Deglitching procedure for XAFS

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A computer program for eliminating artifacts such as glitches and Bragg peaks of the polarized XAFS spectra is presented. It permits to easily locate and to eliminate from the EXAFS spectra the additional signals originated from the Bragg scattering by crystalline samples. The test of the procedure on the spectra with specially introduced artifacts and on the experimental polarized XAFS spectra showed its high effectiveness.

Keywords: XAFS, data analysis, computer program

1. Introduction

Experimental spectra often contain additional signals - peaks that originated from diffraction by a single-crystal sample or artifacts by the single-crystal monochromator. The artifacts considerably distort the spectra and can introduce significant errors into results. In the case of Bragg reflections the problem is usually solved by applying special experimental approaches such as the oscillating of samples (Revenant-Brizard *et al.*, 1997), adjustment of single crystal sample to avoid the presence of Bragg reflections in the wavelength region of interest (Shuvaeva *et al.*, 1997) or by using oriented polycrystalline samples for polarized XAFS studies (Yang *et al.*, 1988). However, these methods require special experimental equipment or sample preparation techniques and are not applicable in some cases. The study of effectiveness of the deglitching procedures included into modern XAFS packages (Ressler, 1997; www.ixs.iit.edu) for removing artifacts with different positions, shapes and widths has not been reported.

The aim of this work is to study the possibility of analytical elimination of artifacts from experimental data, to work out an optimal deglitching procedure and to study the limits of its effectiveness.

2. Localizing

The problem can be divided into two parts. The first is the localizing of the positions of the artifacts and their separating from the EXAFS signal. Our approach for the solution of this part of the problem is based on the fact, that the artifacts, which as a rule can be approximated with sufficient accuracy by the Gauss function, are usually much more narrow and strong comparative to the XAFS signal, so the first derivative of the absorption coefficient μ(k), where k is a wave number, should display sharp peaks in these parts of spectra. In order to formalize the search of the artifacts we used the function

$$f(k_i) = k^n \cdot \left(\left| \left(\frac{\partial \mu}{\partial k}\right)_{k_i} - \left(\frac{\partial \mu}{\partial k}\right)_{k_{i-1}} \right| + \left| \left(\frac{\partial \mu}{\partial k}\right)_{k_i} - \left(\frac{\partial \mu}{\partial k}\right)_{k_{i+1}} \right| \right) \quad (1)$$

calculated for each point of the experimental spectra with corresponding wave number value k_i. For automatic artifact positions location we use the method disseminated widely in digital signal processing (Saulnier *et al.*, 1985, Zhuchkov, 2000) and radiophysics (Jeffer & Gupta, 1972, Zerguine *et al.*, 1996). The function f(k) is delayed on several points and is multiplied by itself:

$$g(k_i) = f(k_i) \cdot f(k_{i+s}). \quad (2)$$

where s = 1 or 2.

This function significantly enhances the amplitude of the artifacts relative to EXAFS signal that makes it easy to reveal and locate them. At the Fig.1 the real Nb K-edge EXAFS spectra obtained from the single crystal sample of $KNbO_3$ together with the corresponding f(k) and g(k) functions are presented. It can be seen that even those artifacts whose amplitude is quite small relative to XAFS signal are

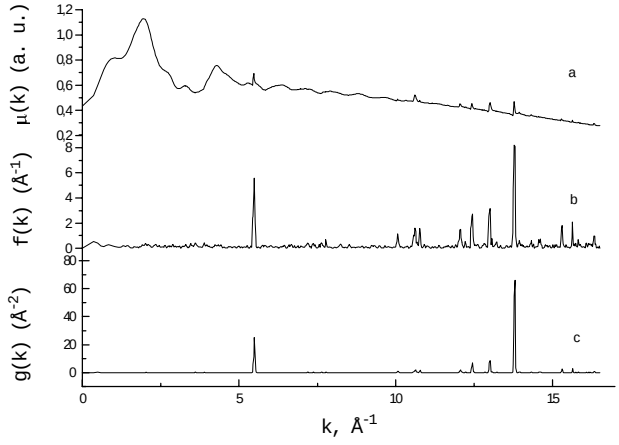

Fig 1 (a) The experimental Nb K-XAFS spectra of $KNbO_3$ and corresponding functions (b) f(k) and (c) g(k).

clearly distinguished at this function. So it is easy to find and to separate these points by setting the upper level of g(k), and all points that lie above it can be automatically marked to be 'bad' points, which are affected by the artifacts.

3. Eliminating

The second part of the problem is eliminating of the artifacts from the spectra. We tried two approaches for elimination:

1. simple deleting of the 'bad' points from the spectra
2. polynomial fitting of the parts of the spectra affected by the artifacts by the least squares method. Smooth parts of the spectrum to the right and to the left of an artifact are fitted by 4-th order polynomial and μ (k) function in the region of the artifact is approximated by this polynomial.

In order to test correctness and accuracy of these deglitching procedures we applied them to regular experimental spectra, obtained from a powder sample, with artificially introduced additional peaks. Artifacts were modeled by adding the Gauss function $B*\exp(-(k-a)^2/2*\sigma^2)$ to the experimental data. After the application of the deglitching procedures normalized EXAFS function of the resulting spectra χ_{rest} were compared to the function of the initial spectra χ_{norm} using the factor

$$\delta = \frac{\int_{k_{min}}^{k_{max}} (\chi_{rest} - \chi_{norm})^2 \, dk}{\int_{k_{min}}^{k_{max}} \chi_{norm}^2 \, dk} \qquad (3)$$

as a criterion of accuracy.

