Introduction: Historical Perspective on XAS

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Historical perspective of XAS and a brief introduction to the book
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1. Historical overview on 100 years of X-ray absorption: a focus on the pioneering 1913–1971 period

The X-ray absorption spectroscopy (XAS) adventure started about one hundred years ago and has travelled some way since. The technique remained a curiosity for much of this time, representing a minor branch of science, developed by only a few highly motivated and enthusiastic scientists. without any apparent possibility of practical applications and without a solid and comprehensive theory able to describe and predict the experimental observations, on gases, liquids and solid (crystalline and amorphous) systems. In 1971, Sayers, Stern, and Lytle made ground-breaking progress when they applied Fourier analysis to the point-scattering theory of X-ray absorption fine structure, so as to formally invert the experimental data (primarily collected in the photoelectron wave-vector space) into a radial distribution function. For the first time they were able to quantitatively determine structural parameters, such as bond distance, coordination number, as well as thermal and disorder parameters [1]. In the 44 years following that key publication the field developed exponentially. Nowadays it is impossible to imagine frontier research in materials science, solid state physics and chemistry, catalysis, chemistry, biology, medicine, earth science, environmental science, cultural heritages, nanoscience, etc. without the contribution of XAS and related techniques. In the following chapter we provide a brief sketch of the main events that have established XAS and related techniques as a leading scientific characterization tools.

After the discovery of X-rays in 1895 by Röntgen [2,3] it took a while before the first X-ray absorption spectrum was observed by de Broglie in 1913 [4]. De Broglie mounted a single crystal on the cylinder of a recording barometer, using the clockwork mechanism to rotate the crystal around its vertical axis at constant angular speed. As the crystal rotated, the X-rays scattered at all angles between the incident beam and the diffraction planes hence, according to the Bragg law ($2d_{hkl} \sin \theta = \lambda = hc/E$, being c the speed of light, c = 2.9979 10^{+8} m/s, and h the Plank constant h = 6.626 × 10^{-34} J s [5], so that hc = 12.3984 Å keV) [6-8], changing X-ray energies E. X-rays of varying intensities were recorded on a photographic plate. Two distinct discontinuities were observed on the film, which were found to be independent of the setting of the X-ray tube. These proved to be the K-edge absorption spectra of silver and bromine atoms contained in the photographic emulsion. As the spectrographic dispersion was poor at these short

wavelengths, the spectra were of low energy resolution and the fine structure was not resolved. Successive works by De Broglie in this field proved remarkable[9,10]. *A posteriori*, it is curious to note that de Broglie's famous intuition concerning the association of a wavelength (λ) to any massive particle with momentum (*p*): $\lambda = h/p$ [11], is actually the key for understanding the phenomenon related to the fine structure of the X-ray absorption spectra.

Moseley published in 1913 his empirical law describing the frequencies (energies, $E = h\nu$) of certain characteristic X-rays emitted from pure elements; named K_α and L_α lines according to the successive Siegbahn notation. Emission energies were found to be approximately proportional to the square of the element atomic number Z [12]. This finding supported Bohr's model of the atom [13-15] in which the atomic number corresponds to the positive charge of the nucleus of the atom measured in |e| units: |e| =1.602 10^{-19} C. Almost 50 years after Mendeleev's milestone work Moseley's findings suggested that atomic weight A was not a significant player in the periodicity of physical and chemical properties of the elements within the periodic table. In contrast, the properties of the elements varied periodically with atomic number Z. This X-ray emission study is historically important because it quantitatively justifies the nuclear model of the atom, where the atom's positive charge is located in the nucleus and associated on an integer basis with atomic number. Until Moseley's work, "atomic number" was merely a label to identify the place of each element in the periodic table, and was not known to be associated with any measureable physical quantity.

In 1916 Lund, Sweden, Siegbahn and Stenström [16-18] developed the first vacuum X-ray spectrometer [19,20] (Figure 1a), making a fundamental technological step toward X-ray spectroscopy advancement. With this kind of innovative technology, the fine structure beyond the absorption edges of selected atoms was - for the first time - experimentally observed by Fricke in 1920 [21] and by Hertz [22]. Frick detected the K-edges for the elements from magnesium (Z = 12, E_0 = 1.3 keV) up to chromium (Z = 24, E_0 = 6.0 keV) [21], whereas Hertz canvassed the L-edges of cesium (Z = 55, E_0 = 5.0 keV) up to neodymium (Z = 60, E_0 = 6.2 keV) [22]. In the period before World War II, other authors reported analogous behaviors on several different absorption edges [20,23-37].

