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Review

EXAFS Spectroscopy: a Brief Introduction*

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EXAFS spectroscopies extract structural information from a sample by analyzing its X-ray absorption spectrum. They make it possible to determine the chemical environment of an element in terms of the number and type of its neighbors, inter-atomic distances and structural disorders. This determination is confined to a distance of 4 to 8 Å radius from the element. The paper gives a short overview of the basic principles of EXAFS spectroscopy, EXAFS experimental techniques and data analysis methods.

INTRODUCTION

EXAFS spectroscopy provides structural information about a sample by way of the analysis of its X-ray absorption spectrum. It allows determining the chemical environment of a single element in terms of the number and type of its neighbours, inter-atomic distances and structural disorders. This determination is confined to a distance given by the mean free path of the photoelectron in the condensed matter, which is between 5 and 10 Å radius from the element.[1–3]

These characteristics make EXAFS a powerful structural local probe, which does not require a long-range order. It is an important technique in several fields of natural sciences, from earth sciences to biochemistry. Since EXAFS is a technique selective for a particular element and sensible only for a short-range order, it is one of the most appropriate spectroscopies to be applied in the following cases:

- amorphous solids, *e.g.,* ceramics,
- liquids, *e.g.,* solutions of ionic compounds or gels which cannot be studied by X-ray diffraction,
- biomolecules, *e.g.,* solutions of metalloproteins,
- homogeneous and heterogeneous catalysts.

Furthermore, EXAFS does not require any particular experimental conditions, such as vacuum (at least in principle). There are several types of sample-holders that allow collecting experimental data under varying temperature and pressure, or while the sample is undergoing a chemical reaction (*in-situ* studies); see for instance the cell described by J. A. van Bokhooven *et al.*[4]

Measures taken under working conditions are of critical importance in the case of heterogeneous catalysts in

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** Author to whom correspondence should be addressed. (E-mail: vlaic@elettra.trieste.it) order to understand their behavior during catalysis, and in studying temperature and pressure induced changes.

On the other hand, there are some problems associated with this spectroscopy. First, the necessity of synchrotron light as a source, which is expensive and not easily available.

Second, the use of simulation and best-fit procedures to obtain structural parameters; these methods are time-consuming and they sometimes give ambiguous or unreliable results. However, if the system under study is properly chosen, EXAFS is able to supply useful and even essential information.

In the following paragraphs, theoretical bases underlying EXAFS and data analysis methods are briefly illustrated.

ORIGIN OF THE EXAFS SIGNAL

The X-ray absorption coefficient for an atom, indicated as μx, is directly proportional to the probability of absorption of one photon and is a monotone decreasing function of energy. It shows several discontinuities known as absorption edges: they occur when the energy of the incident photons equals the binding energy of one electron of the atom and are classified with capital letters (K, L, M...) according to the principal quantum number of the electron in the ground state (n = 1, 2, 3...). There are many tables describing the energy position of all existing absorption edges for all types of atoms. One of the most complete tables available on the web is that by Pathikrit Bandyopadhyay.[5]

Figure 1 shows this behavior for Rh atoms: it is possible to recognize four edges due to K and L (LI, LII and LIII) electrons in the diagram of the absorption coefficient of atomic rhodium.

The edge energy is characteristic of each atom. In the case of an isolated atom (monatomic gas), the absorption coefficient decreases monotonously with energy between two subsequent edges. In all other situations, the spectrum also shows oscillations that start at the edge and finish a thousand eV above; *e.g.,* Figure 2 shows the absorption spectrum for metallic Rh at edge K.

