CGE 2024 – Cristallographie et Grands Equipements

November, 04th-08th, 2024

Synchrotron SOLEIL, Saint-Aubin, France

Summary

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- Programme
- List of Courses, Tutorial, Practical works, Conference
- Posters

Organizing committee :

Eliott COGNE - Synchrotron SOLEIL, Saint-Aubin

Frédéric DATCHI - Institut de Minéralogie, de Physique des Matériaux et CosmoChime - Sorbonne Université, Paris

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Jean-Marc LUCACCHIONI - Synchrotron SOLEIL, Saint-Aubin

Sylvie PAVAN - Synchrotron SOLEIL, Saint-Aubin

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Programme

Monday, November 4th

10:30 - 11:00	Welcome & registration
11:00 - 11:15	Welcome by SOLEIL's Scientific Director, *Amina Taleb*
11:15 - 12:30	SOLEIL Main Building Amphitheater **Course:** Geometric Crystallography, symetry part. I *Delphine Cabaret*
12:30 - 13:30	*Lunch*
13:30 - 15:30	SOLEIL Main Building Amphitheater **Course:** Geometric Crystallography, symetry part. II *Delphine Cabaret*
15:30 - 16:00	*Coffee break*
16:00 - 17:15	SOLEIL Main Building Amphitheater **Tutorials:** Crystal, direct lattice *Greg Cabailh*
18:00 - 19:30	Poster Session
19:30 -	*Self-Diner at SOLEIL restaurant*

Tuesday, November 5th

9:00 - 10:30	SOLEIL Main Building Amphitheater **Course:** Thomson scattering, Kinematic theory part I *Sylvain Ravy*
10:30 - 11:00	*Coffee break*
11:00 - 12:30	SOLEIL Main Building Amphitheater **Course:** Thomson scattering, Kinematic theory part II *Sylvain Ravy*
12:30 - 13:30	*Lunch*
13:30 - 14:30	SOLEIL Main Building Amphitheater **Course:** SR, instrumentation *Pierre Fertey*
14:30 - 16:00	**Tutorial:** **PHENIX room** GR A: Group *Lise-Marie Chamoreau* **Trainning room T5** GR B: Structure factors *El Eulmi Bendeif*
16:00 - 16:30	*Coffee break*
16:30 - 18:00	**Tutorial:** **Training room T5** GR. B: Group *Lise-Marie Chamoreau* **PHENIX room** GR. A: Structure factors *El Eulmi Bendeif*
18:30 - 20:00	SOLEIL Visit Pt I
20:00 -	*Self-Diner at SOLEIL restaurant*

Wednesday, November 6th

9:00 - 10:30	SOLEIL Reception Building Amphitheater **Course:** Single-crystal data analysis *El Eulmi Bendeif*
10:30 - 11:00	*Coffee break*
11:00 - 12:30	SOLEIL Reception Building Amphitheater **Course:** Powder data analysis *Erik Elkaïm*
12:30 - 13:30	*Lunch*
13:30 - 17:30	**Practical work:** **Salle PHENIX** A group: Pratical Single Crystals *Lise-Marie Chamoreau and El Eulmi Bendeif* **Training room T5** B group : Practical Powders *Erik Elkaïm and Benoît Baptiste*
18:00 - 19:00	SOLEIL Main Building Amphitheater Public conference *Virginie Chamard*
19:00 -	*Self-Diner at SOLEIL restaurant*

Thursday, November 07th

9:00 - 10:45	SOLEIL Reception Building Amphitheater **Course:** Neutrons and magnetic diffraction *Françoise Damay and Sylvain Petit*
10:45 - 11:15	*Coffee break*
11:15 - 12:30	SOLEIL Reception Building Amphitheater **Course:** Pdf, neutrons and X-ray *Pierre Bordet*
12:30 - 13:30	*Lunch*
13:30 - 17:30	**Practical work:** **Training room T5** A group : Practical Powders *Erik Elkaim et B. Baptiste* **Salle PHENIX** B group: Pratical Single Crystals *Lise Chamoreau and El Eulmi Bendeif*
18:00 - 19:30	SOLEIL Visit Pt II
19:30 -	*Conference Diner at SOLEIL restaurant*

