IMEKO International Conference on
Metrology for The Sea
Naples, Italy, October 11-13, 2017

Signal denoising using the Stationary Wavelet Decomposition

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***Abstract* — We propose a method to denoise 1D experimental signals using wavelet transform. Noise affecting experimental signals is indeed a problem shared by many different scientific and engineering fields and a proper strategy of denoising, avoiding the loss of useful information embedded in the original signal, is often essential. This is especially true for spectroscopic data, where significant features may be hidden by noise or covered by undesired components, which are not related to the physical content of the signal. In particular, we have applied the Discrete Wavelet Transform (DWT) to infrared spectra collected at a synchrotron source, overcoming the limitations of other filtering strategies conventionally employed. The good results here obtained, and the other attempts presented in the recent literature, suggest that wavelet transform can represent a valuable tool, finding its ideal application in a number of many and diverse fields, including spectroscopy, marine science, meteorology, and engineering.**

***Keywords* — Wavelets, Stationary Wavelet Decomposition, SWD, DWT, signal denoising, filtering, infrared spectroscopy.**

I. INTRODUCTION

Experimental signals are often tricky to study. Usually, major difficulties arise from a poor Signal-to-Noise Ratio (SNR) or from the presence of irrelevant components blending into the signal and making it difficult to extract significant information. Such components may be due to interfering physical or chemical processes not under control, imperfections of the experimental apparatus, or many other causes resulting in random and systematic (or coherent) spurious fluctuations of the signal recorded by the detector. During the last decades, several methods have been developed aimed to improve the quality of experimental signals, such as the Gaussian smoothing [1], the time averaging [2], the Fourier transform filtering procedure [3, 4], the median filter technique originally introduced by Tukey [5], the windowed smoothing algorithm based on moving average due to Savitzky and Golay [6], and others based on Artificial Neural Networks [7, 8]. Unfortunately, it is not unusual to deal with circumstances where all these conventional filtering methods are not effective. Although noise removal and SNR increase are goals achieved by almost all the most widespread filtering methods, it is much more difficult to find a strategy capable of properly removing undesired components from raw data and reliably retrieving the original signal. This turns out to be especially true in case of weak signals with a magnitude close to that of noise or with significant and undesired components of comparable magnitude [9, 10]. One of the most powerful tools recently introduced to overcome the limitations imposed by traditional filtering, smoothing, and denoising algorithms is the wavelet transform. Despite the wavelet transform is usually employed to analyse time series (see, among many, [11-13]), wavelet decomposition can be also successfully used for building up powerful filtering strategies of frequency or time signals, as proposed in this work and recently confirmed by other authors [14-16]. In particular, we have applied the Discrete Wavelet Transform (DWT) to filter a set of infrared (IR) spectra collected at the synchrotron SOLEIL (Saint-Aubin, France). The main goal of our experiment was to investigate the temperature and pressure evolution of vibrational features of water confined in a mesoporous silica matrix known as MCM-41. We focused on two vibrational bands: one due to the stretching motion of the water molecule OH bond, and the so-called connectivity band, arising from the collective motion and distortions of the hydrogen bond network. The effectiveness, versatility, and clear advantages offered by DWT are proven by its rapid spread among the scientific community, so much so that it is already finding extensive use in several applications, such as signal and image processing, data compression, pattern recognition, finance, detection of aircraft and submarines, study of the atmospheric turbulence layer and marine seismic data [17]. However, to the best of our knowledge, DWT is an original solution to the specific problem of spectra collected on a synchrotron beamline, as no alternative and efficient strategies have been proposed in the literature so far. Rather, when similar features have been identified in IR spectra (see, for instance, [18]), no specific solution has been proposed.

The paper is organised as follows: in section II a brief description of the main properties of wavelet transforms is provided; section III describes the experimental procedure and the filtering strategy applied to the IR spectra; section IV shows and discusses the results of this work; finally, section V draws the conclusions supported by our findings.

