

Some notes on data analysis for nuclear resonant inelastic x-ray scattering

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Abstract Nuclear Resonant Inelastic X-ray Scattering (NRIXS) is a spectroscopy method to study atomic vibrations and dynamics, currently done with synchrotron radiation at a few high energy third generation facilities. It finds a wide range of applications in condensed matter physics, materials science, chemistry, biophysics, geosciences, and high-pressure researches. Many atomic dynamics and lattice thermodynamics information can be derived from NRIXS measurements. Phonon Density of States (DOS) characterizes lattice dynamics of a material and can be derived under the quasi-harmonic approximation. Combined with modeling and simulations, results from NRIXS can provide unique and clarifying insights into many fields of research. As for a spectroscopic technique, in order to be able to provide reliable information, close attention should be paid to many issues during experiments and data analysis afterwards. Here we discuss several issues relevant to its data analysis, namely, those of multiple sites, background treatments, and error estimates for some derived quantities.

Keywords Nuclear resonant scattering · Data analysis · Atomic dynamics in solids · Lattice dynamics

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1 Introduction

Nuclear Resonant Inelastic X-ray Scattering (NRIXS), also called Nuclear Inelastic Scattering (NIS), and Nuclear Resonant Vibrational Spectroscopy (NRVS), is a well established synchrotron radiation technique at major light sources around the world and has a large user base consisting of researchers from a diverse collection of fields. Using nuclear resonances as probes, it can measure atomic vibrations in a unique way. This necessitates a thorough understanding of the scattering process and sophisticated data analysis methods to extract information from measurements. There are many excellent reviews of this method in the literature [1–6].

We will discuss a few aspects of its data analysis process. In Section 2 we investigate the case of multiple nonequivalent sites. Noise and background in a measured spectrum is a critical issue. However, post experiment, it is a very difficult problem to deal with. We try to frame the problem and give a brief discussion in Section 3. Lastly, in Section 4, we list formulae to estimate error bars of the derived moments of a spectrum.

2 Multiple sites

In most of NRIXS studies, the resonant isotope resides at one particular crystal site in the samples. However, many solids have nonequivalent sites for atoms of the same species. One example is magnetite (Fe_3O_4), where Fe ions occupy two sites with different coordinations. Specifically, the tetrahedral site holds Fe^{3+} ions, while the octahedral site houses both Fe^{2+} and Fe^{3+} ions. Two studies have considered different contributions to phonon DOS from the two sites in magnetite [7, 8]. In cases of amorphous materials, all the lattice sites are nonequivalent in principle. Nonequivalent sites imply different surroundings, often different coordinations, which may lead to different force constants applying to atoms at the sites. Nonequivalent sites should contribute differently to phonon density of states.

In the following pages we address the questions of how to interpretate measured NRIXS spectrum when there are nonequivalent sites in the sample, and can phonon DOS be extracted and under what conditions. Some of these issues were discussed briefly in the context of Lamb-Mössbauer factor and second-order Doppler shift [9].

NRIXS is an incoherent inelastic process. It measures the number of nuclear resonance absorption events as a function of energy transfer. The typical setup of NRIXS precludes any distinction among resonant nuclei. Thus measured phonon excitation spectrum consists of contributions from all sites with resonant isotope. The cross section per nucleus is given by [3, 10]

$$\sigma(\mathbf{k}, \omega) = \frac{\pi}{2} \sigma_0 \Gamma S(\mathbf{k}, \omega) \quad (1)$$

where $\hbar\omega = E - E_0$ is the difference between incident X-ray energy and the nuclear resonance energy. The measured spectrum is proportional to $\tilde{N}\sigma(\mathbf{k}, \omega)$ and \tilde{N} is the number of resonant nuclei, which may be smaller than N , the number of all atoms in the sample. The cross section factorizes into the properties of the probe - the maximum nuclear resonant absorption cross section σ_0 and the total natural linewidth of the excited nuclear level Γ - and the dynamical property of the scattering system, which is a Fourier transform

$$S(\mathbf{k}, \omega) \equiv \frac{1}{2\pi} \int dt d\mathbf{r} e^{i(\mathbf{k}\mathbf{r} - \omega t)} G_a(\mathbf{r}, t) \quad (2)$$