Friday, November 8th

9:00 - 10:00	Amphithéâtre SOLEIL **Course:** Pump-probe diffraction *Claire Laulhé*
10:00 - 11:00	Amphithéâtre SOLEIL **Course:** Small angle scattering *Thomas Bizien*
11:00 - 11:30	*Coffee break*
11:30 - 12:30	Amphithéâtre SOLEIL **Course:** Coherence *Vincent Jacques*
12:30 - 13:30	*Lunch*
13:30 - 15:00	Amphithéâtre SOLEIL **Course:** Surfaces & interfaces *Alessandro Coati*
15:00 - 16:00	Conclusions

Speakers List CGE2024

(Courses, Tutorial and Practical works, Conference)

COURSES

Single-crystal data analysis

El Eulmi BENDEIF - *Synchrotron SOLEIL, Saint-Aubin*

Small angle Xray scattering in crystallography

Thomas BIZIEN - *Synchrotron SOLEIL, Saint-Aubin*

PDF neutrons + X-rays

Pierre BORDET - *Institut Néel, Grenoble*

Geometric crystallography, symmetry

Delphine CABARET - *Institut de Minéralogie et de Physique des Milieux Condensés, Paris*

Surfaces & interfaces

Alessandro COATI - *Synchrotron SOLEIL, Saint-Aubin*

Diffraction and neutrons

Françoise DAMAY - *Laboratoire Léon Brillouin, Saclay*

SR, instrumentation

Pierre FERTEY - *Synchrotron SOLEIL, Saint-Aubin*

Coherence

Vincent JACQUES - *Laboratoire de Physique des Solides, Orsay*

Pump-probe diffraction

Claire LAULHE - *Synchrotron SOLEIL, Saint-Aubin*

Introduction to neutron scattering

Sylvain PETIT - *Laboratoire Léon Brillouin, Saclay*

Thomson scattering, kinematic theory

Sylvain RAVY - *Laboratoire de Physique des Solides, Orsay*

TUTORIAL

Crystal, direct lattice

Greg CABAILH *- Institut des NanoSciences de Paris, Sorbonne Université, Paris*

Structure Factor

Lise-Marie CHAMOREAU *- Institut Parisien de Chimie Moleculaire, Paris*

Groups

El Eulmi BENDEIF *- Synchrotron SOLEIL, Saint-Aubin*

PRACTICAL WORKS

Practical Single crystals

Lise-Marie CHAMOREAU *- Institut Parisien de Chimie Moleculaire, Paris*

El Eulmi BENDEIF *- Synchrotron SOLEIL, Saint-Aubin*

Practical powders

Erik ELKAÏM *- Synchrotron SOLEIL, Saint-Aubin*

Benoît BAPTISTE *- Institut de Minéralogie et de Physique des Milieux Condensés, Paris*

CONFERENCE

Coherent diffraction imaging at Synchrotron source

Virginie CHAMARD *- Aix-Marseille Université, CNRS, Centrale Marseille, Institut Fresnel, Marseille*

Coherent Diffraction Imaging at Synchrotron Source

Virginie Chamard

Aix-Marseille Université, CNRS, Centrale Marseille, Institut Fresnel UMR 7249, 13013 Marseille, France

ABSTRACT

Imaging tri-dimensional complex materials at the nanoscale is a major challenge of nanoscience, which calls for a microscopy method combining sensitivity to density distribution, in situ compatibility and high spatial resolution. In this context, the recent advents of x-ray lens-less imaging methods, based on coherent diffraction, have opened promising perspectives as they fill the gap between direct microscopies (AFM, SEM, TEM) and reciprocal-space based x-ray scattering or Bragg diffraction analysis. This family of modalities has been proposed to circumvent the lack of efficient focusing optics in the x-ray regime. They are based on the acquisition of far-field coherent intensity patterns, from which the phase of the diffracted field is retrieved with inversion iterative algorithms, providing access to truly quantitative information in the object plane, such as the density distribution inside the sample or the lattice distortions in a crystalline material.