An incident photon is able to extract a core electron if its energy is equal to or greater than the edge energy. The ejected electron is called photoelectron and it has the characteristics of both a particle and a wave. Its kinetic energy is given by:

$$E = E_x - E_0 \tag{1}$$

where E_x is the energy of the X-ray photon and E_0 the energy of the edge. Its wave vector modulus is given by:

$$|\boldsymbol{k}| = \frac{2\pi}{\lambda} = \sqrt{\frac{8\pi^2 m}{h^2}(E_x - E_0)} = \sqrt{0.2624 \cdot E} \tag{2}$$

If the absorbing atom is isolated in space, the photoelectron propagates as an unperturbed isotropic wave (Figure 3A), but in most cases there are many other atoms around the absorber. These become scattering centers of the photoelectron wave (Figure 3B). The final state of the photoelectron can be described by the sum of the original and scattered waves. This leads to an interference phenomenon that modifies the interaction probability between core electrons and incident photons. Constructive interference increases while destructive interference decreases the absorption coefficient of the atom. This interference phenomenon, for a given energy of the photoelectron, depends on the distance between emitting and scattering atoms, and their atomic numbers.

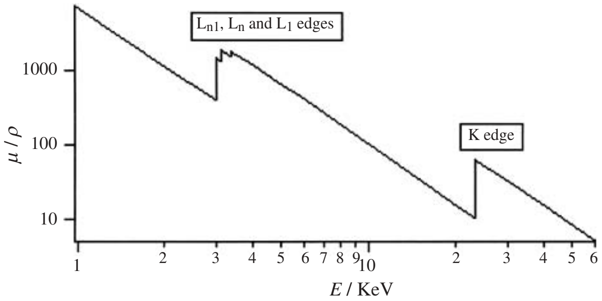

Figure 1. Absorption spectrum for Rh atoms.

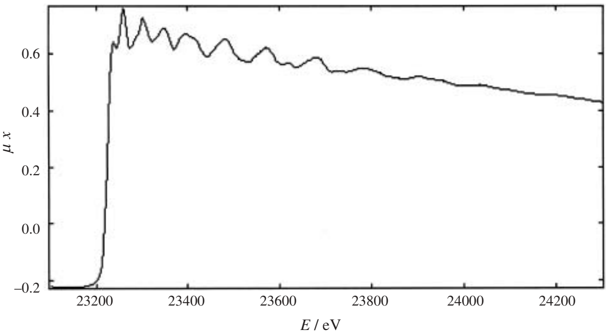

Figure 2. Absorption spectrum for metallic Rh (K edge) showing EXAFS signal.

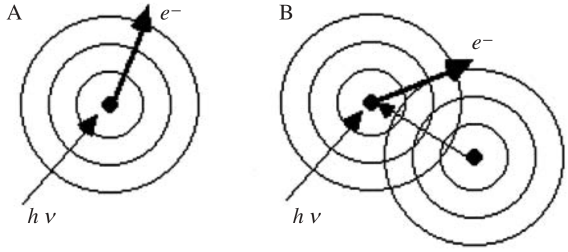

Figure 3. Schemes of scattering processes.

The EXAFS signal $\chi(k)$ is defined as a function of the wave vector $\boldsymbol{k}$. It is mathematically defined as:

$$\chi(k) = \frac{\mu x - \mu_1 x}{\mu_1 x} = \frac{\mu x}{\mu_1 x} - 1 \tag{3}$$

where μx is the experimental absorption coefficient and $\mu_1 x$ is the intrinsic atomic absorption coefficient. Dividing by $\mu_1 x$ normalizes the signal. Such a definition means that $\chi(k)$ contains only the oscillatory part of the absorption coefficient.

ANALYTICAL EXPRESSION OF THE EXAFS SIGNAL

In order to extract structural information from experimental spectra, a simple analytical expression that relates the EXAFS signal to the structural parameters is required. To obtain a simplified EXAFS formula we must accept some approximations. First of all, the dipole approximation, which describes well the interactions between core electrons and hard X-ray photons. This approximation allows writing the absorption cross-section as:

$$P_{\mathrm{if}} = \frac{2\pi^2 e^2}{m^2 \omega} |M_{\mathrm{if}}|^2 \rho(E_{\mathrm{f}}) \tag{4}$$

where i and f stand for initial and final states of the electron, e and m are its charge and mass, $\rho(E_{\mathrm{f}})$ is the state density available to the electron (it is considered as a free electron so there is a continuous distribution of states), ω is the incident photon frequency and $|M_{\mathrm{if}}|$ is a dipole matrix element related to the transition of the electron from i to f state.

$$|M_{\mathrm{if}}| = \left\langle \Psi_{\mathrm{f}} \middle| \boldsymbol{p}\cdot\boldsymbol{e} \middle| \Psi_{\mathrm{i}} \right\rangle \tag{5}$$

where $\boldsymbol{p}$ is the momentum operator, $\boldsymbol{e}$ is the electric field vector of the X photon, Ψ_{i} and Ψ_{f} are wave functions for i and f states.