of the particle autocorrelation function of a many-body system [11],

$$G_a(\mathbf{r}, t) = \frac{1}{\tilde{N}} \left\langle \sum_{\nu} \int d\mathbf{r}' \delta(\mathbf{r} + \mathbf{r}_{\nu}(0) - \mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}_{\nu}(t)) \right\rangle_T \tag{3}$$

where ν enumerates resonant nuclei, and \mathbf{r}_{ν} is the position of the ν -th nucleus. The statistical average at a given temperature T is indicated by $\langle \dots \rangle_T$. It is similar to the dynamic structure factor $S(\mathbf{q}, \omega)$, a function of energy and momentum transfer defined by the same equation but with the particle pair correlation function instead. Phonon dispersions can be determined by measuring the dynamic structure factor with inelastic X-ray scattering and coherent inelastic neutron scattering. In contrast, the function $S(\mathbf{k}, \omega)$ obtained from NRIXS is a function of energy transfer and the incident X-ray momentum instead of momentum transfer. It can be interpreted as the phonon excitation probability density.

With the help of sum rules [12], one can properly normalize measured spectrum and obtain the inelastic part of the dynamical function $S(\mathbf{k}, \omega \neq 0)$. The elastic $S(\mathbf{k}, 0)$ is then calculated according to the fact that normalization of S with respect to ω is 1. This is the recoil-free fraction, or Lamb-Mössbauer factor. From this phonon excitation probability density function, one can also calculate certain dynamical properties of the nuclei involved. These include averaged kinetic energy and second order Doppler shift, and averaged force constant in the incident photon direction.

Many dynamic and thermodynamic properties can be inferred from phonon DOS. Its detailed structure is obviously the focus of many lattice dynamics studies. So one would want to know if it can be extracted from NRIXS measurements. Phonon DOS is related to one-phonon excitation spectrum in a stright forward way, which will be shown below. However, scattering from multiple phonons has appreciable probabilities at finite temperatures. In order to derive DOS, we need to separate one-phonon spectrum from $S(\mathbf{k}, \omega)$.

Now we seek to interpret the measured phonon excitation probability density function in terms of DOS, and in doing so to reveal the method by which, and more importantly under what conditions, one may derive DOS from this function.

Let us introduce an intermediate scattering function $F(\mathbf{k}, t)$, as the inverse Fourier transform of the phonon excitation probability density function with respect to ω , so that

$$S(\mathbf{k}, \omega) = \frac{1}{2\pi} \int F(\mathbf{k}, t) e^{-i\omega t} dt, \tag{4}$$

and

$$F(\mathbf{k}, t) = \int d\mathbf{r} e^{i\mathbf{k}\mathbf{r}} G_a(\mathbf{r}, t) \tag{5}$$

$$= \frac{1}{\tilde{N}} \left\langle \sum_{\nu} e^{-i\mathbf{k}\mathbf{r}_{\nu}(0)} e^{i\mathbf{k}\mathbf{r}_{\nu}(t)} \right\rangle_T. \tag{6}$$

In harmonic lattice model, we can calculate the intermediate scattering function as defined in (6) to be [11],

$$F(\mathbf{k}, t) = \frac{1}{\tilde{N}} \sum_{\nu}^{\tilde{N}} e^{-2W_{\nu}(\mathbf{k})} e^{2M_{\nu\nu}(\mathbf{k}, t)} \tag{7}$$

where

$$2W_\nu(\mathbf{k}) = \sum_s \left(\frac{\hbar}{2\tilde{m}N\omega_s} \right) (\mathbf{k} \cdot \epsilon_s^\nu)^2 (2n_s + 1) \tag{8}$$

$$2M_{\nu\nu}(\mathbf{k}, t) = \sum_s \left(\frac{\hbar}{2\tilde{m}N\omega_s} \right) \times (\mathbf{k} \cdot \epsilon_s^\nu)^2 \left\{ (n_s + 1)e^{i\omega_s t} + n_s e^{-\omega_s t} \right\} \tag{9}$$

and \tilde{m} is the mass of resonant isotope. We use s to label phonon modes, of which ω_s and ϵ_s^ν are the phonon frequency and the polarization vector respectively, and n_s the phonon occupation number. In a crystal, sets of polarization vectors are the same at all equivalent sites, so that these sites share the same $2W_\nu(\mathbf{k})$ and $2M_{\nu\nu}(\mathbf{k}, t)$. We can then group the equivalent site terms together and rewrite the right hand side of (7) into sums of non-equivalent sites, and suppose there are n of them,

