

## How to assess the structure of glasses ?

USTV/CNRS thematic school on the characterization of glass structure

EPN Campus - Grenoble - France 18 – 22<sup>nd</sup> November 2019

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Programme

Abstracts

List of Posters

**Sunday 17<sup>th</sup> November 2019**  
**Cafeteria onsite**

18:00 - 20:30 Welcome Party "Wine and Cheese" at the Cafeteria onsite

**Monday 18<sup>th</sup> November 2019**  
**ILL Chadwick**

08:15 Registration in ILL entrance hall

08:45 - 09:00 Francesco Sette, ESRF, France  
Helmut Schober, ILL, France

Welcome

09:00 - 10:30 D. Neuville, CNRS – IPGP, France  
General Introduction

10 :30 - 11:00 Coffee break – EPN Campus Restaurant ground floor

11:00 - 12:30 G. Vaughan, ESRF, France and G. J. Cuello, ILL, France  
X-ray and neutron scattering for the characterization of glass structures

12:30 - 14:00 Lunch - EPN Campus Restaurant ground floor

14:00 - 15:30 Y. Joly, Institut Néel, France  
X-ray Absorption Spectroscopy

15:30 - 16:00 Coffee break – EPN Campus Restaurant ground floor

**Monday 18<sup>th</sup> Novmber 2019**  
**PRACTICALS**

16:00 – 18:00 Neutron Scattering – G. CUELLO ILL Chadwick

16:00 – 18:00 XANES (XAS) – O. PROUX MD-1-21

16:00 – 18:00 X-Ray Scattering – G. VAUGHAN CIBB Seminar room 214

**Tuesday 19<sup>th</sup> November 2019**  
**ILL Chadwick**

**09:00 - 10:30** **P. Glatzel, ESRF, France**  
Chemical information in X-ray emission spectroscopy

**10:30 - 11:00** **Coffee break** – EPN Campus Restaurant ground floor

**11:00 - 12:30** **M. Cotte, ESRF, France**  
Synchrotron-based micro-analyses for the study of ancient glasses

**12:30 - 14:00** **Lunch** - EPN Campus Restaurant ground floor

**14:00 - 15:30** **D. Foix, IPREM, Université Pau & Pays Adour, France**  
X-ray Photoelectron Spectroscopy

**15:30 - 16:00** **Coffee break** - EPN Campus Restaurant ground floor

**Tuesday 19<sup>th</sup> November 2019**  
**PRACTICALS**

**16:00 – 18:00** **X-Ray Photoelectron Spectroscopy – D. FOIX** ILL Chadwick

**16:00 – 18:00** **X-Ray Imaging – M. COTTE** MD-1-21

**16:00 – 18:00** **X-Ray Emission Spectroscopy – M. RETEGAN** CIBB Seminar room 214

**Wednesday 20<sup>th</sup> November 2019**  
**ILL Chadwick**

09:00 - 10:30 **B. Hehlen, CNRS-Université de Montpellier, France**  
Inelastic light scattering by atomic vibrations

10:30 - 11:00 **Coffee break** – EPN Campus Restaurant ground floor

11:00 - 12:30 **D. De Sousa Meneses, Université Orléans, CNRS, CEMHTI, France**  
Contribution of infrared spectroscopy to the analysis of the glass structure

12:30 - 14:00 **Lunch** - EPN Campus Restaurant ground floor

**Wednesday 20<sup>th</sup> November**  
**PRACTICALS**

14:00 – 16:00 **Raman Spectroscopy – B. HEHLEN** ILL Chadwick

14:00 – 16:00 **EXAFS – F. d’ACAPITO** MD-1-21

14:00 – 16:00 **Infrared Spectroscopy – D. de SOUSA** CIBB Seminar room 214

16:00 - 16:30 **Coffee break** – ILL Chadwick Entrance hall

16:30 - 18:00 **Beamline visit**

**MEETING POINT 16:30 ILL Chadwick Entrance**

**Social Dinner**  
**Wednesday 20<sup>th</sup> November 2019**

19:30 – 22:30 **Social Dinner “Restaurant Le 5”**  
5 Place Lavalette, 38000 Grenoble

**MEETING POINT 19:00 at the Guesthouse**

**Thursday 21<sup>st</sup> November 2019**  
**ILL Chadwick**

- 09:00 - 10:30** **D. Massiot, Université Orléans, CNRS, CEMHTI, France**  
Solid-State Nuclear Magnetic Resonance: from basics to more advanced concepts
- 10:30 - 11:00** **Coffee break** - ILL Chadwick Entrance hall
- 11:00 - 12:30** **P. Florian, Université Orléans, CNRS, CEMHTI, France**  
Dynamic Nuclear Magnetic Resonance
- 12:30 - 14:00** **Lunch** - EPN Campus Restaurant ground floor
- 14:00 - 15:30** **B. Ruta, Université Lyon 1 and CNRS, France**  
Dynamical properties of glass formers probed with coherent X-rays
- 15:30 - 16:00** **Coffee break** - ILL Chadwick Entrance hall

**Thursday 21<sup>st</sup> November 2019**  
**PRACTICALS**

- 16:00 - 18:00** **X-Ray Photon Correlation Spectroscopy – Y. CHUSHKIN/F. ZONTONE** ILL Chadwick
- 16:00 - 18:00** **NMR spectra simulations – P. FLORIAN** MD-1-21
- 16:00 - 18:00** **NMR spectra simulations – D. MASSIOT** CIBB Sem room 214