II. THE CONTINUOUS AND DISCRETE WAVELET TRANSFORM

Wavelets are a relatively recent instrument developed in applied mathematics around thirty years ago [19, 20]. Their interdisciplinary origin (from engineering, physics, and mathematics) is the key to their success and wide applicability, as well as the reason that explains their appeal to scientists and engineers of many different backgrounds. The wavelet transform is similar to the Fourier transform, but with fundamental differences. Both are invertible and based on the decomposition of the signal in terms of orthogonal basis functions other than the original coordinates. However, while the Fourier transform basis sets consist only of sine and cosine functions, there exists an infinite number of "waves" that can be used as basis in the wavelet transform. In particular, each set of orthogonal basis functions can be obtained from a single function (the so-called "mother" wavelet) by shifts acting on time and dilations acting on frequency. Moreover, Fourier basis are completely localized in the frequency (transformed) domain but extend infinitely in the time (physical) domain, whereas the wavelet basis functions are dually localized (i.e. are finite) in both time and frequency domains. Roughly speaking, the wavelet transform is simply a series of band-pass filters with a known response function (i.e. the wavelet basis) of uniform shape and varying location and width. As a consequence, wavelet analysis comes across as particularly suitable to analyse localised variations of power within time series [21], which can be decomposed in the time-frequency space in order to determine both the dominant modes of variability and how those modes vary with time [22]. Thus it is not a coincidence that wavelet analysis is finding large and numerous applications in aerodynamics and fluid dynamics [23-25], geophysics [26-28], and meteorology [28-31].

Let us consider time and frequency as an example of physical and transformed spaces. From a mathematical point of view, the continuous wavelet transform (CWT) of a time signal $x(t)$ consists of a projection over a basis of compact support functions obtained by dilations and translations of a mother wavelet $\psi(t)$, localised both in the physical and transformed spaces. The wavelet coefficients resulting from the signal decomposition are function of time t and scale s, which is inversely proportional to the frequency [28]. Therefore, the CWT of a time signal $x(t)$, $W_x(t,s)$, can be defined as:

$$W_x(t,s) = C_{\psi}^{-\frac{1}{2}} \int_{-\infty}^{+\infty} x(\tau)\psi^{*}\left(\frac{t-\tau}{s}\right)d\tau \qquad (1)$$

where $C_{\psi}^{-1/2}$ is a constant characteristic of each wavelet function and $\psi^{*}((t-\tau)/s)$ is the complex conjugate of the dilated and translated mother wavelet $\psi(t)$, with $\tau, s \in \mathcal{R}$ and $s \neq 0$. The wavelet function is also called wavelet kernel. The parameter s is the scale and measures the degree of compression, while τ is the translation parameter which determines the time location of the wavelet. If $|s| < 1$, then the wavelet is compressed compared to the mother wavelet and corresponds mainly to higher frequencies. On the other hand, if $|s| > 1$, then ψ is dilated and corresponds to lower frequencies. For examples and detailed description of the huge number of wavelet basis and functions commonly used, we refer to [32, 33]. Remarkably, the decomposition of a time series into basis functions is calculated for different segments of the time-domain signal at different frequencies. This point makes clear the main hallmark of the wavelet transforms: they offer "variable time-frequency" resolution, in contrast with Fourier transform which only offers frequency resolution. A discrete version of the wavelet transform can be also adopted to decompose a time signal $x(t)$, where $t = n\delta t$ is the discretized time variable, with n an integer index. According to [34], if the discretised scales s_j are arranged on a dyadic distribution, i.e. $s_j = 2^j$, and the translations are multiple of the scale s_j, the orthonormal basis $\psi(t)$ can be expressed as:

$$\psi_{[k]}^{(j)}(t) = 2^{-j/2}\psi\left(\frac{t-2^{j}k}{2^{j}}\right) \qquad (2)$$

Hence, the discrete wavelet coefficients, $w_x^{(s)}(n)$, are obtained as:

$$w_x^{(s)}(n) = \sum_{-\infty}^{+\infty} \psi^{(s)}(n-2^{s}k)x(k) \qquad (3)$$

The last equation tells us that, by varying the wavelet scale s and translating ψ along the localised time index n, it is possible to build up a picture showing both the amplitude of any feature versus the scale and how this amplitude varies with time.

Some of the main advantages of wavelets can be summarized as follows:

(a) since wavelets are simultaneously localised in time and frequency domains, they are adequate to analyse both stationary and non-stationary signals;

(b) wavelet-based algorithms are computationally very fast;

(c) given their ability to separate the fine details in a signal, wavelets allow multi-scale analysis. Smaller wavelets can be used to isolate very fine details, while larger wavelets can identify coarse details;

(d) wavelets allow for signal compression or denoising without appreciable degradation.

For a more general introduction to wavelet decomposition methods and a comprehensive review of mathematical aspects of wavelet transforms, the reader is referred to several recent monographs [19, 21, 22].