Hanawalt made remarkable observations in 1931 [20], observing that the chemical and physical state of the sample affects the fine structure of the corresponding XAS spectra. Using the experimental set-up reported in Figure 1a, consisting of a quartz cell allowing XAFS spectra of different molecules sublimated in the vapor phase to be acquired, and collecting XAFS spectra on a photographic plate (Figure 1b), he was able to reach two empirical observations of fundamental importance. Firstly, he proved that substances sublimating in the molecular form, like arsenic ($4As_{solid} \rightarrow (As_4)_{gas}$) or $AsCl_3$ (Figure 1c), are characterized by XAFS spectra exhibiting different fine structures above the edge when measured in the solid or in the vapor phases. Secondly, he observed that the monatomic vapors of zinc (Figure 1d), mercury, xenon, and krypton elements exhibit no secondary structure. These incredibly advanced experiments already captured the main messages of EXAFS spectroscopy, but needed several years for correct interpretation and decades before quantitative data could be extracted and the full potential of EXAFS exploited [1].
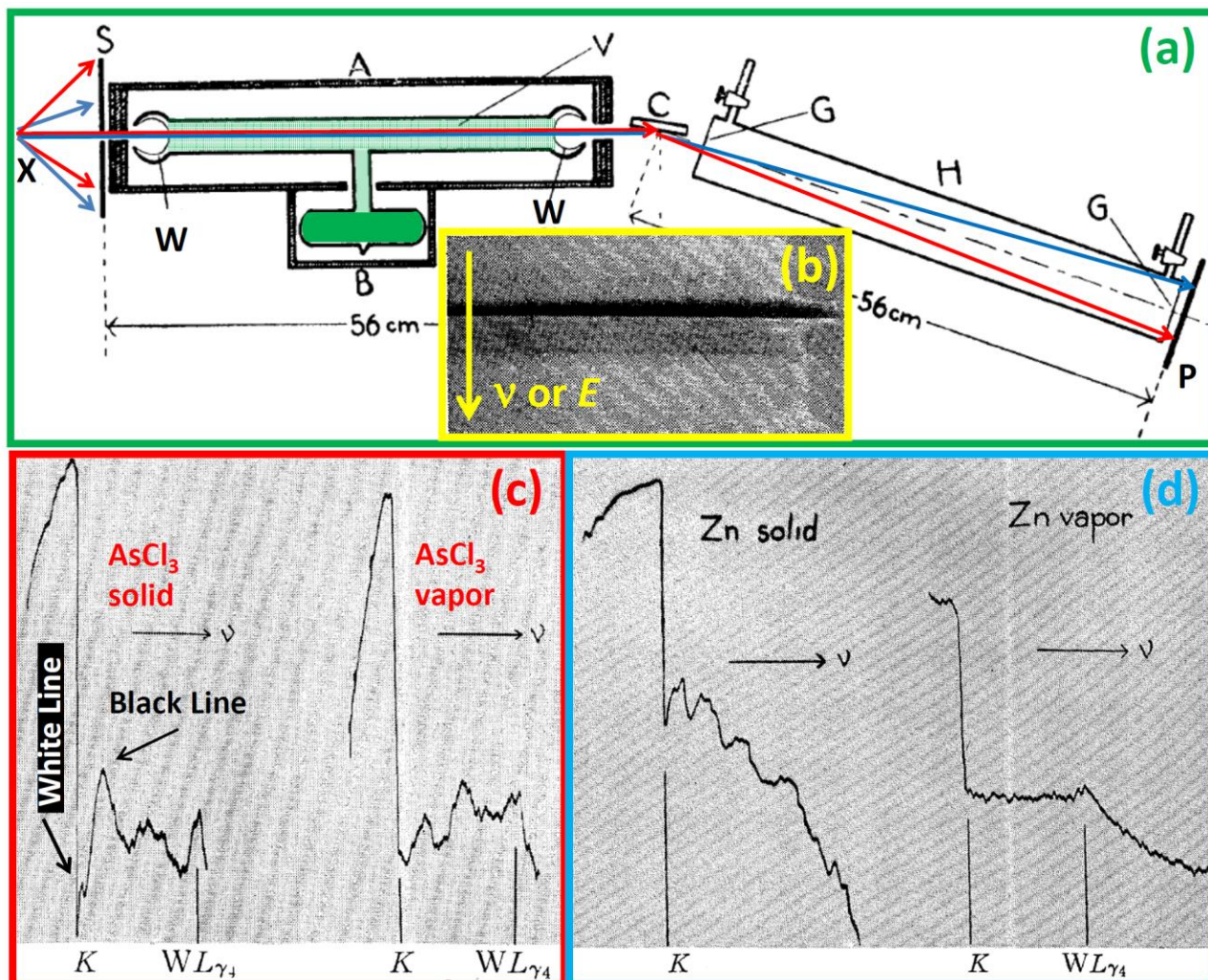
Figure 1. Part (a): Scheme of the vapor cell and X-ray spectrometer used by Hanawalt [20] to measure the fine structures in K-edge X-ray absorption spectra of molecules in the vapor phase. The cell was composed of: two furnaces (B and A), the former for hosting the solid phase and controlling the vapor pressure via the temperature, the latter for preventing re-condensation of the evaporated phase; a long quartz tube hosting the vapor phase (V) equipped at the end by two concave windows (W) as thin as 3 μm so as to maintain a vacuum and remain sufficiently transparent to X-rays. The spectrometer consists of: an X-ray tube of the Siegbahn type (X); slits used to collimate the incoming X-rays (S); a calcite ($CaCO_3$) crystal used as monochromator (C); a quartz tube fluxed with H_2 (H) and equipped with biological X-ray transparent membranes (G) acting as windows; and a photographic plate used as detector (P). This spectrometer was able to cover the 4.9−12.4 keV spectral region, corresponding to 2.5 Å > λ > 1.0 Å and represents the historical prototype of a dispersive spectrometer (see chapter 8 of this book [38]). Depending on the absorbing gas, a time ranging from 4 to 30 h is needed to impress the photographic plate as shown in part (b), where the energy increases from top to bottom. The adsorption edge and the successive modulations are clearly visible in part (b). The photographic images were then converted into absorption-energy plots like those reported in parts (c) and (d) for $AsCl_3$ (As K-edge at 11.8 keV) and Zn (K-edge at 9.6 keV), respectively. Because only I_1 is measured in the set-up, the spectra appear *inverted*. The first resonance after the edge, representing a maximum in the absorption was named *white line* while the successive minimum in the absorption spectrum was named *black line*. The former term is retained in the current terminology, whereas the latter is lost. Adapted with permission from Ref. [20]. Copyright 1931 American Physical Society.