**Friday 22<sup>nd</sup> November 2019**  
**ILL Chadwick**

**09:00 -  
10:30**



**M.A. Gonzales, ILL, France**  
Computer simulation of glasses

**10 :30 -  
11:00**



**Coffee break-** ILL Chadwick Entrance hall

**11:00 -  
11:30**



**F. d'Acapito, CNR-IOM-OGG c/o ESRF, France and E. Mitchell, ESRF, France**  
Access to large scale facilities: opportunities for industry and academia

**11:30 -  
13:00**



**Discussion and Conclusion**

**13:00 -  
14:00**

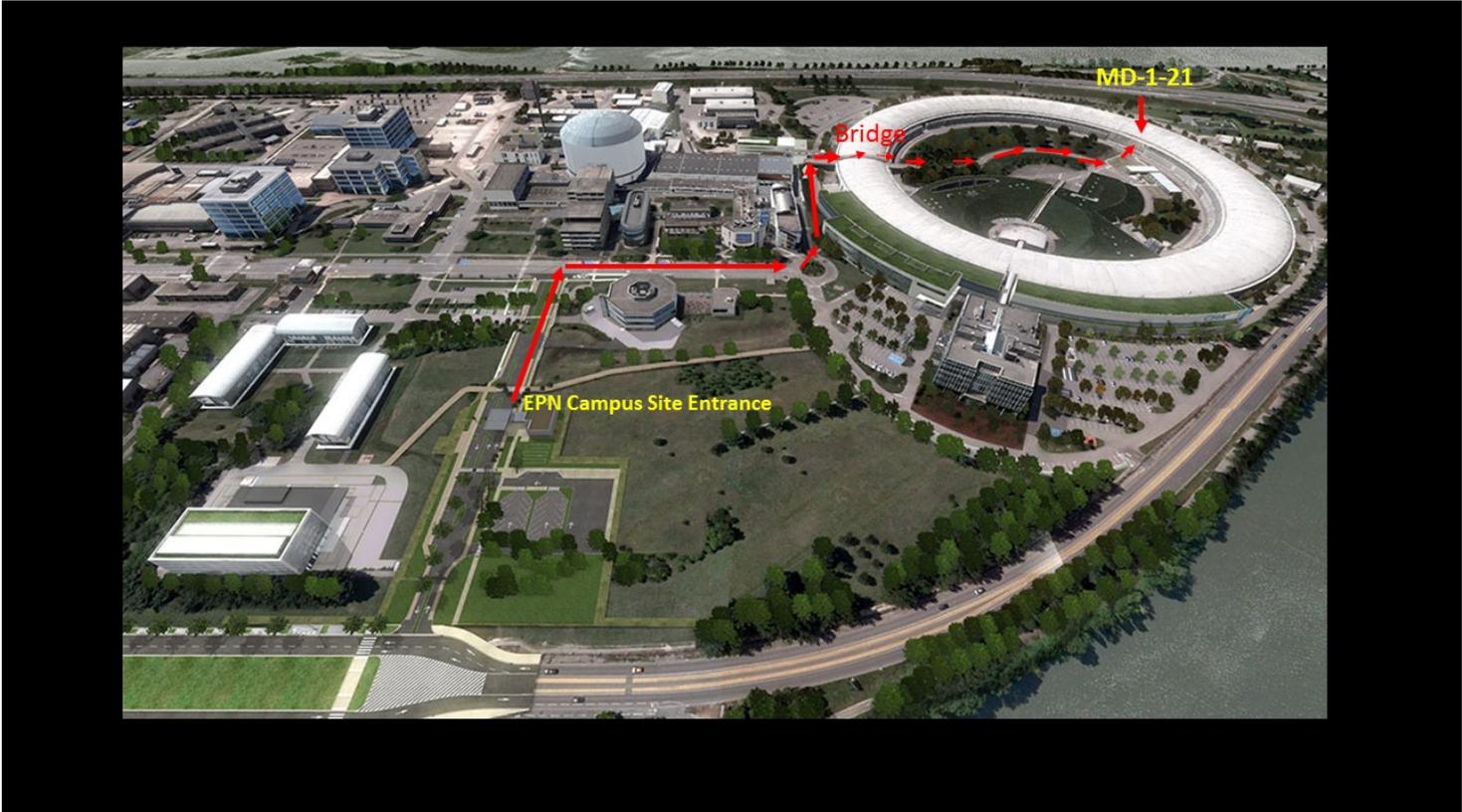


**Lunch -** EPN Campus Restaurant ground floor

# EPN Campus and seminar rooms



## How to reach MD1-21



# X-ray and neutron scattering for the characterization of glass structures

G.J. Cuello<sup>1</sup> G.B.M. Vaughan<sup>2</sup>

<sup>1</sup>Institut Laue Langevin, 71, av des Martyrs, BP 156, F-38042 Grenoble, France, [cuello@ill.fr](mailto:cuello@ill.fr)

<sup>2</sup>ESRF, The European Synchrotron, 71, av des Martyrs, BP 156, F-38042 Grenoble, France, [vaughan@esrf.fr](mailto:vaughan@esrf.fr)

X-ray and neutron scattering are powerful tools for the study of matter at the inter-atomic level, and have been used for over 100 years (in the case of X-rays) to determine precise and quantitative structures of crystalline materials. However, the classical and well-developed methods are based on diffraction from periodic systems, and are thus not directly applicable to amorphous materials such as glasses, where the scattering is not enhanced by constructive interference. Nevertheless, the elastic scattering signal from such materials contains information on their atomic arrangement, albeit in a more diffuse distribution.