III. MATERIALS AND METHODS

A. Experimental details: sample preparation and IR measurements

Infrared spectra were collected at the synchrotron SOLEIL (Saint-Aubin, France), exploiting the new high-pressure/low-temperature set-up available at the AILES beamline. Two spectral regions were investigated: the mid-infrared region (MIR, 1000<ω<6000 cm^{-1}, with ω the vibrational wavenumber) and the far-infrared domain (FIR, 50<ω<600 cm^{-1}), also known as FIR. The investigated system was pure water (H_2O) confined in MCM-41 substrate. MCM-41 is a silica porous matrix characterized by a highly regular structure (2D array of uniform hexagonal channels, arranged in a honeycomb type lattice), a monodisperse distribution of pore size with nanometric dimensions, a high hydrophilicity, and lack of swelling [35]. Our MCM-41 samples (with a pore diameter of 2.8 nm) appeared as a white powder and were synthesised by the Chemistry group of IMPMC (Université Pierre et Marie Curie, Paris), following the procedure described in [36]. After synthesis and calcination at 550°C, the hydration procedure was accomplished by exposing dry MCM-41 powder to a water-saturated environment inside a sealed desiccator at room temperature (~298 K). The time of exposure to water vapour was carefully set to achieve ~90% of pore filling. Pores were not fully filled to avoid water leaking out the pores due to the expected volume expansion of H_2O upon cooling below the crystallization temperature.
Measurements were performed by varying both pressure (less than 1 GPa) and temperature, which ranged from ~140 K up to 293 K. Since all spectra were collected under pressure, a diamond anvil cell (DAC) was used as sample holder. The pressure calibration was performed by means of ruby chips loaded with the sample in the micrometre-sized hole between the diamond faces. In addition, few drops of oil (Fluorolube® in the MIR frequency region and Nujol in the FIR frequency domain) were inserted as pressure transmitting medium. Measurements were carried out using a Bruker IFS 125 Fourier transform spectrometer (FT-IR) and all IR spectra were collected in transmission mode. A bolometer was used as detector, with a resolution of 2 cm^{-1} and 100 scans per spectrum. The MIR region was investigated by means of a Globar lamp, in combination with a KBr beam splitter, whereas the infrared emission of synchrotron radiation was necessary to explore the FIR domain. The synchrotron light was used in combination with a composite Si beam splitter. Further details of the experimental set-up can be found in [37].

B. IR spectra analysis: wavelet denoising

All IR spectra collected at the synchrotron SOLEIL on the AILES beamline were affected by large "oscillations" superimposed to the signal we needed to analyse, as shown in Fig.1. Such oscillations were likely due to multiple reflections of the incident radiation beam on the two windows of the sample container and/or in correspondence of the different interfaces present inside the sample. Attempts of removing these undesired components by means of conventional filtering methods (e.g. smoothing algorithms) were unsuccessful, as only

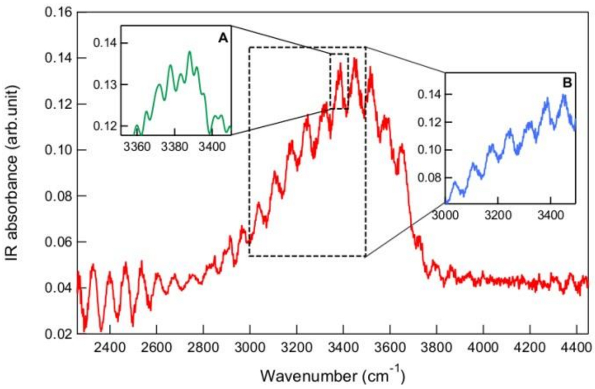

Fig.1. Example of raw data in the MIR frequency domain. The recorded IR absorbance intensity presents some evident oscillations (highlighted in the inset B) superimposed to the signal containing information we were interested in. Inset A indicates very high frequency-low intensity fluctuations resulting from statistical noise.

the high frequency fringes due to statistical noise were correctly removed. The application of a Fourier filter did not give satisfactory results as well, because the unwanted oscillations were not truly periodic and could not be well expressed as a linear combination of sines or cosines. Therefore, we opted for the discrete wavelet transform. In particular, the strategy we adopted is the 1D Stationary Wavelet Decomposition (SWD) technique. We applied a version of the Mallat's algorithm [38], performed by adapting the MATLAB® dedicated toolbox to our specific problem. For the intrinsic characteristics of wavelet transform, discussed in the previous section, wavelet-based filtering can be performed on the scale and time simultaneously. This technique offers an important advantage over the traditional filtering methods, such as Fourier transform: it removes noise (or undesired features in the signal) at *all* frequencies and allows to isolate single events that have a broad power spectrum and multiple events that have different or varying frequency. Indeed, this is exactly what is required in the case of our IR spectra. A complete description of the basic steps of wavelet denoising is reported in [39], while a more in-depth analysis of the advantages of wavelet transform compared to Fourier transform can be found in [17].