The first theoretical attempt to explain fine structure in the XAS spectra was proposed in the years 1931-32 by Kronig [39,40], who developed a model based on the presence of long-range order in the probed system. The Kronig long-range order theory can be summarized in the following equation: $W_n = h^2(\alpha^2 + \beta^2 + \gamma^2)/[8md^2 \cos^2(\theta)]$, where W_n are the energy positions corresponding to the zone boundaries (i.e. not the absorption maxima or minima, but the first rise in each fine-structure maximum); h is the Planck's constant; m is the electron mass; α, β, γ are the Miller indices; d is the lattice parameter and θ is the angle between the electron direction and the reciprocal lattice direction. The Kronig long-range order equation was fundamentally simple to apply and interpret, and experimental spectra presented an approximate agreement with the theory. For any observed absorption features there were always some (α, β, γ) triplet able to match the experiment with the prediction of the Kroning's model. However, the stronger Bragg reflections of the lattice did not always correlate with the most intense absorption features of the EXAFS spectra, as intuitively expected. However, agreement was tantalizingly close and the equation was uniformly implemented as a check for measured data to obtain a "Kronig structure".

As we now know, this theory is intrinsically incorrect owing to its baseline assumptions, which do not accurately explain the EXAFS signals observed in gases, liquids, solutions and amorphous solids. Stimulated by the experiments of Hanawalt [20] (see Figure 1), even Kronig himself presented a new theory in 1932 based on the fundamental role of short-range order to explain the fine structure observed in the spectra of diatomic molecules [41]. The new approach explained the XAFS features in terms of modulation of the wave function of the final state of a photoelectron upon its scattering from the potentials of neighboring atoms. Implemented successively by Petersen [42-44] and by many other authors in the 1930-60s [45-61], this approach represents the basis of the modern concept of XAFS, although it was still unable to provide quantitative information on the local structure of the absorbing atom in the investigated samples. At that stage, XAFS was still just a spectroscopic curiosity and not yet a powerful characterization tool. In most reported cases [20,21,25,30,34,50,60,62] the discussion was limited to a table containing a list of the observed maxima and minima of the fine structure of a given material, and a comparison of these values alongside those predicted by the other theories of the time, *vide supra*. No quantitative information was extracted and only qualitative conclusions could be reached. Some relevant, although qualitative, conclusions are mentioned here: (i) several authors observed that the amplitude of the XAFS oscillations decreases with increasing temperature [31,57,59,61], (ii) it was observed that metals with the same crystal structure had similar fine structures [24,30,33,34], (iii) in 1957 Shiraiwa *et al.* [54] measured the X-ray absorption spectra of crystalline and amorphous germanium observing that the shape of the fine structure was the same on the two materials though oscillations were less intense and disappeared at lower energies in the amorphous phase than in the crystalline phase. Similar conclusions were reached in 1962 by Nelson *et al.* [58] who measured germanium(IV) oxide in the amorphous state and in both hexagonal and tetragonal crystalline forms.

From an experimental point of view, a fundamental improvement in the instrumentation was achieved in the sixties when commercial diffractometers were modified so that absorption spectra of much better quality could be obtained, although still using conventional X-ray tubes as a source [62-64]. A silicon crystal, acting as a single-crystal monochromator, was positioned on a goniometer configured to allow step scaling. Diffraction experiments carried out using this assembly allowed scientists to scan the energy through the desired absorption edge. By mounting and dismounting the sample in the beam path, both I_1 and I_0 could be detected, thereby

allowing a precise determination of the absorption coefficient $\mu(E) = \ln[I_0(E)/I_1(E)]$. With this experimental set-up Van Nordsthand [63,64] performed a systematic study on many transition metal compounds and classified their XANES spectra according to the atomic structure and valence of the metal element in the compound, also noting the chemical shift with valence. This fingerprint classification was used to identify the structural/valence form of elements of interest in catalysts, which are usually so highly dispersed that their diffraction patterns cannot be measured. This work by Van Nordsthand was the first example of the application of XANES in catalysis.

The crucial advance in the interpretation of the post-edge oscillations (now referred to as EXAFS) occurred in 1971 [1], when it was shown by Sayers, Stern, and Lytle that a Fourier transform of the background-subtracted oscillations (Figure 2a) gives a pattern in R-space close to the function of radial distribution of atomic density (Figure 2b). From the EXAFS spectra collected on crystalline and amorphous germanium they were able to extract the following quantitative structural information: (i) the crystalline distance to first and second neighbors in amorphous germanium within 1% accuracy; (ii) by comparing the relative second-shell-peak intensities of the crystalline and amorphous samples, the authors were able to conclude that the Debye-Waller factor is six times larger in the amorphous phase; from this they deduced that the tetrahedral bonds are distorted by about 5° in the amorphous phase [1]. To achieve these insights must have been extremely exciting. It is remarkable that such accurate conclusions were obtained while working with experimental spectra collected using an X-ray tube as a source.
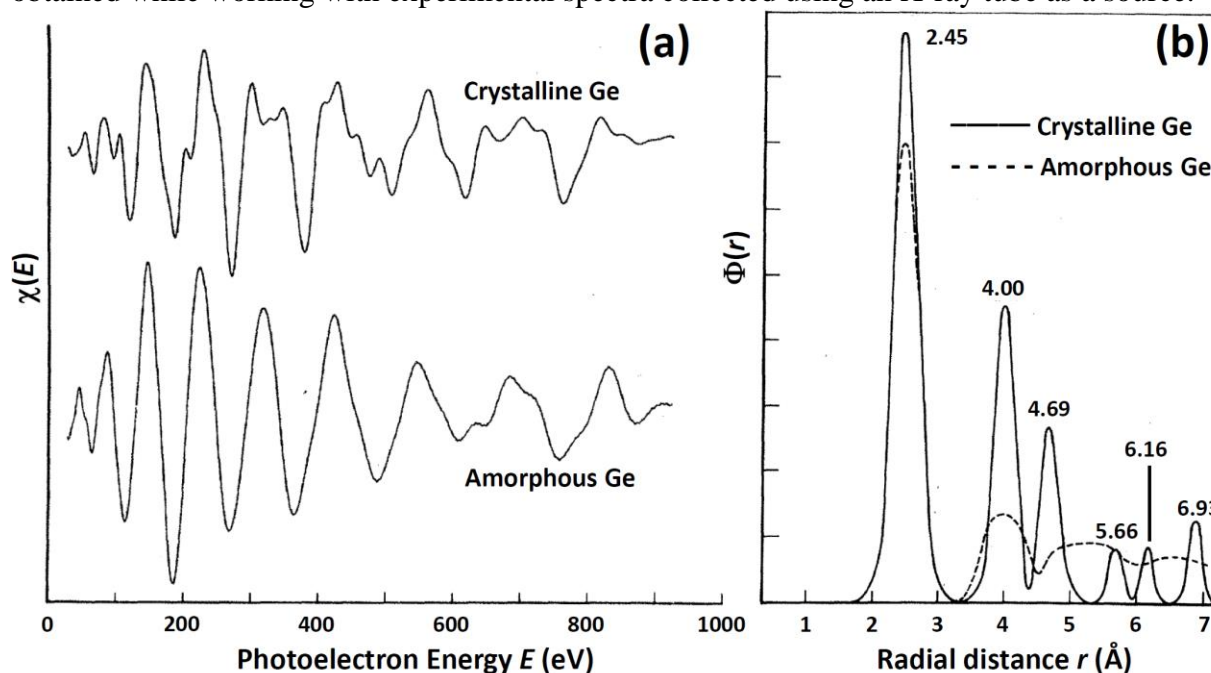
Figure 2. Part (a): Smoothed experimental EXAFS data for crystalline (top) and amorphous (bottom) germanium, plotted as a function of the photoelectron energy E. Part (b): Fourier transform of the EXAFS functions reported in part (a). The numbers over the peaks indicate the measured distances in Å. Adapted with permission from Ref. [1], copyright APS, 1971.