Although the scattering from amorphous materials has been analysed for many years to give semi-quantitative descriptions of their structure, methods have been developed particularly over the last few decades to model these materials based on the Pair-Distribution function (PDF, see [1] for a recent review). These methods rely on scattering data measured in a (much) higher Q-range than traditional diffractions, as well as very careful treatment of background and other parasitic scattering for their application.

The advent of neutron sources and later high energy synchrotrons have allowed the collection of such data, and this, along with advances in analytical methods and available software have greatly increased the power and popularity of these methods in recent years. In these lectures we will describe the acquisition, reduction and analysis methods used to collect and treat the data in order to arrive at qualitative descriptions of local glass structures. The various methods employed and their relative advantage will be discussed, with examples drawn from recent work to illustrate the scope of the PDF method.

## References

[1] - Billinge, S. J. L., *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* **377**, 20180413 (2019) doi:10.1098/rsta.2018.0413.

# **X-ray absorption spectroscopy**

Y. Joly

Institut Néel 25 Rue des Martyrs 38042 Grenoble, France, **yves.joly@neel.cnrs.fr**

X-ray absorption spectroscopy is a synchrotron technique able to give information on the geometrical and electronical structures around chosen chemical element in all classes of material. Because it does not need long range order, it can be used to study glass. Our purpose will be to present the basics of this spectroscopy, the selection rules, the polarization dependence... We shall see the differences when using the extended part of the spectra (EXAFS) or the energy range close to the edge (XANES). The very close X-ray Raman Spectroscopy will also be presented with its specificities and sensitivity. The main paths to simulate the corresponding signals will be briefly given. Finally different examples will illustrate the ability of such tools to solve specific parameters.

# Chemical information in X-ray emission spectroscopy

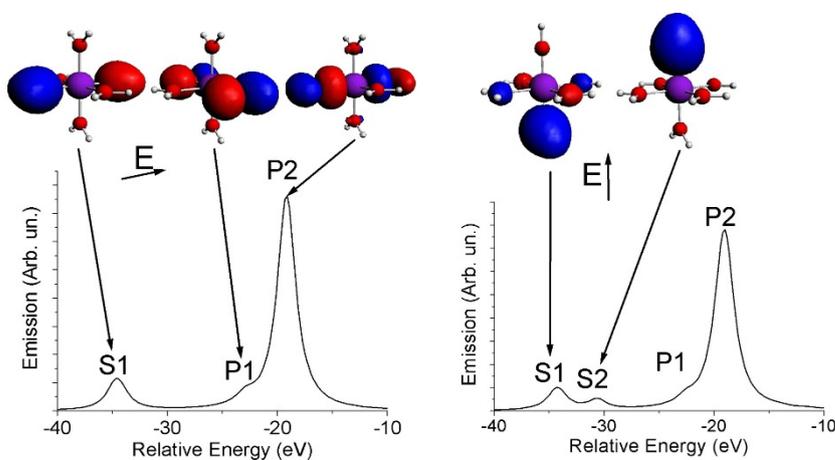
P. Glatzel<sup>1</sup>

European Synchrotron Radiation Facility, 71, avenue des Martyres, 38000 Grenoble, France, [glatzel@esrf.fr](mailto:glatzel@esrf.fr)

X-ray emission spectroscopy is a second order process following core shell ionization. The technique does not require a monochromatic incident X-ray beam and is thus attractive for applications at free electron lasers and pink beam synchrotron radiation beamlines. The past decades have brought significant new insight into the theoretical understanding of X-ray emission spectra which in turn considerably increased the value of the technique for time-resolved experiments.

The strong  $K\alpha$  and  $K\beta$  emission lines have been used with great success to characterize the spin state of a 3d transition metal ion. The much weaker valence-to-core lines give direct access to the valence electron configuration and thus contain a wealth of chemical information. However, obtaining sufficient data quality for a detailed analysis is challenging and pump-and-probe experiments.

The presentation will discuss some fundamental aspect of X-ray emission spectroscopy and address experimental challenges. I will also address resonant inelastic X-ray scattering (RIXS) for chemical applications. RIXS gives access to information that cannot be obtained in standard X-ray absorption spectroscopy.



**Figure 1:** Calculated valence-to-core X-ray emission spectra for  $[\text{Mn}(\text{H}_2\text{O})_6]^{2+}$ . The contributing molecular orbitals are shown.

