users' Meeting at DXC

2 August 2015, Westminster, Colorado



# North American Meetings Key Exhibits & Educational Events • 2015-16

#### **Materials Research Society (MRS Spring 2015)**

San Francisco, CA • 6 - 10 April 2015

### **ACA Summer Course for Chemical Crystallography**

Evanston, IL • 21 June - 1 July 2015
No exhibit; Sponsored financially; Marketing
materials sent

#### American Crystallographic Association (ACA)

Philadelphia, PA • 25-29 July 2015

#### Microscopy & Microanalysis (M&M)

Portland, OR • 2 - 6 August 2015

#### **Denver X-ray Conference (DXC)**

Westminster, CO • 3 - 7 August 2015 PDF Users' Meeting held



ACA, Philly



DXC, Westminster

#### **Technical Committee Meeting** North American Meetings

### Key Exhibits & Educational Events • 2015-16

#### **Materials Science & Technology** (MS&T 2015)

Columbus, OH • 4 - 8 October 2015

#### **Gulf Coast Conference**

Houston, TX • 20 - 21 October 2015

#### American Association of Pharmaceutical **Scientists (AAPS)**

Orlando, FL • 25 – 29 October 2015

Seminar: The Identification of API Polymorphs and Formulation Analysis Using X-ray Powder Diffraction and the PDF-4/ Organics Database

### **Geological Society of America (GSA)**

Baltimore, MD • 1 − 4 November 2015

#### **Materials Research Society** (MRS Fall 2015)

Boston, MA • 29 November - 4 December 2015



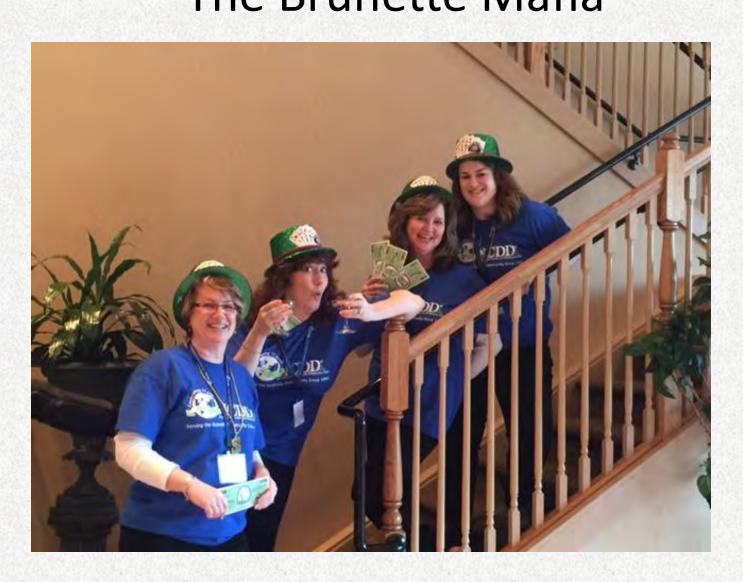
GSA, Baltimore 1

AAPS, Orlando

Page 100 of 144



# Conference Services - The Brunette Mafia



### Marketing and Communications





## REGIONAL CO-CHAIR: South America 2015 - 2016

Miguel Delgado







III School of Advanced Studies in Crystallization and Crystallography for Latin America (ECRISLA 2015)

7 - 18 December 2015 Florianópolis, SC, Brazil

- Module 1: Crystallization (7 11 December)
- Module 2: Crystallography (14 18 December)

Prof. Carlos E.M. Campos – Prof. Silvia Cuffini



Module 1: Crystallization

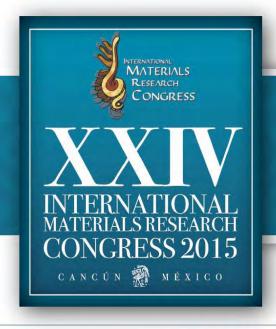


Module 2: Crystallography



## XXI International Materials Research Congress

Cancún, México, 16-20 August 2015



## Symposium 6G

Tom Blanton -Invited Speaker-

## MATERIALS SCIENCE OF PHARMACEUTICAL SOLIDS

Graciela Díaz De Delgado / VENEZUELA / Universidad de Los Andes Magali Hickey / USA / Alkermes Lauro Bucio / MEXICO / Universidad Nacional Autónoma de México