Denoising algorithm

Generally speaking, the recorded experimental signal $X(n)$ is a discretized function that can be written as:

$$X(n) = S(n) + N(n) \qquad (4)$$

where $S(n)$ is the part of the signal that must be extracted, embedding all the information we need to analyse, while $N(n)$ represents the signal components we intend to remove. In particular, if $N(n)$ is a low amplitude-high frequency component, it simply represents what is commonly addressed as "noise". In our particular case, $N(n)$ also includes the pseudo-sinusoidal oscillations superimposed over the IR spectrum. The denoising algorithm here employed for removing $N(n)$ is

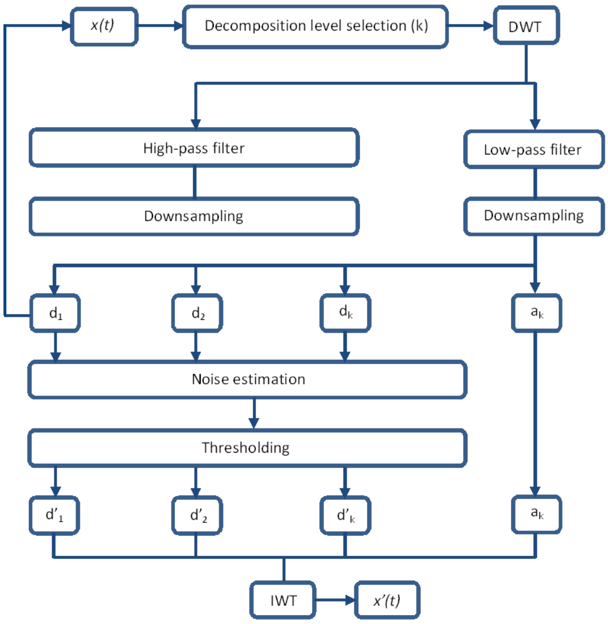

Fig.2. Block diagram of the 1D Stationary Wavelet Decomposition (SWD) method. Downsampling means that only the even indexed elements are kept. The approximation coefficients ($a_1,a_2,...,a_k$) are obtained by convolution with a low-pass filter, whereas the detail coefficients (d_1, $d_2,...,d_k$) result from the convolution with a high-pass filter.

based on the reconstruction of the original signal by means of the discrete inverse wavelet transform (IWT) [40]. This is a “direct” filter because it is applied to the transformed data set, prior to back-transforming it to the signal (physical) domain. A block diagram of the adopted algorithm is displayed in Fig.2. Essentially, the DWT is used to convert a series a_0, a_1, …, a_m (the experimental signal) into two coefficient series: one low-pass series known as *approximation* and one high-pass series known as *detail* ($d_1,d_2,\dots,d_k$), where the length of each series is $m/2$. This decomposition is then applied recursively to the detail series until the desired number of iterations is reached. In other words, the experimental signal, which must be a vector of $N = 2^n$ elements, is numerically transformed into two vectors with 2^{n-1} elements each; one vector contains the approximate coefficients, the other gets the detailed coefficients and serves as an input for each iteration. The unwanted signal components appear in the detail coefficients vector, hence they can be removed from the original signal by setting the detail coefficients related to those particular components to zero. Otherwise, the contribution of a specific component can be reduced by setting a proper threshold on the corresponding detail coefficients. The number of iterations indicates the level of the filter, i.e. the number of detail coefficients used for decomposition. Once the level of the decomposition is established, the inverse wavelet transform can be applied to the semi-processed data to get back the original signal which is now free from noise or any other undesired component.