## References

- [1] – P. Glatzel and U. Bergmann, *Coord. Chem. Rev.* **249**, 65-95 (2005)
  - [2] – E. Gallo and P. Glatzel, *Advanced Materials*, **26**, 7730-7747 (2014)
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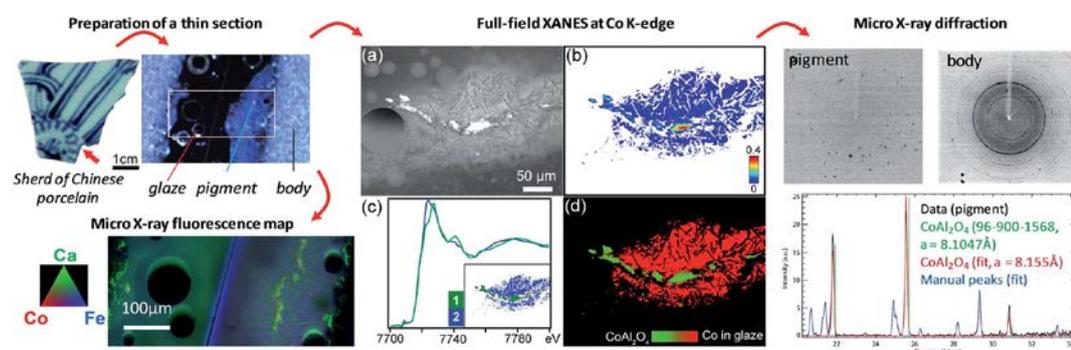
# Synchrotron-based micro-analyses for the study of ancient glasses

M. Cotte<sup>1,2</sup>

<sup>1</sup>European Synchrotron Radiation Facility (ESRF), 71 Avenue des Martyrs, 38000, Grenoble, France, [marine.cotte@esrf.fr](mailto:marine.cotte@esrf.fr)

<sup>2</sup>Sorbonne Université, CNRS, Laboratoire d'archéologie moléculaire et structurale, LAMS, 4 place Jussieu, 75005 Paris, France

Artistic and ancient materials are increasingly studied using synchrotron-based techniques [1]. Among the wide range of materials (from hard materials such as metals and alloys to soft materials such as fibres, passing through hybrid materials such as paintings), those based on vitreous matrices (glasses, ceramics) strongly benefit from the synchrotron beam properties. Notably, X-ray fluorescence can be used to obtain elemental composition. More importantly, X-ray absorption spectroscopy (XAS) is a key technique to obtain information about the speciation of elements of interest, even in amorphous system [2, 3]. In the particular case of ancient and artistic glass and ceramics, element speciation can enclose a memory of the reactions and chemical environment during the synthesis of the objects (choice of the ingredients, firing temperature, firing red/ox conditions). All these parameters, when well controlled, can provide the artisan with a variety of optical effects (color, opacity, lustre effect...) which translate into the quality of the object. XAS analyses can thus reveal how artistic and craft techniques evolved since Antiquity, over space and time. XAS measurements can be complemented with X-ray diffraction characterization, for example to obtain a more accurate identification of crystallized phases, pigments notably [4]. In addition to energy tunability, synchrotron sources offer a high brightness and produce collimated beams, which can be used to focus X-ray beams on probes of few microns, down to few tens of nanometers. This is essential considering the heterogeneity of the artistic materials. Micro-probes are necessary to selectively probe individual crystals and surrounding glassy matrix [5], or even to probe difference of speciation from the core to the surface of pigment particle [6].



**Figure 1:** Analyzing the origin of the colour in Chinese Qinghua blue decors (Ming dynasty) by a combination of  $\mu$ XRF, full-field XANES at Co K-edge and  $\mu$ XRD at ID21. Fragments were sampled from sherds (Top left).  $\mu$ XRF maps show particular concentration of Co and Ca in the pigment regions, and of Fe on the surface (Bottom left). Full-field XANES at the Co K-edge reveals the presence of two main Co species, in the pigment and in the glaze.  $\mu$ XRD offers further determination of Co pigment lattice parameters (right). From [7]

## References

- [1] Bertrand, L., et al., *Physics Reports*, **519**(2), 51-96 (2012).
- [2] Cotte, M., et al., *Accounts of Chemical Research*, **43**(6), 705-714 (2010)
- [3] Farges, F. and M. Cotte, *X-Ray Absorption Spectroscopy and Cultural Heritage: Highlights and Perspectives.*, in *X-Ray Absorption and X-Ray Emission Spectroscopy: Theory and Applications*, J.A.v.B.a.C.L. (eds), Editor. 2016, John Wiley & Sons: Chichester (UK). p. 609-636.
- [4] Wang, T., et al., *Analytica Chimica Acta*, **928**, p. 20-31 (2016).
- [5] Lahlil, S., et al., *Applied Physics A*, **100**(3): 683-692 (2010).
- [6] Verger, L., et al., *Journal of the American Ceramic Society*, **100**(1), 86-95 (2017)
- [7] Cotte, M., et al., *Journal of Analytical Atomic Spectrometry*, **32**, 477-493 (2017).

# X-ray Photoelectron Spectroscopy XPS

D. Foix

CNRS/ Univ Pau & Pays Adour, Institut des Sciences Analytiques et de Physico-chimie pour l'Environnement et les Matériaux, UMR5254, 64000, Pau, France, [dominique.foix@univ-pau.fr](mailto:dominique.foix@univ-pau.fr)

X-ray photoelectron spectroscopy (XPS), also named Electron Spectroscopy for Chemical Analysis (ESCA) allows the characterization of the extreme surface of materials (5-10nm depth). This technique is based on the photoelectric effect. Irradiated by a beam of X-rays, the sample emits photoelectrons. Their kinetic energy (KE) is measured. Knowing the energy of the incident Xray beam ( $h\nu$ ), the energy conservation law leads to the value of the binding energy (BE) of these photoelectrons. This binding energy characterizes a special orbital of one atom, and highlights the chemical environment of this atom. By this method, all the elements present in this surface are detected, except H and He. A photoelectron spectrum is recorded, representing the counts of detected photoelectrons over a range of kinetic energies. Peaks appear for each atom (and each orbital) present in the sample surface, their position (binding energy value) allowing elemental and chemical identification, and their area allowing quantification of each surface elements.