$$F(\mathbf{k}, t) = \sum_j^n p_j f_j(\mathbf{k}) e^{2M_{jj}(\mathbf{k}, t)} \tag{10}$$

where $p_j = \tilde{N}_j/\tilde{N}$ is the fraction of equivalent sites of type j among all the sites occupied by resonant nuclei with $\sum p_j = 1$, and $f_j(\mathbf{k}) = e^{-2W_j(\mathbf{k})}$ is the directional Lamb-Mössbauer factor of that site. The site specific contributions to the intermediate scattering function can be defined as

$$F_j(\mathbf{k}, t) = f_j(\mathbf{k}) e^{2M_{jj}(\mathbf{k}, t)}, \tag{11}$$

so that $F(\mathbf{k}, t) = \sum p_j F_j(\mathbf{k}, t)$.

The expansions of the exponential terms in (10) correspond to various multi-phonon contributions. The first order one-phonon term is related to single phonon excitation probability density and DOS,

$$S_j^{(1)}(\mathbf{k}, \omega) = \frac{f_j(\mathbf{k})}{2\pi} \int 2M_{jj}(\mathbf{k}, t) e^{-i\omega t} dt \tag{12}$$

$$\mathcal{D}_j(\mathbf{k}, \omega) = \frac{\hbar\omega(1 - e^{-\beta\hbar\omega})}{f_j(\mathbf{k}) E_R} S_j^{(1)}(\mathbf{k}, \omega) \tag{13}$$

for every j , and E_R is the recoil energy of nucleus and $\beta = 1/k_B T$.

Now we can express the measured phonon excitation probability density in terms of site specific phonon DOS.

$$S(\mathbf{k}, \omega) = \sum_j^n p_j \frac{f_j(\mathbf{k})}{2\pi} \int e^{2M_{jj}(\mathbf{k}, t)} e^{-i\omega t} dt \tag{14}$$

with

$$2M_{jj}(\mathbf{k}, t) = \int \frac{E_R}{\hbar\omega(1 - e^{-\beta\hbar\omega})} \mathcal{D}_j(\mathbf{k}, \omega) e^{i\omega t} d\omega, \tag{15}$$

$$f_j(\mathbf{k}) = \exp \left(-E_R \int \frac{\coth(\beta\hbar\omega/2)}{\hbar\omega} \mathcal{D}_j(\mathbf{k}, \omega) d\omega \right). \tag{16}$$

Given individual site specific DOS, one can use these equations to simulate the spectrum measured in a NRIXS experiment. The projected partial DOS is defined as

$$\mathcal{D}_j(\mathbf{k}, \omega) = \frac{1}{N} \sum_{s=1}^{3N} (\hat{\mathbf{k}} \cdot \epsilon_s^j)^2 \delta(\omega - \omega_s), \tag{17}$$

where $\hat{\mathbf{k}} = \mathbf{k}/k$ is the unit vector of incident photon direction.

Next, let us look at the question that whether phonon DOS can be derived from the spectrum measured in a NRIXS experiment. The key to understand this is in (10), whose left-hand side is known, the Fourier transform of measured spectrum. The nonequivalent site fractions p_j are also supposedly known as sample characteristics. The other two quantities are unknown and one of them, $2M_{jj}(\mathbf{k}, t)$, is directly related to site-specific phonon DOS through (12) and (13).

For a crystal where the resonant nuclei occupy only the equivalent sites, (10) is simplified to contain only two unknowns, $f(\mathbf{k})$ and $M(\mathbf{k}, t)$, of which the Lamb-Mössbauer factor is solved from moment sum rules and normalization [12, 13]. Then function $M(\mathbf{k}, t)$ is calculated from the inverse Fourier transform of the measured spectrum $S(\mathbf{k}, \omega)$, and from which the one-phonon spectrum and the projected partial DOS are calculated. This is the standard procedure of extracting phonon DOS from a NRIXS spectrum [14].