This work represented the milestone for EXAFS spectroscopy and was supported and further implemented in more formal derivations based on Green's function and generalization to

muffin-tin scattering potentials. This development was performed by successive works by Sayers, Stern, and Lytle and co-authors [65-69] and from other independent groups [70-74].

Starting in the seventies, the cumulative availability of several and progressively more brilliant and broadband synchrotron radiation sources [75-79] established EXAFS and XANES spectroscopies (and successively XES) as a reliable tool to determine and understand the structural and electronic configuration of unknown systems. During the eighties and nineties in particular, development and the distribution of codes for data analysis saw a rapid expansion of EXAFS and XANES spectroscopies into the broader scientific community for the purposes of structural characterization of materials. Among the many data processing packages available we only mention: GNXAS [80-84], developed by Natoli, Filipponi and Di Cicco; EXCURVE [85-88] by Binsted *et al.*, and FEFF [89-101] developed by Rehr *et al.* A plethora of codes developed in the last two decades were conceived with the intention of using theoretical phases and amplitudes generated by the different releases of FEFF. This is particularly relevant because packages, such as FEFFIT [102,103], had a huge impact in making the EXAFS data analysis more "user-friendly" and thus accessible. FEFFIT is developed by Newville, and the ATHENA, ARTEMIS, HEPHAESTUS package are developed by Ravel and Newville [104]. For a more complete overview on the codes developed for EXAFS data analysis see the recent review by Bordiga et al. [105].

Overall the impact of XAS on a variety of scientific disciplines was boosted by (i) the existence of a solid theory allowing a quantitative analysis of the XAS spectra [1], (ii) increased availability of beamlines at synchrotron radiation facilities allowing high quality XAS spectra to be collected, and (iii) development of reliable codes allowing data analysis to be made in a safe, reproducible and controllable way. The improved usability of XAS is self-evident on *ISI web of Science* in the period between 1971 and (main part of Figure 3). The milestone of one hundred papers per year was reached and passed in the year 1981. At that stage, the community was sufficiently mature to organize the first XAFS conference (XAFS I) at Daresbury (United Kingdom), with a total of 27 papers published in the proceedings. The community progressively grew, reaching 1000 published papers in 1995 and more than 1500 from 2005 onwards. Statistics concerning papers published in the proceedings of the XAFS conferences from XAFS I to XAFS XIV (Camerino, Italy) has been reported in Table 1 of Ref. [105]; XAFS XV conference (Beijing, China) published 136 papers in its proceedings in *J. Phys.: Conf. Ser.*, **430** (2013). Strong correlations are observed between the date of conference proceedings and the number of papers published by the XAFS community (the years labeled with a Roman numeral correspond to the conference which proceedings were published that same year). Notwithstanding this fact, the trend is clear - the community publishes close to 2000 papers per year. When X-ray emission is included in the tally, this number is in excess of 2000 (inset in Figure 3). We believe that the number of possible publications is limited by access to synchrotron radiation. At synchrotrons, X-ray absorption beam lines are among those with the highest oversubscription. High oversubscriptions clearly indicate the high demand of XAS experiments from the overall scientific community and suggest that a larger number of papers per year would be published if more beam time were available.

The inset of Figure 3 describes an analogous bibliographic research for the papers related to XES in the 1985-2014 time span. The number of papers is much lower but a similar upward trend is observed. This community has passed the threshold of 50 papers per year in 1988, doubling in volume since 2010. In this case, the number of papers per year is even more severely limited by the accessibility to high flux beamlines equipped with sophisticated crystal analyzers