The fundamental principles of XPS will be presented, and we will discuss how this technique is suitable to assess "glass structure".

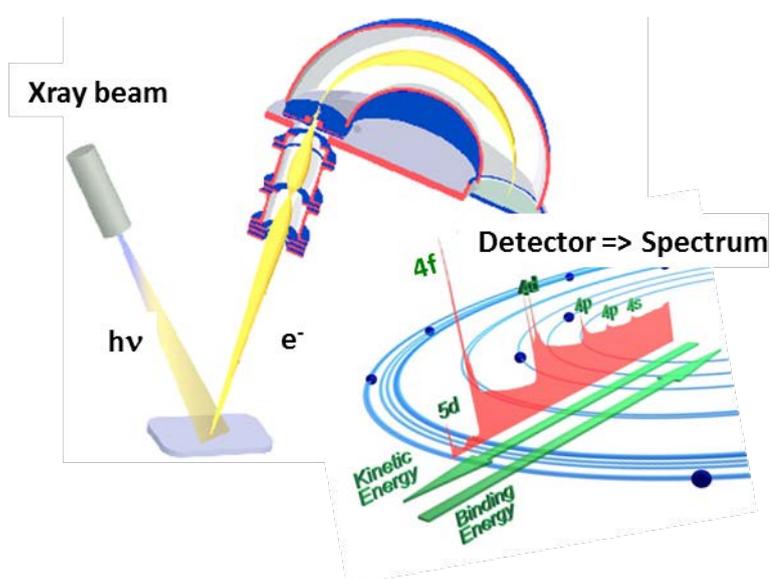


Figure 1: Xray Photoelectron Spectroscopy (XPS)

# Inelastic light scattering by atomic vibrations

B. Hehlen

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An introduction to the linear response theory will allow us to define the concepts of susceptibility, fluctuation spectra, autocorrelation function... and to connect these quantities through the fluctuation-dissipation theorem. We will then determine the origin of the scattering of light and calculate the Raman and Brillouin spectra within a (classical) macroscopic theory [1]. These calculations will reveal selection rules that will be applied to few examples taken from crystalline solids, liquids, and glasses [2].

## References

- [1] – B. Hehlen and R. Vacher “Light scattering by atomic vibrations” in “Teaching Glass Better” Ed. A. Takada, J. Parker, A. Duran, and K. Bange. ISBN 978-84-17528-04-1 (<https://www.sgt.org/books>).
- [2] – B. Hehlen and B. Rufflé, “Atomic Vibrations in Glasses”, to be published in “Encyclopedia of Glass” Ed. P. Richet, cond-mat arXiv:1908.08321.

# Contribution of infrared spectroscopy to the analysis of the glass structure

D. De Sousa Meneses<sup>1</sup>

<sup>1</sup> CNRS, CEMHTI UPR3079, University Orléans, F-45071 Orléans, France, [desousa@cnrs-orleans.fr](mailto:desousa@cnrs-orleans.fr)

Infrared spectroscopy is a unique tool to retrieve information on the glass structure from polar vibrational modes and its temperature dependence. This course gives clues to select, for fixed measurement conditions, the most adapted measurement technique. Particular lighting will be given on the use of thermal radiation to characterize the infrared response of glasses and melts. We will show using the Kirchhoff's law, that emission spectroscopy constitutes a very efficient mean to deal with the high temperature range [1]. Dielectric function models able to reproduce the electromagnetic response of disordered materials [2, 3], that is to say capable of taking into account a homogeneous and inhomogeneous broadening of vibrational modes, will be introduced (Figure 1).

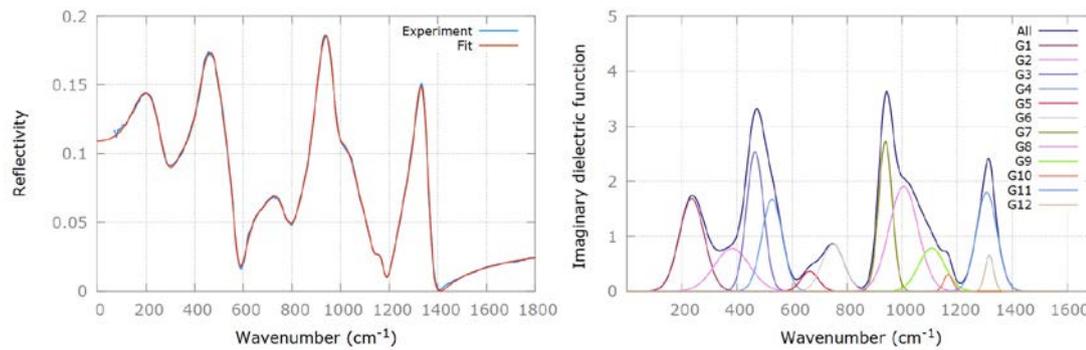


Figure 1: Reflectivity spectrum of a glass of the CaO-PO<sub>4</sub> system and its band decomposition.