When there are n nonequivalent sites occupied by the resonant nuclei, we can see that in (10) we have $2n$ unknowns. There are n normalization conditions, one for each site-specific spectrum. It applies to the whole spectrum as well. So as discussed above, from moment sum rules we can get an averaged Lamb-Mössbauer factor,

$$\overline{f(\mathbf{k})} = \sum_j p_j f_j(\mathbf{k}). \tag{18}$$

We have an underdetermined system. To be able to solve it, one has to find additional $n - 1$ equations in order to derive site specific phonon DOS. If the site specific contributions to the measured spectrum can be distinguish and identified, that is, the following sum can be resolved,

$$S(\mathbf{k}, \omega) = \sum_j p_j S_j(\mathbf{k}, \omega) \tag{19}$$

which generally require only $n - 1$ additional conditions, then the system is broken down into n single-site problems and each is solved as outlined above.

Now, to answer the question stated earlier, additional conditions and/or experiments are needed for one to be able to derive phonon DOS from the spectrum measured in a NRIXS experiment. The procedure described above for extracting phonon DOS in a single site system breaks down when multiple sites exist. If we ignore this fact, and still apply the algorithm outlined above for unique site, the then derived DOS and the separation of multiphonon spectra are quite questionable. Since in doing so, we are forcing the following condition in (10),

$$F(\mathbf{k}, t) = \sum_j p_j f_j(\mathbf{k}) e^{2M_{jj}(\mathbf{k}, t)} = \overline{f(\mathbf{k})} e^{2M'(\mathbf{k}, t)}. \tag{20}$$

It is not difficult to see that $2M'(\mathbf{k}, t)$ is definitely not the sum of all $2M_{jj}(\mathbf{k}, t)$'s. There is no simple way to relate them.

Even though for multiple site cases we cannot derive phonon DOS, as we have shown, the NRIXS spectrum can still be quite helpful in modeling of materials. If we have models for the site-specific DOS, then $S(\mathbf{k}, \omega)$ can be calculated using some of the equations shown above, and compared to a NRIXS measurement. Of course in doing so one has to be very careful, since uniqueness is lacking in this approach. Quite different sets of components can yield same sum.

Now let's consider some special cases when phonon DOS can be obtained. One exception is the case of amorphous materials. There, if the local order is preserved, or the local environment is sufficiently similar, we can expect every lattice site has almost identical

vibrational frequency distribution. Thus we have recovered the single-site condition as an approximation.

Another special case where phonon DOS can be derived is when multiphonon contribution to $S(\mathbf{k}, \omega)$ can be neglected and all the nonequivalent sites share same Lamb-Mössbauer factor, or at least approximately. Multiphonon contribution is negligible when $f(\mathbf{k})$ is high, for example, when sample is at low temperatures. Then DOS is calculated according to (13) with $S^{(1)}(\mathbf{k}, \omega)$ replaced by the measured $S(\mathbf{k}, \omega)$. This is demonstrated in the following approximation of (10),

$$\begin{aligned} F(\mathbf{k}, t) &= \sum_j p_j f_j(\mathbf{k}) e^{2M_{jj}(\mathbf{k}, t)} \\ &\simeq \sum_j p_j f_j(\mathbf{k}) [1 + 2M_{jj}(\mathbf{k}, t)] \end{aligned} \quad (21)$$

$$= \frac{1}{f(\mathbf{k})} \left[1 + \sum_j \frac{p_j f_j(\mathbf{k})}{f(\mathbf{k})} 2M_{jj}(\mathbf{k}, t) \right]. \quad (22)$$

In this case, the DOS derived is a weighted sum of those from all NR sites.

3 Noise background in a NRIXS spectrum

A measured NRIXS spectrum can be modelled in terms of counts as a function of energy,

$$I(E) = \int [A S(E') - B \delta(E')] R(E - E') dE' + X_E \quad (23)$$

where $S(E)$ is the phonon excitation probability density function defined in (2) with $E = \hbar\omega$ the energy difference between incident X-ray and the nuclear resonance. The measured spectrum is the result of a convolution of $S(E)$ with an instrumentation resolution function $R(E)$ determined by the high-resolution monochromator used in the measurement. This resolution function is measured by the way of nuclear forward scattering (NFS). The factor A is an unknown normalization factor. The term with a factor B describes the phenomenon of “elastic peak deficit” which has been discussed in many places [13, 15, 16]. The factors A and B can be estimated by using moment sum rules [12]. This term was discussed in Ref. [9, 13].