In this presentation, I will introduce the basis of x-ray coherent diffraction imaging and will further focus on two modalities, finite-support coherent diffraction imaging and ptychography, and their crystalline counterparts, in the Bragg geometry. A series of recent examples will be presented to illustrate their interest in material and life science related problems. Finally we will see what are the new research perspectives that are now made possible by fourth generation synchrotron sources.

Posters List

PO-01	TiVCr-based high entropy alloys for solid-state hydrogen storage ***Léa Abou-Samra*** *- Institut Néel, Grenoble, France*
PO-02	Mineralogical and optical properties of rock samples from hydrous asteroids ***Kana Amano*** *- Institut de Minéralogie, Physique des Matériaux et Cosmochimie & Muséum National d'Histoire Naturelle, Paris, France*
PO-03	A New Bi_2Se_3-polytype : $RbKBi_7Se_{12}$ ***Amélie Galodé*** *- Laboratoire CRISMAT, Caen, France*
PO-04	Search of magnetic texture in the pseudo-gap of cuppers superconducting ***Mariame Sakho*** *- Laboratoire Léon Brillouin, Gif-sur-Yvette, France*

TiVCr-based High Entropy Alloys for Solid-state Hydrogen Storage

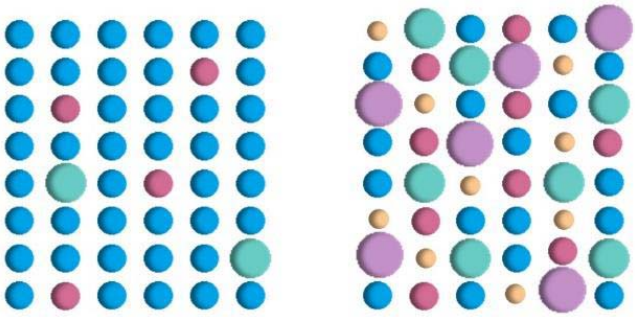
L. Abou-Samra, A. Bailly, R.Haettel, E. Verloop,
P. De Rango, L. Laversenne

Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France

ABSTRACT

High entropy alloys (HEA) have recently emerged as a new class of materials that garnered interest for hydrogen storage applications due to their interesting sorption properties. Unlike conventional alloys, HEAs are composed of five or more chemical elements in proportions that might range from 5 at. % to 35 at. %. The resulting high mixing entropy promotes the formation of multi-element solid solution phases, usually exhibiting simple crystallographic structures (BCC, FCC or HCP). This unique feature enhances the HEAs' ability to absorb and desorb hydrogen and makes them promising candidates for hydrogen storage applications.

Our work targeted HEAs composed of Ti, V, Cr, Mn and/or Fe. These alloys were already shown to be promising in terms of hydrogen sorption properties under reasonable pressure and temperature conditions [MAR23]. However, the compositions studied then exhibited a mixing of several phases of different crystallographic structures, preventing to study the structural effects on the alloys' properties. The aim of our work was therefore to explore other chemical compositions in order to possibly i) synthesize single-phase alloys and ii) tune the equilibrium pressures at ambient temperature. The present contribution focuses on three alloys, namely $Ti_{25}V_{35}Cr_{32}Mn_8$, $Ti_{25}V_{35}Cr_{34}Fe_6$ and $Ti_{23}V_{37}Cr_{30}Mn_5Fe_5$. The complementarity of X-ray and neutron diffraction, coupled to fine MEB-EDX analyses, sheds light on the subtle differences that exist at the micrometric scale, in terms of crystallographic structure and chemical composition. These investigations were complemented by pressure-composition isotherms, measured by the Sievert's volumetric method, confirming the great interest of these alloys for potential applications, with equilibrium pressures above 1.5 bar at 298 K.



Conventional alloy **HEA**

REFERENCES

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Mineralogical and Optical Properties of Rock Samples from Hydrous Asteroids

K. Amano

Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC)
Muséum National d'Histoire Naturelle (MNHN)

ABSTRACT

Asteroids witnessed the initial stages of the solar system evolution, whereas evolved planetary bodies, i.e., Earth, have lost such primitive information. Hydrous asteroids formed beyond the frost line of water to host hydrated minerals and may subsequently have provided volatile elements to early Earth [e.g., 1]. In this context, the composition of hydrous asteroids is a key to understanding what makes a planet habitable.