A curve fitting software [4] specially developed to analyze infrared spectra allows to implement these kind of dielectric function models based on causal Gaussian and Voigt profiles. The efficiency of these mathematical expressions will be discussed through the fit of a large number of reflectivity spectra. We will discuss also how to extract microstructural information from the band decomposition.

## References

- [1] - D. De Sousa Meneses, P. Melin, L. Del Campo, L. Cosson and P. Echegut, *Infrared Physics & Technology* **69**, 96 (2015).
- [2] - D. De Sousa Meneses, G. Gruener, M. Malki and P. Echegut, *J. Non-Cryst. Solids* **351**, 124 (2005).
- [3] - D. De Sousa Meneses, M. Malki and P. Echegut, *J. Non-Cryst. Solids* **352**, 769 (2006).
- [4]- Focus website: <http://www.cemhti.cnrs-orleans.fr/pot/software/focus.html>

# Solid-State NMR: from basics to more advanced concepts

Dominique Massiot, Pierre Florian

CEMHTI UPR3079 CNRS, Orléans Dominique.massiot@cnrs-orleans.fr & Pierre.Florian@cnrs-orleans.fr

Solid State Nuclear Magnetic Resonance spectroscopy allows to examine the structure and dynamics around the observed nuclei selectively excited at their Larmor frequency. The spectral signatures obtained in NMR experiments translate (i) the shielding of the principal field (chemical shift anisotropy), (ii) the interactions between spin bearing nuclei (dipolar couplings and J couplings) and (iii) the Electric Field Gradient (for quadrupolar nuclei), giving an indirect image of the coordination sphere, possibly up the sub nanometer scale.

We will introduce the basic solid-state NMR methods, discuss the acquisition of one dimensional spectra, measurement of relaxation times and introduce advanced concepts put to work in multi-dimensional experiments. The example will focus on inorganic materials showing order and disorder.

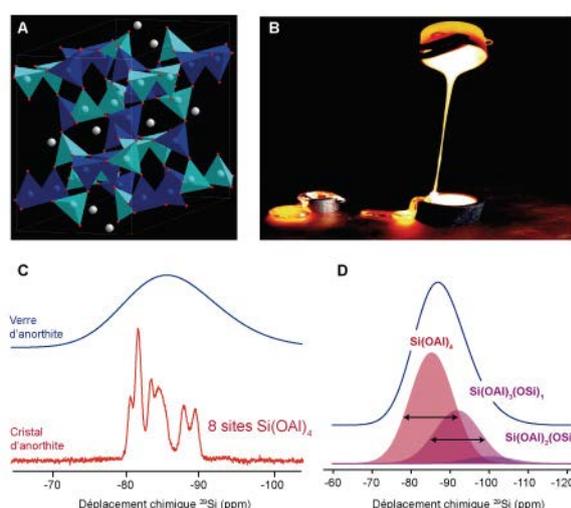


Illustration of  $^{29}\text{Si}$  MAS NMR of crystalline and glassy samples.

## References

- [1] - F.Babonneau, C.Bonhomme, C.Gervais, T.Azaïs, O.Lafon, L.Montagne, J.P.Amoureux, T.Charpentier, F.Angeli, F.Fayon, M.Deschamps, S.Cadars, P.Florian, D.Massiot, 'Les spins nucléaires : des espions pour explorer la structure des matériaux', *Acutalité Chimique*, 364-365 73-81 (2012)  
<http://www.cemhti.cnrs-orleans.fr/Publications/Pubview.aspx?Id=7834>
- [2] - D.Massiot, R.J.Messinger, S.Cadars, M.Deschamps, V.Montouillout, N.Pellerin, E.Veron, M.Allix, P.Florian, F.Fayon, 'Topological, Geometric, and Chemical Order in Materials: Insights from Solid-State NMR', *Accounts Chem. Res.*, 46 1975–1984 (2013) doi:10.1021/ar3003255  
<http://www.cemhti.cnrs-orleans.fr/Publications/Pubview.aspx?Id=10003>

# Dynamical properties of glass formers probed with coherent X-rays

B. Ruta<sup>1</sup>

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The continuous improvement of brilliance and coherent flux in modern X-ray sources has led to the emerging of new techniques able to probe physical properties in hard materials at the atomic level. This is particularly the case for X-ray photon correlation spectroscopy (XPCS), a technique that measures the intensity fluctuations of coherent diffuse scattering to track slow collective dynamics at the nanometric and atomic scale in complex soft and hard materials [1].

In the last years, XPCS has been successfully applied to the investigation of the microscopic relaxation processes occurring in metallic [2-4] and oxide glass formers [5,6] during the vitrification process and in the deep glassy state. These experiments revealed a complex dynamical scenario which cannot be described by any current microscopic theory for glasses.

In this talk, I will discuss these works together with future scientific possibilities offered by XPCS at the current Extremely Brilliance Sources (EBS) upgrade of ESRF. The new source will allow to extend dramatically the dynamical range of XPCS, opening the field to new ground breaking experiments like the investigation of dynamical heterogeneities in complex materials and of the atomic motion under extreme conditions of temperature and pressure.