The hard part of the job is to obtain a good expression of the final state wave function. This can be done by choosing a proper approximation for the potential function that describes the system. In most cases this is solved using the muffin-tin approximation. Moreover, the single electron approximation and the sudden approximation are introduced. Under these conditions, Ψ_{f} depends on the absorbed photon energy and can be written as a linear combination of two terms: the wave function for the photoelectron outgoing the excited atom Ψ_{out} and a perturbing term Ψ_{sc} which represents the backscattered wave.

At this point, keeping in mind that the absorption coefficient is proportional to P_{if}, it is possible to write a theoretical expression of the EXAFS signal:

$$\chi(k) = \frac{\left\langle \Psi_{\mathrm{out}} + \Psi_{\mathrm{sc}} \middle| \boldsymbol{p}\cdot\boldsymbol{e} \middle| \Psi_{\mathrm{i}} \right\rangle}{\left\langle \Psi_{\mathrm{out}} \middle| \boldsymbol{p}\cdot\boldsymbol{e} \middle| \Psi_{\mathrm{i}} \right\rangle} - 1 \tag{6}$$

Starting from this formula and with many boring mathematical transformations and minor physical approximations, it is possible to write an EXAFS analytical expression like the one suggested by E. A. Stern[6] in 1974:

$$\chi(k) = \frac{1}{k} S_0^2 \sum \frac{N_i}{R_i^2} \cdot \exp(-2\sigma^2 k^2) \cdot \exp\left(\frac{-2R_i}{\lambda(k)}\right) \cdot \left|f_i(k)\right| \cdot \sin[2kR + \Phi_i(k)] \tag{7}$$

where:

– k is the wave vector modulus for the photoelectron;

– N_i is the number of atoms of type i at distance R_i from the absorber;

– the exponential term $\exp(-2\sigma^2 k^2)$ takes account of fluctuations of distances due to a structural and/or thermal disorder, under the assumption of small displacements and Gaussian distributions of distances;

– the exponential term $\exp\left(\frac{-2R_i}{\lambda(k)}\right)$ takes account of finite elastic mean free paths of photoelectrons $\lambda(k)$ (between 5 and 10 Å for photoelectron energies from 30 to 1000 eV);

– S_0^2 is an average amplitude reduction factor; its value is the percent weight of the main excitation channel with respect to all possible excitation channels; its value is usually 0.8–0.9;

– $|f_i(k)|$ is a scattering amplitude function characteristic of the i-th atom;

– $\Phi_i(k)$ is a phase function that takes account of the varying potential field along which the photoelectron moves; it can be expressed as the sum of two potential terms, $\Phi_i(k) = 2\,\delta(k) + \varphi_i(k)$, the former given by the absorber, the latter given by the scatterer.

Equation (7) is valid in the case of non-oriented samples (crystalline powders, solutions and gases) and/or in the case of a non-polarized light source. Using polarized light, like synchrotron radiation, with monocrystals implies a correction of the equation: it must be multiplied by $3\cos^2\Theta$ where Θ is the angle between the absorber-scatterer axis and the polarization direction.

Non-oriented samples do not require this correction, because the angle is isotropically distributed in space.

Equation (7) is able to describe only single scattering processes. However, it has been demonstrated that considering also multiple scattering processes leads to a very similar analytical expression. Introducing multiple scattering allows one to obtain also stereochemical information about the local structure.[7]

EXPERIMENTAL METHODS

Since EXAFS spectroscopy requires an intense polychromatic X-ray source, the most suitable light source is a synchrotron storage ring.