The last term in the above model represents background noise in the measurement. At any energy point E , X_E is a sum of single measurements of many stochastic variables having the noise spectra when the monochromator is tuned to energy E at different times during a measurement. It is a sum typically, due to the fact that a measurement consists of many so called energy scans.

Ideally, all these stochastic variables follow identical probability density distributions, which describes a constant noise spectrum over the course of a measurement. This is almost never the case in practice. The best an experimenter can do is to increase the signal to noise ratio, thus making the first term much larger than the second, to the extent that it can be ignored safely, over the relevant and interested energy range.

A common practice in data processing is to subtract a constant background from the measured spectrum $I(E)$ and treat the result as the first term on the right-hand side of (23). Thus one has pushed the variations into the reduced $S(E)$ effectively. Another attempt is to exploit both ends of an energy spectrum, extend the approximation to the first order. If

one is reasonably sure about the noise levels at both ends, then an interpolation in-between the two end points can be used as an appoxy for background noise. Indeed a NRIXS code SciPhon [17] employs this method to remove background.

As mentioned before, the factors A and B can be estimated using sum rules. Here we give the results,

$$A = \frac{I_1}{E_R} + \left(1 - \frac{r_1}{E_R}\right) I_0 + \frac{r_1}{E_R} x_0 - \frac{1}{E_R} x_1 \tag{24}$$

$$B = \frac{I_1}{E_R} - \frac{r_1}{E_R} I_0 + \left(1 + \frac{r_1}{E_R}\right) x_0 - \frac{1}{E_R} x_1 \tag{25}$$

where various moments are defined as the following,

$$I_n = \int (E - E_R)^n I(E) dE \tag{26}$$

$$r_n = \int E^n R(E) dE \tag{27}$$

$$x_n = \sum_i E_i^n X_{E_i} \tag{28}$$

The moments of background noise x_n are very small compared to other terms in (24–25). The odd moments of noises could be even smaller due to possible cancellation from the negative energy side of the spectrum. If the resolution function used in an experiment is reasonably symmetric, that is, its first moment r_1 is negligible compared to E_R , then the normalization factor A is almost not influenced by the sum of the background. However, in many low temperature studies, the energy range over which data is taken is often highly skewed to the positive side, which would likely result in a large contribution from x_1 . The factor B is relevant only under the elastic peak. It is influenced by both moments of the noises. This will add uncertainties to the derivation of the f -factor, f_{LM} .

4 Error estimates of NRIXS moments

Moments of the phonon excitation probability density function $S(E)$ provide information of atomic dynamics of a sample studied. The 0-th moment is relevant to the Lamb-Mössbauer factor f_{LM} ; the first moment is the nucleus recoil energy; the second moment is the mean kinetic energy, thus related to second order Doppler shift; and the third moment is the mean force constant experienced by the resonant nucleus.

Let us define central moments of $S(E)$ [16],

$$R_k \equiv \int_{-\infty}^{+\infty} (E - E_R)^k S(E) dE \tag{29}$$

which is related to the moments I_n of measured spectrum, r_n of resolution function, and x_n of noises, (26–28), in the following way,

$$I_n = A \sum_{k=0}^n C_n^k r_{n-k} R_k - B \sum_{k=0}^n C_n^k (-E_R)^{n-k} r_k + \sum_{k=0}^n C_n^k (-E_R)^{n-k} x_k \tag{30}$$

where C_n^k are the binomial coefficients.

To simplify the discussion and estimate error contributions from various factors, we assume a perfect resolution function $R(E) = \delta(E)$, a constant background $X_E = x$, and no

elastic peak deficit $B = 0$. The no elastic peak deficit assumption can be made for moments calculations, because $S(0)$ does not contribute to R_k except for $k = 0$ which is a trivial case. We also write the relation for discrete values of E_i as in an energy scan. In doing so, we have the much simplified (23),

$$I_i = A S_i + x \tag{31}$$

and for moments,

$$R_k = \sum_i (E_i - E_R)^k S_i \Delta_E \tag{32}$$

Next we will consider several contributions to the error bars of derived R_k from a measurement. This is to supplement previous discussions of error estimates [9, 16].