that are described in Chapter 6 of this book [106]. More and more beamlines are installing crystal analyzers, heralding a steep development of this technique in the near future.
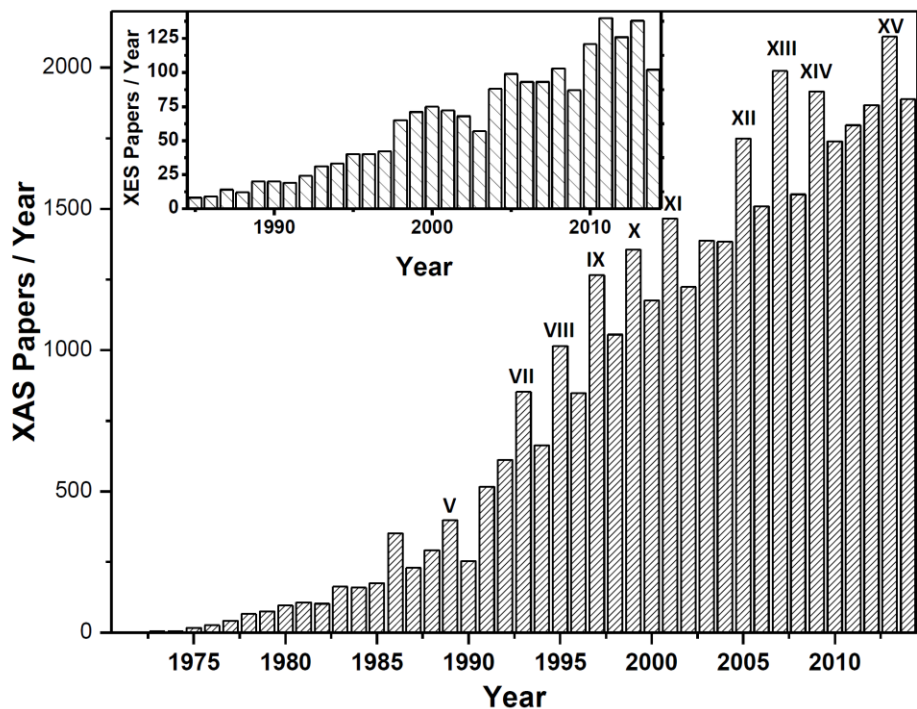
Figure 3. Main part: number of papers published per year found using (*XAFS* OR *EXAFS* OR *XANES* OR *"X ray absorption spectroscopy"* OR *"X-ray absorption spectroscopy"* OR *"X ray absorption fine structure"* OR *"X-ray fine structure"*) as the search key. Spanned period 1971 – December 2014; total number of papers > 35000. Roman numerals mark the years where the proceedings of the XAFS conference were published in journals indexed by *ISI Web of Science*. Inset: number of paper published per year found using (*XES* OR *RIXS* OR *XANES* OR *"X ray emission spectroscopy"* OR *"X-ray emission spectroscopy"*) as the search key. Spanned period 1985 – December 2014; total number of papers 1910 (1987 in the 1971 – December 2014 period). Source *ISI Web of Science*. Unpublished figure.

If we consider the birth of X-ray spectroscopy in 1913 against appearance of the paper by de Broglie [4], as discussed above, the 1971 milestone paper by Sayers, Stern, and Lytle [1] appears roughly in the middle. Partial and more complete reviews of the pioneering 1913-1971 (58 years) period of X-ray absorption spectroscopy can be found in the literature[60,95,105,107-114], from which the present section has drawn inspiration. The remaining 26 chapters provide a detailed account of the progress made by X-ray absorption and X-ray emission spectroscopy in almost all scientific directions in the period 1971–2014 (43 years), while providing perspectives for the following years.

2. About the book: a few curiosities, some statistics and a brief overview.

The idea and ambition for compiling a book that updates the famous book edited by Koningsberger and Prins [115] in 1988 was born in the summer of 2013, during a dinner between van Bokhoven and Lamberti in the typical Piedmont restaurant *Le tre galline* (literally *The three hens*) in downtown Torino. Catalyzed by excellent food and wine, that evening produced the very first list of chapters and prospective authors. The project was then pitched to Wiley, who accepted it with rapid enthusiasm and the invitation letters were then sent to the

invited authors. We are proud that most of the names on that list are now authors of chapters to this book.

With respect to the outline of the book as it was after consultation with anonymous reviewers of the proposed plan, only three chapters are missing. These were supposed to cover the following aspects: (i) theoretical methods for XES spectra simulation; (ii) combined techniques: XAFS and XES experiments performed simultaneously with other data collections (XRD, SAXS, IR, Raman, UV-vis, etc.); and (iii) biological and medical applications of XAS. Point (i) has been partially covered by Rehr and coworkers (sections 2.3.3, 2.3.5 and 2.3.6) [101] and by Glatzel and co-authors [106] (section 2). Point (ii) was largely covered by Fernández García [116] (section 6) while point (iii) remains unfortunately absent. We recommend that interested readers refer to the literature for more information on this topic [117-173]. Overall, we are very happy to deliver 29 out of the initial 30 subjects, and especially proud to present the outstanding work of so many prestigious researchers.

The author selection was a fundamental starting step of this project. In all cases, an accurate bibliographic analysis was made with a view towards inviting the most authoritative scientists in each specific sub-field. Of course, in the many cases of comparable prestige, our choice was most likely biased by our personal network and relationships. Notwithstanding this systematic bias, this book comprises the contributions of 57 authors from 11 countries (Canada, France, Germany, Italy, Japan, Poland, Russia, Spain, Switzerland, the United Kingdom and the USA), on three different continents (main part of Figure 4). Most of the authors are affiliated to Universities or to synchrotron radiation sources, but public and private research centers are also fractionally represented (inset of Figure 4).

