Adaptive time-frequency analysis of signals in AFM

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Abstract. The probe-sample interactions during the AFM experiments represent a case of a multi-frequency behaviour, since they are characterized by the simultaneous excitation of cantilevers eigenmodes and/or their harmonics. Analysis of the data obtained as a result of the interaction between the probe and the sample is of a particular interest not only from a practical point of view, i.e. obtaining information about the surface of the sample, but also this is an interesting methodological task, since the instantaneous processes resulting from the interaction of the probe with the sample surface carry a huge amount of information. To obtain this information, it is necessary to provide an analysis method that is capable of characterizing all of the excited cantilevers frequencies simultaneously and without averaging. In other words, it is necessary to obtain the complete spectral response of the cantilever interacting with the sample surface, i.e. information about the dynamics of cantilever behaviour in time. The aim of the present work is to show the possibilities of time-frequency analysis techniques in analysing the signals of AFM experiments.

1. Introduction

Atomic Force Microscopy (AFM) [1] experiments are aimed at gaining information about the sample surface, not only depicting its topography, but also revealing its physical properties. In AFM experiments, cantilevers are used to probe the sample, and thus information about the sample surface is coded in its dynamics. Cantilevers are micromechanical oscillators and the dynamics of the cantilevers has a multi-frequency nature, inasmuch as it consists of simultaneously excited cantilevers eigenmodes and/or their harmonics originated while the probe interacts with the surface distinctive features. All this information can be obtained only if the behaviour of the cantilever is properly described and analysed. This task requires accurate and adequate signal analysis.

The main difficulty in solving this task is that the dynamics of the cantilever is not only of a multi-frequency nature, but also that each of the frequencies combining the resulting signal is changing in time, and sometimes abruptly. Hence, in terms of the signal processing, the AFM signals are non-stationary ones. The analysis of such signals demands for special thoroughness that can be provided if the signal analysis is adaptive.

2. Signal analysis approaches

Commonly, analysis of the signals in AFM is carried out by applying Fourier transform (FT) to the signal. This well-known approach is used due to its high accuracy and analysis speed [2]. However, despite its many benefits, FT provides a full spectral analysis only when stationary signals are investigated, which are caused by its working principle implying displaying of the integrated spectrum of the studied signal. This results in a loss of information about cantilever dynamics in particular time

moments, which ultimately may lead to incorrect conclusions about the system behaviour. To avoid such situation, a time-frequency analysis needs to be implemented. The most powerful time-frequency analysis approach is a wavelet transform (WT) method [2].

Wavelet transform is a known method for image processing and recently it has found its applications in data analysis, when non-stationary signals need to be studied [3-4]. The distinctive difference between FT and WT is an availability of the time scale in the last technique. This possibility stems from the working principle of the WT, in which scaled and delayed wavelets are used unlike cosines infinitely spread on time scale from minus to plus infinity as in FT. It is worth to notice that the only basis functions in FT are cosines of various amplitudes, frequencies, and phases, while in WT basis functions are of different shapes and should be chosen in accordance with the form of the analysed signal. The correct choice of the basis wavelet function or so called mother wavelet allows outperforming standard FT and, hence, this task need to be solved individually in each case [5]. WT has already been successfully implemented to study experimental data in dynamic AFM experiments and for those tasks the Morlet wavelet has been used [6-9] since it has superior time-frequency resolution [10].

Morlet wavelet is formed by multiplying a complex exponential with fixed carrier frequency by a Gaussian shape envelope [2]:

$$\psi(t) = \frac{1}{\sqrt[4]{\pi c^2}} e^{-\frac{t^2}{2c^2}} e^{idt} \tag{1}$$

where $\psi(t)$ is the mother wavelet, c and d are positive parameters controlling the carrier frequency of the mother wavelet and its time spread, i.e. time-frequency resolution. The product of these parameters is a dimensionless parameter $G_S = cd$, known as Gabor shaping factor. It is worth to notice that Morlet wavelet satisfies the admissibility criterion.

Mother wavelet in WT provides a source function, which is scaled and delayed to obtain so called daughter wavelets, and to obtain the WT spectrum of the analysed time signal; the projection of the signal onto daughter wavelets in the entire time-frequency range is calculated.

The WT provides adaptive time-frequency resolution of the signal spectrum due to its working principle. However, it also satisfies the uncertainty principle, which implies that the higher the frequency resolution, the lower the time resolution.

In most AFM data analysis tasks, the joint use of FT and WT fulfils the requirements imposed on the accuracy of the mapping of signal spectral characteristics. However, some tasks require a higher frequency resolution or higher signal to noise ratio than conventional wavelet transform analysis can provide. In these cases, the approach can be used that in the present work is referred to as up-chirplet and down-chirplet transform, (U)CT and (D)CT, respectively. The principal concept of the chirplet transform has been previously introduced [11-13]; however, without consideration of the difference between the up-chirplet and down-chirplet transform and up to present days it is rarely used in real experimental data analysis tasks.