## References

- [1] - A. Madsen, A. Fluerasu and B. Ruta, *Synchrotron Light Sources and Free-Electron Lasers*, Springer International Publishing, 2015, pp. 1–21.
- [2] - B. Ruta et al. Topical Review, *J. Phy.: Cond. Matter* **29**, 503002, 2017
- [3] - A. Das et al. *Nat. Commun.* **10**, 50006, 2019
- [4] - S. Hechler et al. *Phys. Rev. Mat.* **2**, 085603, 2018
- [5] - B. Ruta et al. *Scient. Rep.* **7**, 3962, 2017
- [6] - G. Pintori et al. *Phys. Rev. B*, **99**, 224206, 2019

# Computer simulation of glasses

Miguel A. González<sup>1</sup>

<sup>1</sup>Institut Laue-Langevin, 38042 Grenoble, France, [gonzalezm@ill.fr](mailto:gonzalezm@ill.fr)

Computer simulations are an excellent method to complement experimental probes in order to study the structure of glasses. They can provide reliable microscopic models of the arrangement of the atoms in the glass, allowing to get detailed insights on the short and medium-range structure. Here I will present briefly the basics of Monte Carlo and Molecular Dynamics simulations, in combination either with effective interaction potentials or using Density Functional Theory to perform fully *ab initio* simulations. Then the possibilities offered by simulation will be illustrated through a few selected examples.

# Access to large scale facilities: opportunities for industry and academia

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Large scale facilities offer powerful analysis methods for the comprehension of the glass structure – and are arguably *the* ultimate means of characterisation in our age. Unfortunately the use of these techniques requires specialised skills that could refrain potential users from carrying out experiments and measurements. To mitigate this ‘knowledge gap’ several initiatives dedicated to both industry and academia have appeared with the aim of supporting users in their access to these facilities.

Moreover, in Europe and worldwide, funding agencies are requesting and demanding a stronger economic return from the significant public investments made in such research facilities and this is resulting in firm pressure for stronger interactions with industry. In this context, new business models are springing to life, with more partnerships, more services, and nimble small start-ups bridging the gap between the oft “ivory tower” nature of research infrastructure and the commercially driven industry world. In most facilities Business or Industry Liaison Offices have the mission to engage with industry with the aim to generate income and impact in supporting work to solve real-world R&D problems. These offices put in place specific commercial services, access models, dedicated platforms and beamline environments, as well as creative partnerships to attract industry.

Also from the point of view of academic users there are initiatives such as the IPANEMA [1] platform dedicated to scientists in the cultural heritage field or the NFFA platform [2] for nanosciences. The scope of these platforms is to provide the potential users with the tools to access different experimental techniques and support them in the phases of proposal submission and experimental design.

## References

[1] - <http://ipanema.cnrs.fr/>

[2] - <https://www.nffa.eu/>

# X-ray Absorption Near Edge Spectroscopy simulations

O. Proux<sup>1</sup>, Y. Joly<sup>2</sup>

<sup>1</sup>Univ. Grenoble Alpes, CNRS, IRD, Irstea, Météo France, OSUG, FAME, 38000 Grenoble, France,

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X-ray Absorption Spectroscopy (XAS) allows to probe the speciation of a target element, *i.e.* its valence state and the local order around it, by analysing the variation of the absorption cross-section crossing an electronic level characteristic of the element of interest, close to this edge (the X-ray Absorption Near Edge Spectroscopy or XANES region) or from ~50eV to ~1000eV after the edge (the Extended X-Ray Absorption Fine Structure or EXAFS region). This analytic technique can be apply to every kind of material, in their amorphous to crystallized states, and so is very well-adapted to the study of glass or glassy structure.

XANES can be analysed by i) comparing the “unknown” spectra to reference ones and/or ii) by simulating them using reference structure or distorted ones. The aim of the tutorials is to use this second approach to show the XANES sensitivity to several crystallographic and electronic parameters using the FDMNES code [1]. This code can be used either using the multiple scattering calculation approach (using the muffin-tin approximation of the electronic potentials) or by solving the Schrödinger equation in the cluster using the Finite Difference Method (FDM). The first method is faster than the second one, but the made approximation can limit its application to high-symmetry site-geometry. During the tutorial we will performed numerical experiments on different samples described as on the input file (Fig. 1).

# Introduction to EXAFS data analysis

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This tutorial is focused on the quantitative analysis of EXAFS data. The free code 'DEMETER' [1] will be used at this purpose on a simple case of metallic copper. In the first part the methods for data extraction and normalization will be described evidencing the pitfalls typically encountered by the beginners. A second part will be devoted to the analysis of the first coordination shell with the ab-initio calculation of backscattering functions and quantitative fit of the data. In the third part a multi-shell fit of the data will be presented evidencing the use of multiple-scattering paths and methods for reducing the number of free fit parameters. Participants will carry out the complete analysis on their laptops.