The most common EXAFS beam-line works in transmission. It collects data measuring how the beam intensity decreases as it passes through the sample while scanning energy using a crystal monochromator. Experimental spectra are usually recorded by scanning energy from about 200 eV below the explored edge to 1000 eV above it. Energy steps can be of 0.1–2.0 eV, depending on the energy interval and the experimental setup.

As it is known, the Lambert-Beer law relates intensities I_0 and I to the absorption coefficient:

$$\ln\frac{I_0}{I} = \mu x \qquad (8)$$

Because of the angular rotation of the crystals inside the monochromator, the beam can shift up or down. Light must pass through the sample always at the same position, so either the sample follows the beam by placing it on a micrometric table, or it is necessary to change the monochromator mechanism to obtain a fixed beam.

There is also a different experimental set-up, useful for collecting data from diluted samples: it measures the fluorescent photons emitted by absorbing atoms. A complete description of these different detection schemes, with a very interesting discussion on the obtainable signal-to-noise ratios was published by Lee *et al.*[8]

A spectrum recording takes from 15 minutes up to three hours. However, there are two other EXAFS techniques, which take shorter recording times and allow kinetic studies to be performed. One is known as Quick-EXAFS[9] and requires up to a couple of minutes to record a spectrum, and the other is Dispersive-EXAFS[10] and requires, at most, a couple of seconds.

In Figure 4, counts obtained in the transmission mode using two ionization chambers as detectors are reported for a foil of metallic rhodium.

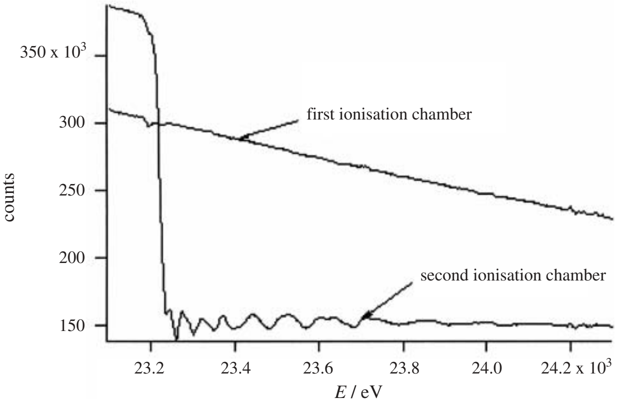

Figure 4. Raw data spectrum for metallic Rh (recorded in transmission mode).

DATA ANALYSIS

The purpose of EXAFS analysis is to obtain the parameters of the local structure of the absorbing atom from its experimental cross-section. Many analysis methods have been developed and in this section we will describe one of the most general and simple ones. The software package used in the following examples was designed by Alain Michalowicz.[11]

The first step in data analysis is signal extraction by background removing. This delicate operation can be divided into three steps:

a) choosing the threshold energy, for wave vector definition;
b) pre-edge extrapolation (named $\mu_0 x$);
c) atomic absorption modeling (named $\mu_1 x$).

After these steps, it is possible to obtain the EXAFS signal as:

$$\chi(E) = \frac{\mu x(E) - \mu_1 x(E)}{\mu_1 x(E) - \mu_0 x(E)} \qquad (9)$$

In Figure 5, the EXAFS signal for metallic rhodium is reported.

The EXAFS signal contains the contributions of all of the coordination shells. Each contribution can be approximated to a damped sinusoidal function in k-space, whose frequency is proportional to the absorber-scatterer distance.

The EXAFS signal is Fourier transformed to obtain a radial distribution function. Fourier transform (FT) is the standard tool used for frequency separation. In fact, this operation transforms each sinusoidal component in a FT modulus peak, going from the k(Å^{-1}) space to R(Å) space. To minimize distortions and to avoid the presence of ripples (peak side-lobes which arise from the truncated integration) in the FT modulus, $\chi(k)$ is multiplied by a window W(k).