4.1 Error due to counting statistics

Due to counting statistics, $S(E)$ has uncertainties at each spectral point,

$$S_i \pm \sigma_{S_i} \tag{33}$$

According to (31), with respect to counts I_i ,

$$\sigma_{S_i}^2 = \frac{1}{A^2} \sigma_{I_i}^2 \tag{34}$$

Assuming Poisson statistics, $\sigma_{I_i}^2 = I_i$, we have

$$\sigma_{S_i}^2 = \frac{1}{A^2} I_i = \frac{1}{A} S_i + \frac{1}{A^2} x \tag{35}$$

Thus for the moments we have,

$$\begin{aligned} \sigma_{R_k}^2 &= \sum_i \left[\Delta_E (E_i - E_R)^k \right]^2 \sigma_{S_i}^2 \\ &= \frac{\Delta_E}{A^2} I_{2k} \end{aligned} \tag{36}$$

$$= \frac{\Delta_E}{A} R_{2k} + \frac{x \Delta_E}{A^2} \sum_i (E_i - E_R)^{2k} \Delta_E \tag{37}$$

4.2 Error due to spectrum normalization

With respect to normalization factor A ,

$$\sigma_{S_i}^2 = \frac{(I_i - x)^2}{A^4} \sigma_A^2 \tag{38}$$

For the moments we have,

$$\begin{aligned} \sigma_{R_k}^2 &= \sum_i \left[\Delta_E (E_i - E_R)^k \right]^2 \sigma_{S_i}^2 \\ &= \sigma_A^2 \frac{\Delta_E}{A^4} \sum_i (E_i - E_R)^{2k} (I_i - x)^2 \Delta_E \end{aligned} \tag{39}$$

It should be noted that the uncertainty of normalization factor σ_A is not an independent variable, as one can tell from (31) that it is related to counts and background,

$$A = I_0 - x_0 \tag{40}$$

The above result can be used to estimate the effect of normalization on the derived moments.

4.3 Error due to background subtraction

With respect to the assumed constant background x ,

$$\sigma_{S_i}^2 = \frac{1}{A^2} \sigma_x^2 \tag{41}$$

For the moments we have,

$$\begin{aligned} \sigma_{R_k}^2 &= \sum_i \left[\Delta_E (E_i - E_R)^k \right]^2 \sigma_{S_i}^2 \\ &= \sigma_x^2 \frac{\Delta_E^2}{A^2} \sum_i (E_i - E_R)^{2k} \end{aligned} \tag{42}$$

In addition to this uncertainty, we can also estimate the effect on derived moment caused by background subtraction. The sensitivity of R_k to a change in x is,

$$\frac{\Delta R_k}{\Delta x} = -\frac{\Delta_E}{A} \sum_i (E_i - E_R)^k \tag{43}$$

4.4 Errors due to energy scale uncertainties

Another major source of systematic errors come from energy scale of a measurement. In an NRIXS experiment, the energy value at each point during a scan is derived from the high-resolution monochromator parameters, including the temperatures of its crystals. Let us represent these uncertainties in the following way. At each energy point,

$$E_i = \tilde{E}_i + \epsilon + \epsilon_i + \delta \tilde{E}_i \tag{44}$$

with \tilde{E}_i represents the true energy at each point. There could be a uniform shift ϵ of the energies, *i.e.*, a shift of energy zero reference, which might be resulted by fitting the elastic peak, while ϵ_i allows for a random uncertainty in the energy calculation at each point. A scaling error of $1 + \delta$ might happen as well. Higher order deviations can be added into the above model. However, they ought to be very small in a reasonably well calibrated system.

The effects of random energy variations ϵ_i and scaling error of δ were considered in Ref. [16]. Here we only list the sensitivity of moments to an energy shift,

$$\Delta R_k = \sum_i \left[k (E_i - E_R)^{k-1} S_i \Delta_E \right] \epsilon = k R_{k-1} \epsilon \tag{45}$$

5 Concluding remarks

After 20 years of exciting developments and applications, NRIXS method has matured, as users of this technique now ask for ever more precise and quantifying results from measurements. While this will ultimately come from hardware improvements and innovations in light sources, x-ray optics, and detectors, developments in data analysis can help researchers better understand what information is contained in a measurement and get the most out of existing data sets. Here we only mentioned a few aspects of NRIXS data analysis. There are many other topics need further investigations and developments, *e.g.*, elastic peak treatment, sound velocity derivation, spectrum de-convolution, anharmonicity, just to

name a few. With the availability of increasing computing power and sophisticated statistical methods, we expect to be able to provide more reliable results tailored to specific needs of individual research groups.

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