Academic contributions came from Bologna (I), Davis (CA, US), Hokkaido (Jpn), Kielce (PO), L'Aquila (I), Madrid (S), Manchester (UK), Paris (F), Potsdam (D), Rome "La Sapienza" (I), Stanford (US), Turin (I), Wuppertal (D) and Zaragoza (S), and from EPFL Lausanne (CH), ETH Zürich (CH), Northwestern University (US), Southern Federal University (Russia) and Universidad Politécnica de Valencia (S). We are also pleased to offer contributions from many of the world's most important synchrotron radiation facilities: Argonne National Laboratory (US), Canadian Light Source Inc. (CA), Diamond Light Source (UK), European Synchrotron Radiation Facility (F), European XFEL Hamburg (D), Japan Synchrotron Radiation Research Institute (Jpn), SLAC National Accelerator Laboratory (US), SPring-8 (Jpn), Swiss Light Source (CH), SwissFEL (CH) and Synchrotron SOLEIL (F). We are confident that the DESY Hamburg (D), Advanced Photon Source (Argonne, US) and BNL (US) institutions are represented by the respective contributions of Prof. R. Frahm in Chapter 7, L. X. Chen in Chapter 9 and B. Ravel in Chapter 11, because these authors spent an important fraction of their scientific carrier working at these establishments. As for the contribution coming from research centers, we have authors from French CNRS, the Institut NÉEL in Grenoble, the IMPMC in Paris, Muséum National d'Histoire Naturelle de Paris, the National Institute of Standards and Technology in US and UOP LLC (a Honeywell company in Des Plaines, IL). We consider the chapter on industrial use a unique addition to the book.
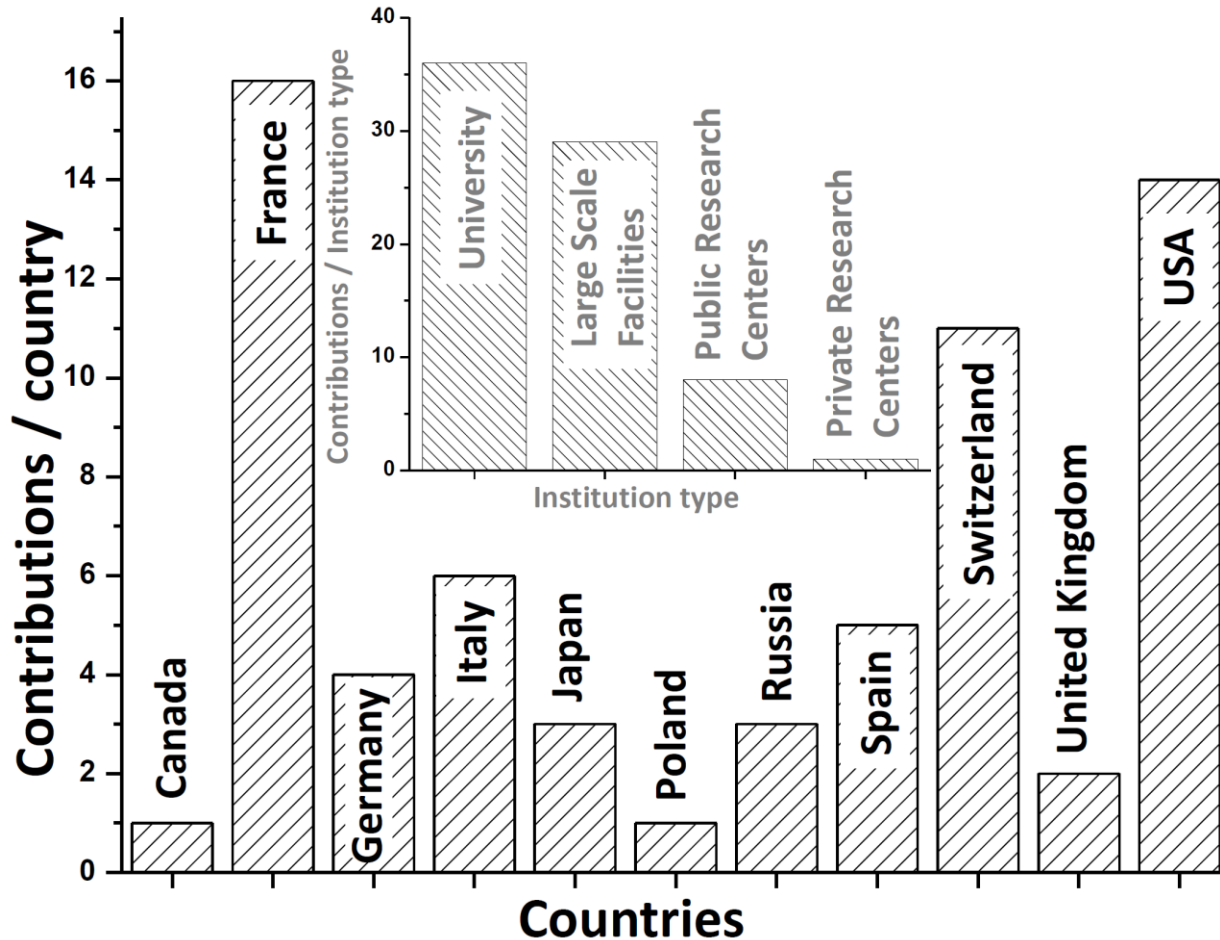
Figure 4. Main part: number of contributions to the book coming from the different countries, from left to right, in alphabetical order. The indicated country reflects the affiliation of the authors, not their citizenship. Inset: number of contributions to the book coming from the types of institution of the authors. In both cases, authors contributing to more than one chapter have been counted more than once. Unpublished figure.

The book is structured in two sections. The first part includes Chapters 1 to 12, and mainly deals with the experimental and theoretical aspects of X-ray absorption and emission spectroscopies. After this Introduction, it continue with Margaritondo' Chapter 2 [174], where the physics of photon emission by accelerated charged particles in bending magnets, wigglers, undulators and free electron lasers is described in a pedagogic and rigorous way. The concepts of photon flux and source brightness are introduced, as well as the time structure of synchrotron radiation so important for pump and probe experiments [175]. Elements of beamline optics like mirrors, monochromators, focusing elements as well as X-ray detectors are included. In Chapter 3, the Rehr group reviews the progress made in recent years towards both theory and *ab initio* codes for calculating XAS spectra with a particular emphasis on the EXAFS part [101]. The Real-space Multiple Scattering Approach is discussed in detail, as well as its close connection with the excited state electronic structure. In Chapter 4, Joly and Grenier [176] discuss the general equations used to describe the X-ray absorption process by matter in the XANES region. They describe the primary codes used to compute XANES spectra and explain how the Finite Difference Method allows researchers to avoid the muffin-tin approximation typical of the multiple scattering approach.