The height of peaks depends on the amplitude parameters of the EXAFS equation, while their position depends on phase parameters. Total or partial overlapping of more peaks often occurs.

The position of a peak depends in the first approximation on the distance between absorber and scatterer and in the second approximation on the phase function. Since $\Phi(k)$ depends on k (always with a negative slope), peaks are shifted to lower R values.

Figure 6 shows the FT modulus for metallic rhodium. Peaks corresponding to different Rh–Rh distances are clearly visible.

In simple cases, when a peak is well separated by the others and is determined by only one distance, it is possible to obtain information on the interatomic distance directly from FT.

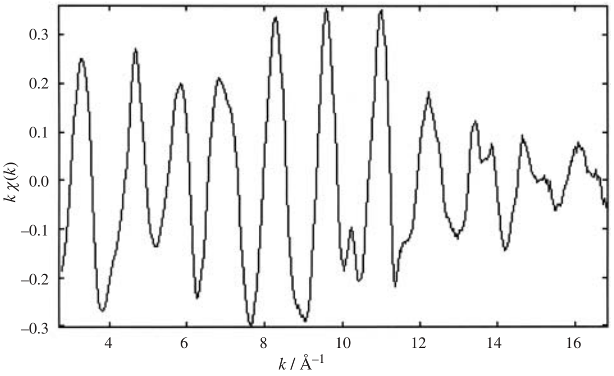

Figure 5. EXAFS signal of metallic rhodium.

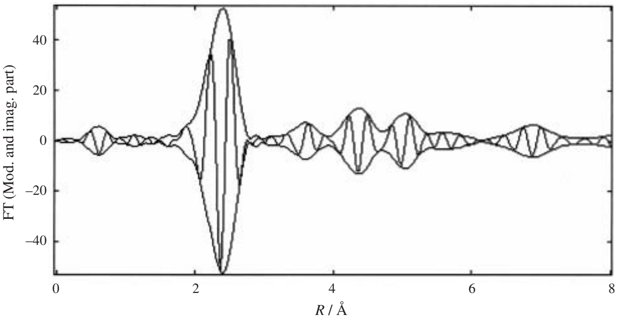

Figure 6. FT (modulus and imaginary part) of metallic rhodiium.

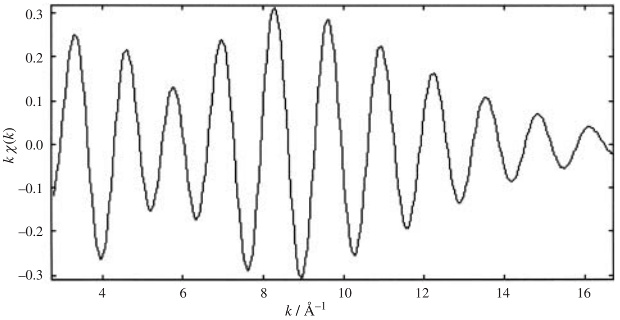

Figure 7. Inverse FT of the first peak for metallic rhodium.

It suffices to multiply the EXAFS signal by $\exp(-i\,\Phi_j(k))$ to remove the phase dependency of the position of the peak due to the absorber-jth atom pair.

Once the peak associated to a single coordination shell has been recognized in the Fourier transform of the EXAFS, its contribution to the total signal can be obtained by an inverse Fourier transform carried out over the limits of the peak in R-space (otherwise the filter is calculated in a region containing more than one contribution). The outcome of this operation is the $\chi_i(k)$ function related to absorber-scatterer pairs whose interatomic distances belong to that specific integration interval. Figure 7 shows the inverse FT (FT^{-1}) of the first peak in Figure 6, which corresponds to the first Rh–Rh atomic pair.

Structural parameters can be obtained from $\chi_i(k)$ by means of a fitting procedure using known phase and amplitude functions. EXAFS analysis allows obtaining coordination numbers, interatomic distances and an estimate of the disorder around the central atom.