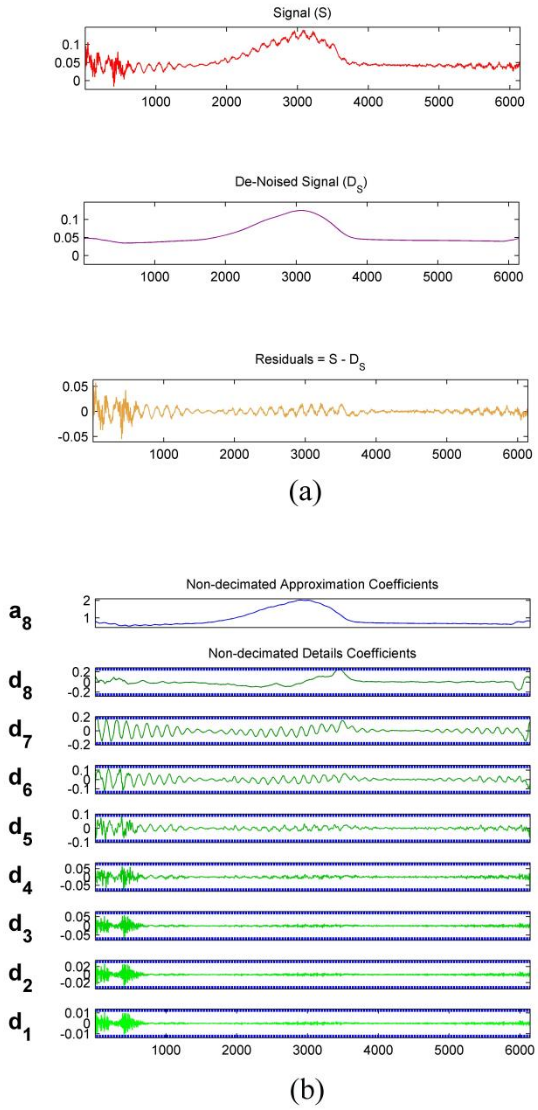

Fig.3. In panel (a) there are (from top to bottom): the raw signal (red), the denoised signal as a result of the application of the SWD technique outlined in Fig.2 (purple), and the residuals calculated as the difference between raw and denoised signal (yellow). In panel (b) all the coefficients (approximation and detail) of the wavelet decomposition are individually shown.

To ensure the generality of the adopted approach, we have checked that results presented in the following are independent of the specific choice of the wavelet kernel. As illustrated in the next section, the decomposition procedure described above appears to be particularly suited for our aims, since it allowed us to analyse the noise level separately at each wavelet scale and adapt the denoising algorithm accordingly, with no particular assumption on the structure of the original signal.

IV. RESULTS AND DISCUSSION

Fig.3 shows an example of the application of the denoising wavelet-based algorithm, described in the

previous section, to a MIR spectrum. All coefficients are individually displayed: d_1-d_8, which represent the detail coefficients at the respective decomposition levels, and a_8, that is the corresponding approximation coefficient at the highest decomposition level.
We remind that our aim is not simply to remove the high frequency fringes due to statistical noise, but to identify and remove all components (with a lower frequency but higher intensity compared to statistical noise) giving rise to the large oscillations shown in Fig.1.
Since the filtered signal was verified to be not dependent on the particular wavelet basis used for decomposition, we adopted the simplest wavelet kernel, i.e. the Haar function. In addition, a soft thresholding method [15, 41] was employed, establishing a denoising level equal to 7. The reason for this choice can be pinpointed looking at panel (b) of Fig.3: d_8 does not look like noise but as a significant part of the signal; if it is removed from the reconstructed signal, some evident physical features would be lost. A good strategy to be sure of the selected level is to observe the residuals of the experimental raw signal and the reconstructed one: if just the noisy components have correctly been removed, the residuals are expected to be structureless. The detail coefficients reported in panel (b) of Fig.3 clearly show that levels from 5 to 7 represent the undesired large oscillations we want to remove, thus the corresponding coefficients were set to zero. On the other hand, levels from 1 to 4 simply reproduce the high frequency noise (statistical noise) that is possible to remove also with other denoising techniques. We do not have any strong reason to completely remove it. However, if we choose to delete even the statistical noise components, we can set the corresponding coefficients to zero; otherwise, we can define a threshold able to remove from those coefficients only the high amplitude oscillations occurring at the lowest wavenumbers. An example of the results obtained by applying to a MIR spectrum the SWD technique, with a signal decomposition approximated at the 7^{th} level of denoising, is shown in Fig.4 and Fig.5. Likewise, satisfying results have been obtained in the case of FIR spectra (data not shown).
In general, the final result is expected to be dependent on the filtering level and on the threshold established for each level. However, the identification of the undesired components of our experimental signals was straightforward after wavelet decomposition. As a consequence, the choice of the filtering level was quite easy and unambiguous for our data. We notice that a convincing proof of the accuracy of the selected filtering level comes from the post-processing stage. After denoising, IR spectra were deconvoluted using a sum of Gaussian functions (data not shown). Since with a decomposition level equal to 7 we identified all the expected Gaussian components in the denoised signal, giving each component a reasonable physical interpretation, we can be confident that the filtering level was correct and that we have removed only the unwanted components without loss of information.