In Chapter 5, Gianolio provides a concise and efficient guide that directs experimenters in all practical aspects that have to be faced prior to and during a XAS experiment in pursuit of optimal data collection [177]. All steps of planning, preparing, and executing XAS experiments are described, underlying the common pitfalls that should be avoided. This chapter is highly recommended for inexperienced users.

Glatzel, Alonso-Mori and Sokaras describe XAS instrumentation in Chapter 6, including the theory and some applications of hard X-ray photon-in/photon-out spectroscopy [106]. In this chapter the authors discuss the first decay of the XAS excited state back to the ground state, and describe XES as a second order optical process which includes resonant inelastic X-ray scattering (RIXS) and high energy resolution fluorescence detected (HERFD) or partial fluorescence yield (PFY) XAS. Standard XAS is contrasted with XES, which provides considerably more detailed information about electronic structure. The critical problem related to experimental artefacts that may occur as a consequence of non-negligible self-absorption processes is also discussed.

Three successive chapters describe the domain of time-resolved XAS experiments at progressively more demanding time scales. In Chapter 6, Nachtegaal, Frahm *et al.* give an overview of QEXAFS setups at several synchrotron radiation sources worldwide and describe the capabilities of the different technical realizations. Some historical aspects and the technical requirements for detectors, angular encoders and hardware and software for fast data acquisition are also discussed. A selection of significant examples illustrates the current state of the art. The energy dispersive XAS technique is detailed in Chapter 7 by Mathon, Kantor and Pascarelli [38]. After a brief historical introduction they enter into the technical details of the essential X-ray source, dispersive optics, and beam detection. Selections of relevant examples at progressively faster time resolutions are reported. Chapter 8, authored by Chen, is devoted to the description of laser pump - X-ray probe experiments [175]. The basic theory and the basic experimental set-up of X-ray transient absorption (XTA) spectroscopy at synchrotrons and at free electron lasers are described. These aspects are supported by a selection of relevant examples. In combination these three chapters illustrate the enormous progress that has been attained in the achievable time resolution of XAS experiments over the last two decades.

With Chapter 10, authored by Suzuki, we enter the domain of space-resolved experiments [178]. The focusing optics of X-rays are reviewed in detail, followed by a selection of relevant examples and a perspective section for future development of the technique.

In Chapter 11 Ravel considers the delicate problem of quantitative EXAFS data analysis [179]. A brief historical overview of EXAFS theory in the period between 1971 and the present is outlined. The author provides a description of the muffin tin potential, of Fermi's golden rule and of Green's function expansion. The most commonly used codes for EXAFS data analysis are reviewed, underlying their peculiarities: the n-body decomposition in *GNXAS*, the exact curved wave theory in *EXCURVE*, and the path expansion in *FEFF*. The relevant aspects of the fitting statistics are treated in detail. Also addressed are: problems arising from limitation of the total number of optimized parameters, adoption of constraints in the fits, as well as the multiple data set analysis approaches. These concepts are illustrated by various practical examples of EXAFS analysis.

In Chapter 12, Fernández García *et al.* [116] emphasize proper use of the so-called "related techniques" in unlocking the full potential of EXAFS. They stress the importance of combining information at long (XRD), medium (PDF) and local range (XAS, DAFS) for achieving a complete structural view of the investigated materials. They show how it is possible

to obtain EXAFS-like information from low Z elements (PDF, EXELFS, XRS), how local-range contributions coming from amorphous and crystalline phases present in the same sample can be disentangled (DAFS), and how EXAFS-like contributions coming from the same element hosted in different crystallographic sites can be separated. Finally, the relevance, advantages, and criticalities of simultaneous data collection with different techniques are discussed.

The second volume of this book covers most of the current applications of X-ray absorption and emission spectroscopies. In Chapter 13, the editors review applications in catalysis [180]. The authors introduce the basic principles of catalysis and discuss the use of simple vacuum cleaved single crystals as models for studying systems under high pressure on more complex, high surface area catalysts. The concepts physisorption, chemisorption, catalytic conversion, and reaction are discussed in conjunction with their effect on structure-performing relations. The significance of space and time-resolved experiments in understanding catalyst operation is thoroughly discussed, with the support of relevant examples.

Physics and chemistry under high pressure is reviewed by Itié *et al.* in Chapter 14 [181], in association with XAS, XMCD and IXS techniques. Examples of pressure-induced phase transitions and amorphization are discussed in detail. Chapter 15, written by Solmon *et al.* [182], reviews use of XAS and XES in structural and electronic characterization of coordination complexes. The authors discuss first information available from XAS experiments at the K-edges of transition metals, and then that accessed through L-edges studies. In both cases they begin by describing simple complexes containing transition metal ions with a single hole in the 3d level, such as Cu(II). Subsequently they move on to more complex ions comprising multiple 3d holes, such as Fe(III) and Fe(II).

Applications of XAS to semiconductor physics are reported by Boscherini in Chapter 16 [183]. Various experimental acquisition modes of XAS spectroscopy (transmission, fluorescence, total, partial and conversion electron yields and photoluminescence yield) are initially reviewed. Determination of the local environment of dopants in semiconductors is then discussed, followed by determination of the bond length strain in thin films and heterostructures and by a summary on dilute magnetic semiconductors. The physics and chemistry of mixed valence oxides is reviewed by García *et al.* in Chapter 17 [184]. After a brief introduction to XAS, XES, and X-ray resonant scattering techniques, the authors provide examples relevant to different classes of mixed-valence oxides such as high-critical-temperature superconductors, manganites and perovskites.