We studied the accuracy of the deglitching procedure depending on the width σ of the introduced peaks. The dependence of δ values on σ is shown at the Fig.2. It can be seen that the both

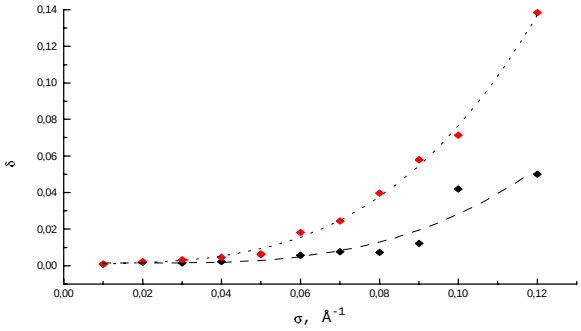

Fig 2 The dependence of the deviation factor δ between normalized χ(k) of the initial and the resulting spectra on the width of the introduced peaks σ (dashed line - elimination of glitches, doted line - polynomial fitting).

procedures give good results for the peak width values less than 0.1 A^{-1}, and give the discrepancy factor less then 0.1 %, which is comparable with the regular values of discrepancy factors in the fitting procedure. However, fitting procedure provided somewhat better results, especially for the larger values of σ.

The stability of the algorithm under the variations of artifact position (parameter a) is revealed.

4. Program description

The above approaches have been incorporated into interactive computer program adapted to IBM PC. It allows to locate those parts of the experimental absorption coefficient function μ(k), which are affected by artifacts, by setting the maximum level of function g(k), and to eliminate the artifacts by the polynomial fitting by least squares method (Press *et al.*, 1996, Stoer & Bulirsch, 1990). It also permits to model the artifacts and so to test the accuracy of deglitching for every specific case.

The code of program is written in Object Pascal. Standard conventions for ©MS-WINDOWS-95 have been taken into account and users familiar with programs like ©MS-WORD etc. should have no problems to use the program. Graphical interface helps to visualize the results of all the operations at every stage of the data treatment. Program needs energy and corresponding absorption factor values from ASCII files, written in two columns. It allows converting the data into k space for convenience of data treatment. The options include also the calculation of g(k) function, the choice of its upper level just at the plot and the automatic marking of the points which lie above this level, approximation of the selected parts of spectra by polynomial fitting, modeling of artifacts by adding Gauss function to the regular spectra. Output data can be exported using OLE-technology or to ASCII-code files optionally.

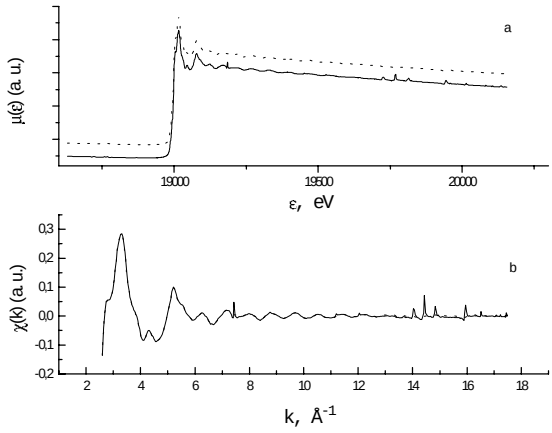

Fig 3 The experimental Nb K-XAFS spectra of $KNbO_3$ (a) and corresponding normalized EXAFS function (b) with artifacts (solid lines) and after application of the program (doted lines).

If the experimental spectrum has artifacts within the different k-regions then we recommend using different values of n in (1) (k^n- is the weight function, included to amplify the contribution of different k-ranges). The program performs estimation of the artifact parameter σ and if its value exceeds 0.1 A^{-1} warning message is displayed.

The proposed algorithm is applied to real experimental polarized XAFS spectra of $KNbO_3$ with artifacts originating from Bragg reflections of the spectra. The standard analysis of the spectra was made before and after application of the deglitching procedure using the ©FTBF code (Bugaev *et al.*, 1999). The Fourier transformation was performed within the k-range from k_{min}=3.0 to k_{max}=15.7 $Å^{-1}$. The comparison of experimental absorption coefficients and normalized χ functions (Fig.3) and Fourier Transform (Fig.4) of the initial spectra and the one treated using the deglitching program indicates that procedure considerably improves the spectra and makes them suitable for further analysis.

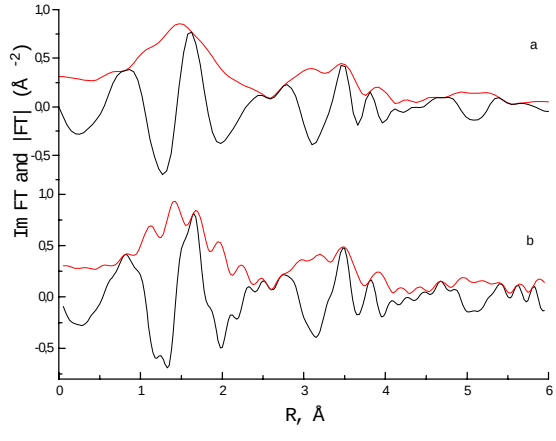

Fig 4 The Fourier Transform imaginary parts and amplitudes of experimental Nb K-XAFS spectra of $KNbO_3$ (b) with artifacts and (a) after application of the program.

5. Conclusion

We have shown that the spectra affected by artifacts with widths less then 0.1 A^{-1} can be successfully corrected by the deglitching procedure. We also have worked out the computer code for deglitching including formalized search of the artifacts, their elimination and spectrum reconstruction by polynomial fitting. The advantage of the suggested program is localizing of artifact positions in a spectrum in automatic mode, which makes it possible to eliminate glitches simultaneously all over the spectrum.

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