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The Phase and Amplitude Corrected Fourier Transform for the Detection of Small Signals

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In many cases one is interested in small EXAFS signals which are present along with large signals. When the small signal has a frequency close to the dominant frequency of the EXAFS spectrum it may be fully obscured in the Fourier transform. Detection may be even more difficult when the radial structure function (RSF) of the dominant signal shows a complicated structure due to the k -dependence of the phase and amplitude functions of the dominant absorber scatterer pair. This k -dependence especially appears for high Z elements. When a suitable reference compound for the dominant signal is available, the RSF may be simplified by using a Fourier transform which eliminates the complex structure of the phase shift function and the backscattering amplitude. This can be done by transforming $\chi(k) \cdot \exp(-i\phi_j(k)) / f_j(k)$ instead of $\chi(k)$ (1-4), where $\phi_j(k)$ and $f_j(k)$ are the phase shift function and the backscattering amplitude for the j th shell of the reference compound, respectively. Such a phase and amplitude corrected Fourier transform reduces the complicated peak in the RSF to a single, symmetrical and localized peak which peaks at the correct distance and exhibits a very simple, symmetrical imaginary part. Small signals in the neighbourhood of the main peak will now appear as distortions from the symmetrical peak.

As an example, the corrected Fourier transform is applied to a very highly dispersed rhodium (0.5 wt%) on alumina catalyst. The EXAFS signal of this catalyst shows besides the very large Rh-Rh contributions, small contributions of a Rh-O distance at 2.7 Å which is very close to the Rh-Rh distance of 2.68 Å. Fig.1a shows a normal k^1 -weighted Fourier transform from $k=3.3 \text{ \AA}^{-1}$.

Clearly visible is the large sidelobe at the left side of the main peak due to the typical behaviour of the rhodium phase shift function and backscattering amplitude. This sidelobe prevents an easy interpretation of the radial structure function after applying a Fourier transform, which was

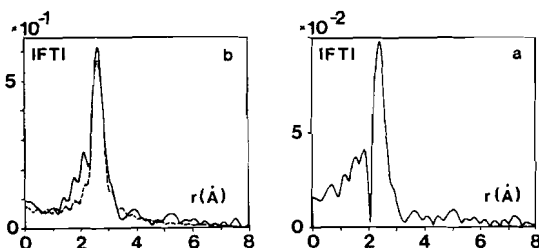


Figure 1

Magnitude of Fourier transform of

- a) experimental data (k^1 -weighted, $k_{\min}=3.3 \text{ \AA}^{-1}$, $k_{\max}=12.7 \text{ \AA}^{-1}$)
 b) experimental data (solid line) and calculated Rh-Rh EXAFS (dotted line) (k^1 -weighted, Rh-Rh phase and amplitude corr.).

corrected for the Rh-Rh phase shift and backscattering amplitude, obtained from rhodium metal foil as reference compound. The dotted line indicates the calculated contribution of the Rh-Rh signal. Since the k -dependence of the Rh-Rh phase shift and amplitude has been removed, the difference at the left side of the main peak is not due to a sidelobe but must be ascribed to a real signal.

The corrected Fourier transform may also be used in the identification of scatterers with approximately the same backscattering amplitude but with a difference in phase shift functions. Applying a FT which is corrected for the right phase shift function will result in a symmetrical imaginary part which peaks positively with the magnitude of the structure function. Small deviations from symmetry might indicate a difference in inner potential between the sample and the used reference compound (5) or a possible asymmetry in the pair correlation function (6), while large deviations may point to a mismatch of the phase shift functions. Again, the above mentioned catalyst may serve as an example. In the catalyst the small signal can be caused by either chlorine, emanating from the used precursor which was used for the preparation of the catalyst, or oxygen from the support. After subtraction of the Rh-Rh content from the spectrum, the RSF of the residual spectrum was examined with the Rh-O and a Rh-Cl phase shift function. In this case, no additional amplitude correction was used since it magnifies the noise to a too large extent, distorting the residual spectrum. The Rh-O corrected FT gives a positively peaking imaginary part (Fig.2a) while a Rh-Cl phase shift results in a negatively peaking imaginary part (Fig.2b), thus indicating the presence of oxygen instead of chlorine as scatterer.

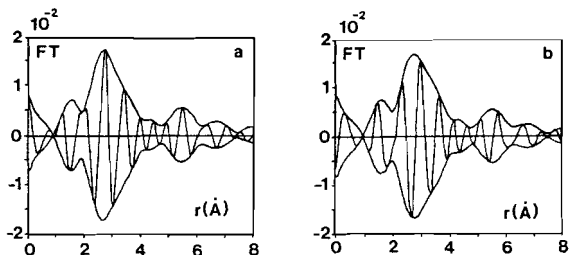


Figure 2

Fourier transform of residual spectrum (k^1 -weighed, $k_{min}=4.2 \text{ \AA}^{-1}$,
 $k_{max}=9.2 \text{ \AA}^{-1}$)
 a) Rh-O phase corr.
 b) Rh-Cl phase corr.

The use of the imaginary part and the magnitude of the phase and amplitude corrected Fourier transform yields the following advantages:

- a) it modifies complicated peak structures to simple symmetrical peaks and thus allows a more direct interpretation of the spectrum (e.g. Cl, O).
- b) once the N constituents of a spectrum are known, the correctness of the parameters may be verified by analyzing each constituent separately to verify that the imaginary part of the phase corrected Fourier transform peaks positively at the maximum of its magnitude.
- c) the oscillating behaviour of the imaginary (and real) part of the transform may cause severe interference effects when several components are contributing in a given region of the spectrum. These interferences may give rise to peaks which do not correspond to real distances in the material.

By studying imaginary parts under different phase (and amplitude) corrections it is possible to unravel complicated transforms and anticipate these interference effects.

d) the imaginary part can be used for the identification of elements with a similar backscattering amplitude.

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