## XXIV International Materials Research Congress

**CANCUN - 2015** 

ICDD Workshop
Practical Applications of X-ray Analysis in
the Study of Pharmaceutical Materials



Symposium 6G
Materials Science of Pharmaceutical Solids

19th August 2015

Prof. Lauro Bucio, UNAM, Mexico Prof. Miguel Delgado, ULA, Venezuela Dr. Thomas (Tom) Blanton, ICDD, USA







#### XXII Reunião da ABCr I Reunião da LACA



9 a 11 de setembro de 2015

Convidamos a todos os cristalógrafos dos países latinoamericanos a participar desta importante Reunião com a qual a LACA inicia sua atuação como membro Regional da União Internacional de Cristalografia.

#### Local da Reunião



Instituto de Física, USP, São Paulo, Brasil

#### Comissão Organizadora Internacional

Marcia C. A. Fantini (Brasil)
Diego G. Lamas (Argentina)
Mauricio Fuentealtaba (Chile)
José Roberto Vega-Baudrit (Costa Rica)
José Antonio Henao (Colombia)
Graciela D. Delgado (Venezuela)
Lauro Bucio Galindo (México)
Alejandro Buschiazzo (Uruguay)
Iris C.L. Torriani (Brasil) – Chair

<u>"Workshop" satélite:</u> "High Pressure Crystallography" 12-14 de set. 2015, Laboratório Nacional de Luz de Síncrotron - LNLS -Campinas, SP, Brasil

O programa científico completo (em elaboração) será divulgado no segundo anuncio do encontro.

#### Contactos:

laca cristalografia@gmail.com - mfantini@if.usp.br - torriani@ifi.unicamp.br

GiA Workshop 8 September 2015 USP – Sao Paulo, BRAZIL ICDD Sponsored
Pre-Congress Workshop
on Powder Diffraction
Techniques and Applications



## The ICDD Grant-in-Aid Program in Brazil



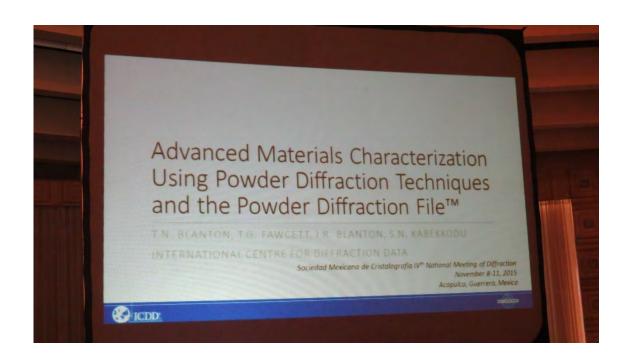
Instituto de Física "Gleb Wataghin"
UNICAMP, Campinas, SP
8 September 2015



## Sociedad Mexicana de Cristalografía A.C. SMCr

IV National Meeting on Difractometry (IV RND), Acapulco, Guerrero. 8 - 11 November 2015





Tom Blanton Plenary Lecture

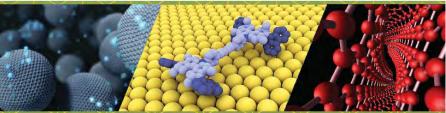


Miguel Delgado Invited Lecture









## 13 y 14 de Noviembre de 2015

#### Instructores:

- Dr. Thomas Blanton (ICDD E. U.A.)
  Dra. Graciela Diaz (UDA Venezuela

#### Valor curricular: 20 Hrs. educación continua

PDF-4+ y PDF-4+/Organics don vigencia hasta el 31 de Diciembre.

#### Cuota de recuperación: \$110.00 M. N

Servicio: Curso Taller Uso del banco de datos PDF-4-

BUAP

PDF-4+ Workshop 13-14 November 2015 Puebla, México











Page 120 of 14 Universidad de Los Andes, Facultad de Ciencias Departamento de Química Laboratorio de Cristalografía Mérida 5101 - VENEZUELA

Technical Committee Meeting

Laboratorio Nacional de Difracción de Rayos X **FONACIT** 

> Prof. Miguel Delgado (migueld@ula.ve)

Dr. Akihiko Iwata (iwata@rigaku.co.jp)

Workshop on Fundamentals of XRD

In the route to the IUCr-UNESCO Rigaku OpenLab Bolivia 2016



La Paz - Bolivia 27-28 January 2016





Technical Committee Meeting
Page 121 of 144







## **NEXT:**



#### ICDD WORKSHOP

Applications of the Powder Diffraction File PDF4+ in the Characterization of Materials

in

Symposium E. Materials Characterization E.4. Structural and Chemical Characterization of Metals and Alloys.