Telescopic surveys of asteroids have been conducted to investigate their compositional distribution [2]. The composition of asteroids is estimated by comparison of reflectance spectra of asteroids with those of meteorites, the latter characterized in the laboratory as well as petrography, mineralogy, and chemistry. However, the accuracy was not tested and what controls the optical properties of asteroids and meteorites, especially dark hydrous bodies, is not fully understood.

As a breakthrough on this issue, space missions have recently been conducted in which the spacecraft brought back rock samples from a hydrous asteroid to Earth [3]. Reflectance spectral properties of the asteroids were examined on various scales: from the observatory (global), from the spacecraft (down to meters), and in the laboratory (millimeter ~ micrometer) [e.g., 4–6]. Laboratory analyses of the collected samples revealed the actual nature of asteroids as the samples avoid reactions with the terrestrial atmosphere, unlike meteorites [6,7].

The samples collected from the hydrous asteroid Ryugu consist of hydrated minerals (up to 90 vol.%), Fe oxides, Fe sulfides, and carbonates, indicating they originated from the outer solar system [6,7]. The mineralogical properties and volatile-rich nature of Ryugu samples are similar to those of CI-type meteorites [6,7], however, the reflectance spectra of CI-type meteorites do not match those of Ryugu samples because oxidation and moisturization in terrestrial environments result in spectral changes in CI-type meteorites [8]. This highlights the need to consider terrestrial weathering effects on meteorite spectra when applying them to those of asteroids, and consequently for better interpretation of asteroidal spectra.

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5. S. Sugita, et al. The geomorphology, color, and thermal properties of Ryugu: Implications for parent-body processes. *Science* 364, 252 (2019).
6. T. Nakamura et al. Formation and evolution of carbonaceous asteroid Ryugu: Direct evidence from returned samples. *Science* 379, 6634 (2022).
7. T. Yokoyama, et al. Samples returned from the asteroid Ryugu are similar to Ivuna-type carbonaceous meteorites. Science379, eabn7850 (2022).
8. K. Amano et al, Reassigning CI chondrite parent bodies based on reflectance spectroscopy of samples from carbonaceous asteroid Ryugu and meteorites.*Sci. Adv.*9, eadi3789(2023).

A New Bi_2Se_3-polytype : $RbKBi_7Se_{12}$

A. Galodé[1] ; D. Pelloquin[1] ; F. Gascoin[1]

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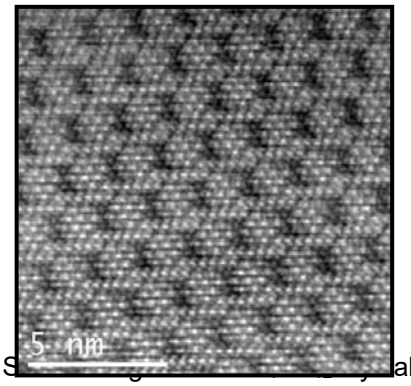
ABSTRACT

In the world, waste heat corresponded to 10% of energy requirements[1]. Many solutions exist to avoid heat lost or to recover waste heat to produce electricity. The latter solution is the subject of numerous studies into thermoelectric materials. Currently, a few thermoelectric materials are in industry, with an efficiency of at least 10%[2]. This is why various studies are focusing on the development of new thermoelectric compounds, starting with the research of new structures[3,4,5,6]. Bi_2Se_3-related materials are well known to often such properties.

In this goal, news prospectives in the system Rb-Bi-Se by means transmission electronic microscopy had allowed to identify a new structure namely $RbKBi_7Se_{12}$. Several techniques are employed to do this. Tomographic electronic diffraction is used to obtain the lattice and define the new framework owing to SUPERFLIP algorithm[7]. By combining tomographic and elemental atomic mapping (energy-dispersive spectroscopy data), we were able to resolve the structure. To validate this structure, Rietveld refinements from powder XRD data and atomic image calculations were carried out.