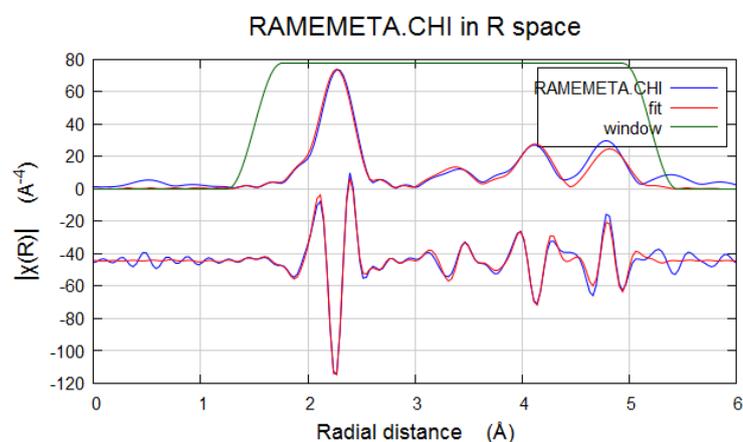


Figure 1 : Example of a multi-shell fit of metallic Cu.

## References

[1] B. Ravel and M. Newville, *ATHENA, ARTEMIS, HEPHAESTUS: data analysis for X-ray absorption spectroscopy using IFEFFIT*, Journal of Synchrotron Radiation **12**, 537–541 (2005) doi:10.1107/S0909049505012719

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# X-ray spectroscopy simulations using Crispy

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Theoretical predictions have played a central role in interpreting experimental measurements. However, despite the insights offered, theoretical methods have remained the domain of experts with limited adoption by the non-specialists.

It is in this context that Crispy was developed. The goal of the project was to provide an intuitive graphical user interface to calculate the experiments performed on spectroscopy beamlines. With the current version, it is possible to easily perform X-ray absorption, X-ray emission, and resonant inelastic X-ray scattering simulations for transition metals, lanthanides, and actinides for different site symmetries of the absorbing atom.

The goal of the tutorial is to familiarize the participants with the simulation of core-level spectra using semi-empirical multiplet approaches. Following a short introduction to the theoretical aspects, hands-on training will be given. This will include examples of simulating X-ray absorption and resonant inelastic X-ray scattering spectra for transition metals.

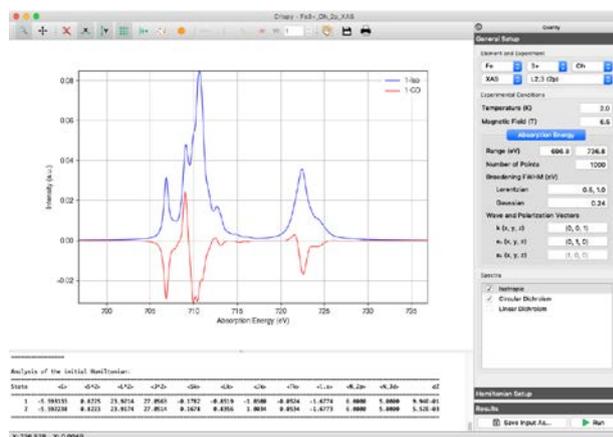


Figure 1: The main window of Crispy showing the calculated spectra for an  $Fe^{3+}$  complex.

# **Measuring structural relaxations and stability of glasses by X-ray Photon Correlation Spectroscopy**

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In the frame of the lecture describing how dynamics in glasses can be revealed by X-ray Photon Correlation Spectroscopy (XPCS), the practical will focus on the coherence properties of the EBS source and the methodology of the XPCS technique. Assessing slow structural relaxation in glasses at the atomic length scale is challenging. Only recently, owing to the increase in coherent flux, progress in detector technology and development of optimized algorithms, XPCS has emerged as a unique and powerful method to study glassy dynamics at microscopic level. In this practical we will show you the essential steps and tools to analyze the measured data and extract useful information such as speckle contrast, structural relaxation time and quantify ageing process. We will use real data to demonstrate all stages of analysis and teach you key concepts applied to glasses.

## **Poster Contribution**

### **1) Pressure-induced densification of vitreous silica: Insight from elastic properties**

Authors: Sébastien Clément, Marie Foret, Marouane Mebarki, Benoit Rufflé, René Vacher, Coralie Weigel

### **2) Towards a better understanding of order and disorder in inorganic materials with NMR spectroscopy**

Authors: Franck Fayon, Dominique Massiot, Laura Piveteau

### **3) Complexity and Boson peak in metallic glasses**

Authors: Emil Babić, Katica Biljaković, Damir Dominko, I. A. Figueroa, Georgy Remenyi, Amra Salčinović Fetić, Suada Sulejmanović, Damir Starešinić

### **4) Semi-amorphous phase in sustainable cements**

Authors: Maria Chiara Dalconi, Ludovico Mascarin, Luca Valentini

### **5) Short Range Order in Amorphous Ice**

Authors: Neta Ellert, Guy Makov

### **6) Mixed network former effect in sodium ion conducting phosphate glasses**

Authors: L. Koudelka, A. Moguš-Milanković, P. Mošner, L. Pavić, A. Šantić, K. Sklepić Kerhač, G. Tricot

### **7) Probing In-Situ Crystallization Pathways in Lead Metasilicate Glass**

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### **8) High-Pressure Plastic Deformation of Lead Metasilicate Glasses Accessed by Vibrational Spectroscopy**

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### **9) Glass transition of antiferroelectric smectic CA\* phase of 3FmHPhF compounds studied with XRD and FT-IR methods**

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### **12) PHASE RELATIONS IN HYDROUS REE-BEARING CARBONATITE AT 1 GPA, 700-1250°C.**

Authors: Patrizia Fumagalli, Marco Merlini, Sula Milani, Stefano Poli, Deborah Sparta