Chapter 18, authored by Ramaker [185], reports application of XAS in the electrochemistry field, with a special emphasis on fuel cells and batteries. In this discipline the advantages of emerging techniques, such as high-energy resolution fluorescence detection and off-resonant spectroscopy, are underlined and compared with the traditional full-yield XAS technique that analyzes the XANES using the differential Δμ approach. Applications related to materials attendant with nuclear energy production processes are reviewed by Denecke in Chapter 19 [186]. The overall cycle of nuclear fuel is described, underlying the relevance of XAS experiments in characterizing radioactive materials. Besides the present and future fuel types, this chapter also discusses different reactor components, and studies related to nuclear fuel recycle and lanthanide/actinide separation, as well as studies concerning nuclear waste disposal.

The impact of XAS and XES spectroscopies in the fields of planetary, geological, and environmental sciences is reviewed in Chapter 20 by Farges and Wilke [187], who report an overview of planetary materials and meteorites, crystalline deep earth materials, nuclear materials with natural origin, magmatic and volcanic materials processes, element complexation

in aqueous fluids, mechanisms and reactivity at the mineral-water interfaces, biomineralization and atmospheric interactions. Chapter 21, written by Farges and Cotte, deals with the application of XAS spectroscopy in the field of cultural heritage [188]. The chapter starts with an overview of the instrumentation needed for space-resolved experiments using both hard and soft X-rays, and discusses spectral resolution of XRF detectors. A large class of materials relevant in the field is presented, covering glasses, ceramics, vitro-ceramics, metallic clusters, pigments and paintings, inks, woods, fossils, bones, ivory, metals and rock-forming monuments.

The present and future application of XAS and XES experiments at the X-ray free electron lasers (XFELs) is reviewed by Gawelda, Szlachetko, and Milne in Chapter 22 [189], making a critical comparison with third-generation synchrotron radiation sources. They report a worldwide overview of the operational and under-construction XFEL facilities, before describing the properties of X-ray pulses from XFELs in terms of number of photon per pulse and pulse duration in time. New, unprecedented, potentialities in terms of time resolved experiments are underlined, complementing the chapters dealing with time-resolution that appear in the first volume of this book [175]. Implementation of single-shot dispersive XAS, high energy resolution off-resonant spectroscopy and XES techniques at XFELs are presented. Finally, this chapter presents several cutting-edge experiments. Rogalev *et al.* review the applications of X-ray magnetic circular dichroism (XMCD) in Chapter 23. The chapter begins with an in-depth historical perspective, followed by a description of the fundamental sum rules of Carra *et al.* Subsequently, experimental considerations and data analysis are described; concluding with a selection of relevant examples.

The industrial applications of XAFS are discussed in Chapter 24 by Bare and Cuttler, considering both patents and the open literature. In this chapter, the authors start with a review of the patent literature with a particular insight into how XAFS has been used to support patent claims. The following topics, relevant for industries, have been treated in detail: semiconductors, thin films, electronic materials, fuel cells, batteries, electrocatalysts, metallurgy, tribology, and homogeneous and heterogeneous catalysts. Successively, the industrial science at light sources is discussed, taking the Canadian Light Source, the SOLEIL synchrotron in France, the National Synchrotron Light Source (NSLS) and the Swiss Light Source (SLS) as examples. The following companies were presented as examples of industrial users of synchrotron radiation: Haldor Topsøe A/S, UOP, General Electric, and IBM.

In Chapter 25 Filipponi and D'Angelo review the applications of XAS in liquid systems [190]. The chapter starts with some thermodynamic considerations followed by a rigorous definition of the concept of pair and higher order distribution functions. Successively, the different computational approaches to model liquid structures are introduced - among them: classical Born-Oppenheimer and Car-Parrinello molecular dynamics simulations, as well as Monte Carlo simulation approaches. Subsequently, the role of XAFS in understanding liquids (and generally in disordered systems) is outlined. XAFS signal decomposition is described and the XAFS signal from the pair distribution is rigorously defined. Selected examples illustrate this concept.

Gates *et al.* [191] review on-surface metal complexes and their applications in Chapter 26. The chapter begins with an introduction on mononuclear (single-metal-atom) complexes on different supports. Several relevant examples are reported and thoroughly discussed. Finally, in Chapter 27 Soldatov and Lomachenko review applications of X-ray absorption and emission spectroscopies to nanomaterials [192]. They discuss nanoclusters, metal and bimetallic

nanoparticles and nanostructures, monoatomic -O-Ti-O-Ti-O- quantum wires embedded in siliceous microporous matrices, as well as defects in solids.

Understandably, the review process for this book has been quite time consuming, as all chapters have been reviewed by at least two independent referees (with the exception of three of the chapters for which only one referee comment was available within the scheduled deadline). This process involved more than 50 referees; in some cases double-duty by referees reviewing two chapters, and in several instances a second or third review of one chapter by the same referees. In adopting such a rigorous review process it is our intention to present the highest quality publication possible. The editors are deeply indebted to all the referees, who worked diligently and anonymously towards this goal. Together with the authors, they significantly contributed to the high quality of the chapters. We are extremely grateful for all the work done by the authors, which has resulted in this voluminous book in two volumes. To prevent publication in three volumes, rigorous limits were set to the length of each chapter. In the early stage of this project, we were strongly encouraged by the very positive and often enthusiastic replies we received from the authors after requesting them to contribute to the book. During the processing and reading of the chapters and observing their development, it has become even clearer that XAS and XES are scientifically mature and extremely widely applied. Evidently, seniority has done little to suppress rapid and global technique development. The new and exciting opportunities and applications described in the contents of this book illustrate tremendous development during the past decades. This leads to the exciting conclusion that the future for XAS and XES is bright.

We thank you for reading.

Zurich and Torino, December 2014

Jeroen A. van Bokhoven   and   Carlo Lamberti.

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