The structure of the compound $RbKBi_7Se_{12}$ subscribes in a known structure family, largely described by M.G. Kanatzidis[4,6] in numerous articles. This family of materials can be described by the combination of NaCl blocks with different orientations. In our case, $RbKBi_7Se_{12}$ crystalizes in a monoclinic structure with lattice parameters: a = 18.57840 Å; b = 4.16651 Å; c = 17.55930 Å; β = 114.16°. The NaCl blocks are organized around the rubidium channels. There are two types of NaCl blocks, firstly the $NaCl^{100}$-type on the side of the channels and the latter type $NaCl^{111}$ on the top and bottom of the Rb channels.



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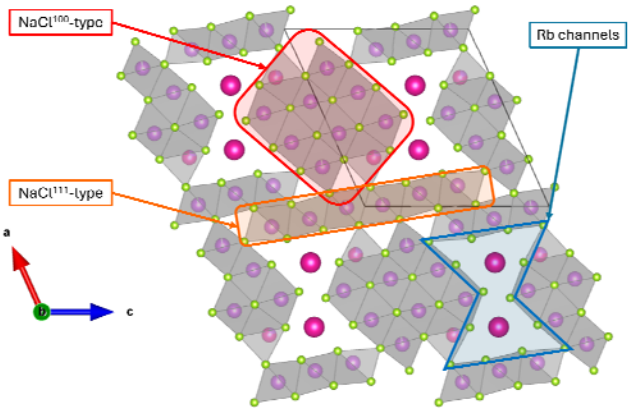
oriented along [010] axis



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Search of Magnetic Texture in the Pseudo-gap of Cuppers Superconducting

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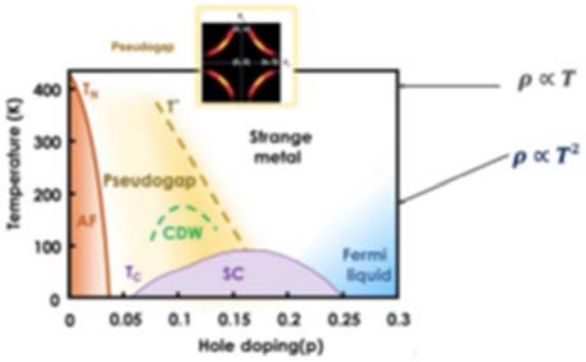
[2]SPEC, CEA, CNRS-UMR 3680, Université Paris-Saclay, Gif sur Yvette Cedex 91191, France

ABSTRACT

Cuprates are superconducting materials characterized by high transition temperatures at ambient pressure, which can exceed the liquefaction temperature of nitrogen (77K) that places them in the family of non-conventional superconductors. At the atomic scale, their crystal structure is made of CuO2 conduction planes and block reservoir planes that facilitate charge carrier transfer upon doping.

Depending on the level of doping, they present a general phase diagram divided into zones with different physical properties. In the underdoped area delimited by T* (fig. 1), a partial opening of a gap at some points on the Fermi surface leads to a loss of density of electronic states. Known as the “Pseudo-Gap (PG)”, this part of the phase diagram could play a role in the emergence of unconventional superconductivity.



The PG contains a magnetic phase, which breaks the symmetries of inversion and time reversal, interpreted as the signature of a magneto-electric quantum state of the “current loops” type [2,3]. However, this phase preserves the translational symmetry of the lattice. It is referred to as “q=0 magnetism”. The recent discovery of additional magnetic correlations induced by these quantum states in CuO2 planes, leading to a doubling of the unit cell (q=1/2 magnetism) in the compound YBa2Cu3O6+x (YBCO), suggests the existence of a magnetic texture that could play a key role in the pseudogap physics [4-6]

With a view to extending this observation to other cuprate families, we are first synthesizing single crystals of Bi2(La, Sr)2Can-1CunO4+2n (with n=1 (Bi2201)) and YBa2Cu3O6+x using the floating zone technique.

These crystals will then be analyzed for magnetic textures by polarized neutron diffraction.

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[1] E.Razzoli et al., New jour of phys, 12 (2010).
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[6] C.M. Varma, Phys. Rev. B, 99 (2019)