> Dr. Tom Blanton, ICDD, USA Prof. Lauro Bucio, UNAM, Mexico Prof. Miguel Delgado, ULA, Venezuela









## Rigaku OpenLab Bolivia

12 - 16 September 2016 Universidad Mayor de San Andrés (UMSA) La Paz – BOLIVIA

### **SARX-2016**

## XV Latin American Seminar of Analysis by X-Ray Techniques

September 18 – 21, 2016 Petrópolis, Rio de Janeiro, BRAZIL



Imperial Museum

## INVITED SPEAKERS Tim Fawcett and Graciela Díaz de Delgado

#### **International Scientific Committee**

- Dra. Lorena Cornejo Ponce, Chile
- Dra. Silvia Lucia Cuffini, Brasil
- Dr. José Miguel Delgado, Venezuela
- Dr. Javier Martínez Juarez, México
- Dr. Héctor Jorge Sánchez, Argentina
- Dr. Germán Tirao, Argentina

- Dr. Joaquim Teixeira de Assis, Brasil
- Dr. René Van Grieken, Belgium
- Dra. Cristina Vázquez, Argentina
- Dr. José Antonio Henao Martínez, Colombia
- Dr. Rodolfo Figueroa Saavedra, Chile

### **SARX-2016**

## XV Latin American Seminar of Analysis by X-Ray Techniques

September 18 – 21, 2016 Petrópolis, Rio de Janeiro, BRAZIL



Imperial Museum

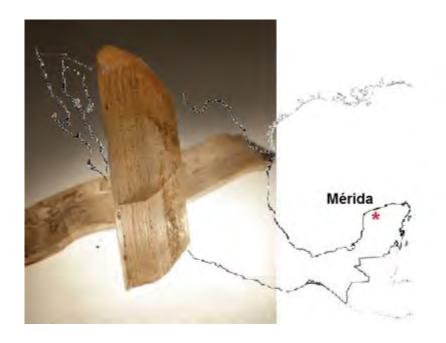
## INVITED SPEAKERS Tim Fawcett and Graciela Díaz de Delgado

## One day ICDD WORKSHOP

#### **International Scientific Committee**

- Dra. Lorena Cornejo Ponce, Chile
- Dra. Silvia Lucia Cuffini, Brasil
- Dr. José Miguel Delgado, Venezuela
- Dr. Javier Martínez Juarez, México
- Dr. Héctor Jorge Sánchez, Argentina
- Dr. Germán Tirao, Argentina

- Dr. Joaquim Teixeira de Assis, Brasil
- Dr. René Van Grieken, Belgium
- Dra. Cristina Vázquez, Argentina
- Dr. José Antonio Henao Martínez, Colombia
- Dr. Rodolfo Figueroa Saavedra, Chile



Joint meeting of

II Meeting of LACA (Latin American Crystallographic Association) and the

VIII National Congress of the Mexican Crystallographic Society

23 - 27 October 2016 Mérida – MEXICO

ICDD Booth and a half-day Workshop

## 2016 New ICDD Member



Prof. Gonzalo González UNAM - Mexico

## 2016 New GiA grantee



Prof. Fabio Furlan Ferreira Federal University of ABC Brazil

## **GRACIAS!**

# Regional Co-Chair's Report for the United Kingdom & Ireland

David Rendle

## Activities since March 2015

- BCA XRF Group Meeting June 17<sup>th</sup>, 2015 held at Leicester University
- 12<sup>th</sup> International Conference on Materials Chemistry July 20<sup>th</sup> – 23<sup>rd</sup>, 2015 held at York University
- British Radiofrequency Spectroscopy Group Christmas Meeting "NMR & Crystallography" December 14<sup>th</sup>, 2015 held at the Institute of Physics, London