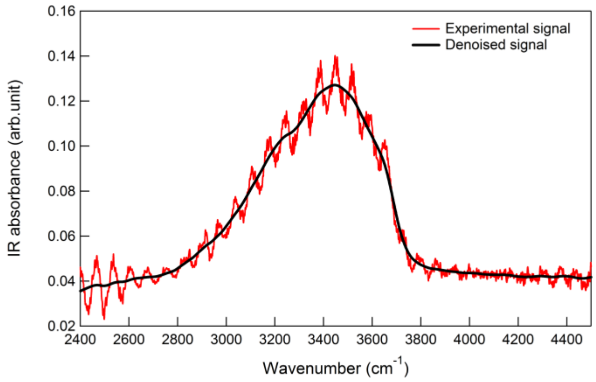

Fig.4. Example of the application of the SWD technique to filter a MIR spectrum (297 K, 0.07 GPa). The raw signal originally recorded is shown as a red line. The black line represents the signal reconstructed after the filtering procedure (7^{th} approximation level). As can be noted, both the undesired oscillations and the statistical noise have been removed.

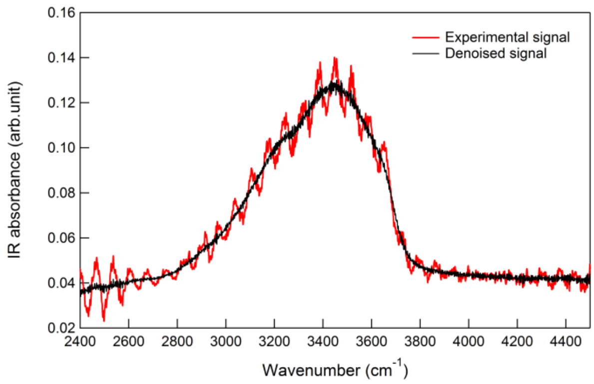

Fig.5. The red line depicts the same signal shown in Fig.4, while the black line represents the denoised signal after the application of the same wavelet-based denoised algorithm, which has deleted all the undesired large oscillation superimposed to the original spectrum. The only difference, in this case, is the presence of the statistical noise: the corresponding detail coefficients have not been set directly to zero, but have been properly thresholded in order to be included in the reconstructed signal.

As far as the results here presented are considered, the wavelet decomposition technique can be regarded as really powerful and easy to apply to treat noise in a huge number of experimental situations. Moreover, it offers high selectivity, stability, and good control and is not time-consuming. This last issue is of particular relevance when large signals or a large number of signals need to be processed, as in the present case of our IR spectra and in many other cases linked with marine and environmental science, meteorology and biology.

V. CONCLUSIONS

In this report we propose a wavelet-based decomposition strategy in order to clean up some IR spectra. Our numerous attempts led us to hold it as the most rapid, versatile and reliable method to realise our purpose. In conclusion, wavelet denoising has made us capable to remove all undesired oscillations affecting the raw spectra in a fast and efficient way, achieving a satisfactory result that any other conventional technique has not provided. Given the efficiency, versatility and reliability of wavelet transforms, we believe that wavelet decomposition-based filtering methods are extremely promising in all cases where data are highly noisy or heavily affected by the presence of interfering signals. As a result, many other applications and research fields may take advantage of the benefits offered by the SWD technique. Therefore, although the method here proposed was tested only on infrared spectra collected at a synchrotron facility, it could be of great interest also for marine science community (e.g. oceanography, meteorology, ecology, biology, geology), as confirmed by other attempts recently appeared in the literature [42-44].

ACKNOWLEDGMENT

The authors intend to thank Prof. Gérald Lelong for providing MCM-41 samples and Prof. Livia Bove for helpful discussions about IR experiments under pressure. Moreover, they also are grateful to all the scientific staff of the AILES beamline and, in particular, to Dr. Frederico Alabarse for his invaluable support during the collection of infrared spectra.

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