Phase and scattering amplitude functions are either theoretical or experimental functions. Teo and Lee calculated theoretical functions in 1977 assuming that the photoelectron wave is a plane wave.[12,13] Better phases and amplitudes were obtained by McKale *et al.* in 1988,[14] within the curved wave approximation; more recently, better theoretical functions were provided by the FEFF program.[15]

Experimental functions are extracted from proper reference samples whose structure is already known. These can be used thanks to the phase and amplitude transferability principle[16] that states: »Phases and amplitudes are insensitive enough to chemical environment in order to be extracted from a well-known sample and transferred to an unknown sample containing the same absorber-scatterer pair at a similar distance«.

Phases and amplitudes can be extracted by filtering FT peaks and using the following formulas:

$$\Phi(k) = \mathrm{arctg}\,\frac{Re}{Im} - 2kR \tag{10}$$

$$A(k) = \exp(-2\sigma^2 k^2)\cdot\exp\left(\frac{-2R}{\lambda(k)}\right)|f(k)| = \sqrt{Re^2 + Im^2}\,\frac{R^2}{N} \tag{11}$$

Experimental amplitude functions include the analyzer's estimate of σ and $\lambda(k)$ for the reference sample, so final fitting values for these parameters will be relative to the initial choice.

Experimental functions are not always available because no proper reference compounds exist or because it is impossible to extract them. For instance, metallic Fe does not allow extracting phase and amplitude for the Fe-Fe pair because Fe is surrounded by 8 atoms at 2.48 Å and 6 atoms at 2.86 Å and these two peaks overlap in the FT modulus. In these cases, the analyzer is compelled to use theoretical functions.

Since ΔE_0 is arbitrarily chosen, the k-scale is not absolute. Therefore, it is necessary to redefine the k scale during the fitting procedures by introducing a ΔE_0 dependence:

$$k' = \sqrt{k^2 + 0.2624\Delta E_0} \tag{12}$$

EXAFS spectroscopy allows estimating structural parameters with a precision highly dependent on the data and analysis quality. Errors are usually about 0.01–0.02 Å for interatomic distances, and 5–15 % for coordination numbers.

DATA ANALYSIS STATISTICS AND ERROR ESTIMATES

Structural parameters are usually obtained by simulating the experimental signal using Eq. (7). This is done by an automatic computer-based minimization procedure. The minimized function is:

$$F(P_i) = A = \sum_k w(k)\,[\chi_{\mathrm{exp}}(k) - \chi_{\mathrm{th}}(k,P_i)]^2 \tag{13}$$

where P_i are the fitting parameters and $w(k)$ is a weighting function. Suffixes exp and th stand for experimental and theoretical EXAFS signals; $w(k)$ usually contains two factors: k^n weighting and the experimental standard deviation. The choice of a particular k^n weighting and of a specific procedure to estimate standard deviation is still controverted and depends on the analysis methods the scientist applies.[17,18]

It is useful also to define a residual factor, for instance:

$$Res = \frac{A}{w(k)\chi^2_{\mathrm{exp}}(k)} \tag{14}$$

The residual factor alone should not be used to compare two models or judge the quality of simulation. More complex methods, based on statistic estimates, are used instead. To describe these methods we have to define some quantities:

a) the number of independent points N_{ind}, which is given by the following formula, since the EXAFS signal undergoes two Fourier integrations:[19]

$$N_{\mathrm{ind}} = \frac{2 \cdot \Delta k \cdot \Delta R}{\pi} + 2 \tag{15}$$

where Δk is the fitting interval (NOT the Fourier integration interval) and ΔR is the filtering interval in real space;

b) the number of parameters used for the fit (N_{par}), which obviously must be lower than the number of independent points N_{ind}; with these definitions the maximum number of fittable parameters is:

$$N_{\mathrm{max\ par}} = N_{\mathrm{ind}} - 1 \tag{16}$$

c) the number of degrees of freedom ν, which is given by:

$$\nu = N_{\mathrm{ind}} - N_{\mathrm{par}} \tag{17}$$

d) chi-squared, which is a function strictly related to the »goodness of fit«, hence the function that »says« how far the fitting curve is from experimental data:

$$X^2 = \sum_i \frac{1}{s_i^2}\,[y_i - y(x_i)]^2 \tag{18}$$

where y_i are experimental data and $y(x_i)$ is the simulated function; s_i is the estimated standard deviation at the i-th point. In the case of EXAFS it is:

$$X^2 = \sum_i \left[\frac{k_i\chi_{\mathrm{exp}}(k_i) - k_i\chi_{th}(k_i)}{s^2(k_i)} \right]^2 \tag{19}$$

e) finally, the reduced chi-squared:

$$X^2_\nu = \frac{X^2}{\nu} \tag{20}$$

X^2 and X^2_ν are of great importance, but we cannot trust their absolute values. Their definition contains a quantity, which is susceptible to large estimate errors and for whose determination no standard method exists (despite its name): standard deviation.[20]

A very simple way of determining standard deviations is to repeat each single measurement three times or more, in order to define an average spectrum with its standard deviation. The average spectrum is given by:

$$\bar{\chi}(k_i) = \frac{\sum_{j=1}^{n} \chi_j(k_i)}{n} \tag{21}$$

and its standard deviation by:

$$s(k_i) = \sqrt{\frac{\sum_{j=1}^{n} = [\bar{\chi}(k_i) - \chi_j(k_i)]^2}{n-1}} \tag{22}$$

In principle, a »good fit« has a reduced-chi-square that tends to unity. Besides, the reduced-chi-square allows comparing, on a statistical basis, two different models for the same data set. This quantity is particularly important; in fact, the value of X^2 can be easily lowered by adding fittable parameters to the model, thus making it more »flexible«. But X^2_ν (Eq. 20) reveals whether the new free parameters have really improved the simulation or not. If its value remains unchanged or even increases as we add a new parameter, it means that the model improvement is statistically negligible.

The reduced-chi-squared function is also useful for comparing different models. There is a quantitative test, called the F-test,[21–23] which says, with a user chosen probability level, whether two models can be discriminated by comparing the X^2_ν ratio of two models to those tabulated on Fisher's tables.

At this point it is important to note that a wrong choice of standard deviation has an impact on X^2_ν values, but it cancels in the F-test.

The results of the EXAFS technique are often ambiguous, especially when dealing with light atoms at similar distances (*i.e.,* coordination chemistry of transition metals with organic ligands). In these cases, it is frequently impossible to obtain only one solution or an acceptable one at all.[24]

Like in any other technique, outgoing values must have their error bars. Ambiguity of the results makes error estimates a delicate matter: many papers have dealt with standard deviation estimates and different approaches to error bar calculations. The International EXAFS Society is still working to produce some standard procedures; these reports are published on the web; the last one was published in 2000.[25]

Common methods involve calculating the standard deviation for a set of spectra or evaluating the noise of a single spectrum by smoothing procedures. Anyway, the uncertainty of experimental data is not fully known yet. Error bars are usually determined by calculating the inverse of the Hessian matrix obtained by a gradient minimization procedure, but more robust techniques, such as the Monte Carlo methods, are preferable in complex cases, though they are used by only a few authors.

Once chi-square has come to a minimum, errors determination becomes possible by varying each parameter separately while refining the others, until X^2 changes of n units, according to a chosen confidence interval. In the case of a confidence interval of 68 % n = 1. Other values of n are tabulated in relevant manuals.

More information on statistics can be found in the books written by Taylor[26] and Bevington and Robinson.[27]

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SAŽETAK

Kratak uvod u EXAFS spektroskopiju

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EXAFS spektroskopija omogućuje strukturne informacije analizirajući apsorpcijski spektar X-zrake uzorka. Tom metodom se može odrediti kemijski okoliš nekog elementa u odnosu na broj i vrstu susjeda, međuatomsku udaljenost i strukturni nered. Određivanje je ograničeno na polumjer od 4–8 Å oko toga elementa. U radu se daje kratki pregled temeljnih načela EXAFS spektroskopije, EXAFS eksperimentalnih tehnika i metoda analize podataka.