Technical Committee Meeting
Page 131 of 144

## XRF Meeting June 17<sup>th</sup>, 2015

(Joint BCA/RSC Atomic Spectroscopy Meeting)

 High quality XRFS analysis of soils and sediments – a combined approach

The challenges of XRF analysis in industrial

catalyst production

Morning session speakers:



## XRF Meeting June 17th, 2015 (continued)

New applications in XRF analysis including small samples, layers and small spots by **WDXRF** 

From pressed powder pellets to Palaeozoic

mantle processes

Afternoon session speakers:



# 12<sup>th</sup> International Conference on Materials Chemistry July 20<sup>th</sup> – 23<sup>rd</sup>, 2015 at York University

- Biennial conference
- Over 600 delegates registered
- Six topics: Energy materials, Soft matter materials, Biomaterials, Electronic & Magnetic materials, Porous materials and Nanomaterials
- Five sponsors, including ICDD
- Perhaps an ICDD booth in 2017?

## Plenary lecture

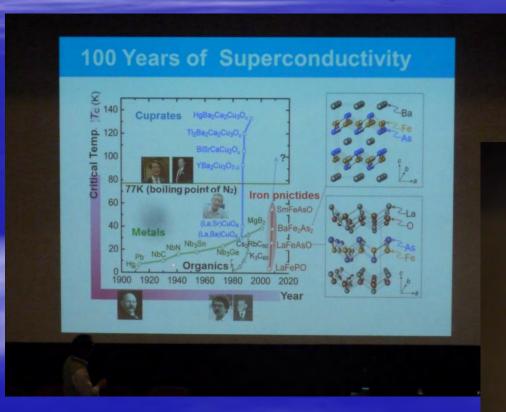
 "The artificial leaf" – Daniel Nocera (Harvard)

Liquid fuel production from solar-driven water splitting



# Iron-based superconductors: recent progress

## Hideo Hosono, Tokyo Institute of Technology



To new superconductors + a list of ~700 materials which were unsuccessful to the superconductors + a list of ~700 materials which were unsuccessful to the superconductors and superconductors and superconductors and functional materials, and fabrication of superconducting tapes and wires of iron pnictides

Hideo Hosono Kelichi Tanabe', Eiji Takayama-Muromachi', Hiroshi Kageyama', Shoji Yamanaka', Hiroshi Kangyama', Hiroshi Kageyama', Shoji Yamanaka', Hiroshi Kangyama', H

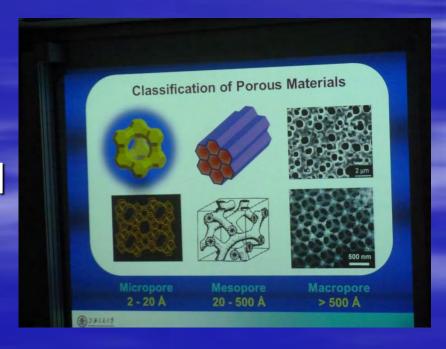
project found several tens of new superconductors by examining ~1000 materials, each of which was chosen by Japanese experts with a background in solid state chemistry. This review summarizes the major achievements of the project in newly found superconducting materials, and the fabrication wires and tapes of iron-based superconductors; it incorporates a list of ~700 unsuccessful materials examined for superconductivity in the project. In addition, described are

new functional materials and functionalities discovered during the project.

## Advanced solid materials with a porous feature

Jiesheng Chen, Jiao Tong University, Shanghai, China

Univalent zinc in ZSM-5 catalyses methane conversion to ethane and hydrogen.



# "NMR & Crystallography" IOP, London, December 14th

- Marek Potrzebowski, Poland
   NMR & crystallography in pharmaceuticals
- Graeme Day, Southampton University
   NMR and crystal structure prediction
- Terry Threlfall, Southampton University
   Defects, disorder, dislocations & amorphicity

## Forthcoming activities

- BCA Spring Meeting April 5<sup>th</sup> April 7<sup>th</sup>, 2016 to be held at Nottingham University
- BCA XRF Group Meeting June 15<sup>th</sup>, 2016 to be held at Leicester University

# UK General Election May 7<sup>th</sup>, 2015



## Brexit - will Britain leave the EU?



IN or OUT? Referendum Day June 23rd, 2016