Up-chirplet /down-chirplet transform can be seen as WT, where the mother wavelet is obtained by multiplying a complex exponential with linearly varying carrier frequency by a Gaussian shape envelope [11]:

$$\psi(t) = \frac{1}{\sqrt[4]{\pi c^2}} e^{-\frac{t^2}{2c^2}} e^{i(a+bt)t} \tag{2}$$

where $\psi(t)$ is the mother chirplet, a and b are parameters defining the starting and final carrier frequencies and chirpyness, i.e. rate of the carrier frequency change. The parameters a and b could be positive or negative, and their signs and values also define whether the carrier frequency increasing (up-chirplet) or decreasing (down-chirplet). Using chirplet instead of wavelet as the mother function allows adding a shear in frequency within existing time-frequency windows, thus improving the frequency resolution. However, this is true only in the case if the choice of the parameters a and b has been carried out in such a way that the mother chirplet resembles the analysed signal.

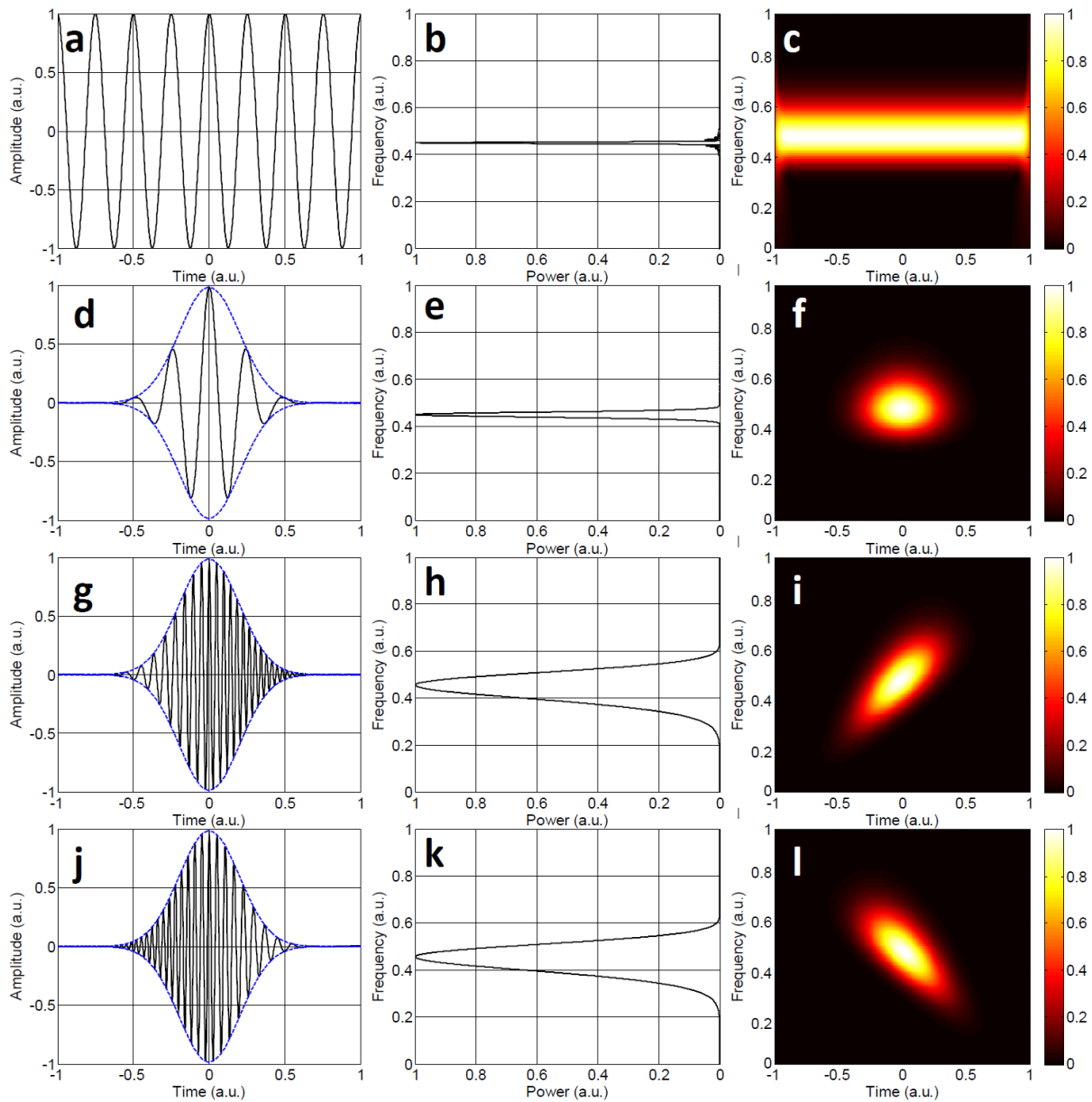Illustrations of the basis functions used in FT, WT, (U)CT, and (D)CT methods are presented in Figure 1.

Figure 1. Basis functions used in signal analysis methods. (a,d,g,j) Temporal representations of basis functions real parts used in FT, WT, (U)CT, and (D)CT methods, respectively. Blue lines – Gaussian shape envelopes. (b,e,h,k) Spectral contents of signals (a,d,g,j), respectively. (c,f,i,l) Time-frequency representations of signals (a,d,g,j), respectively. All scales are normalized and given in arbitrary units.

3. Adaptive analysis of experimental AFM data

To show an example of the approach to data analysis discussed in the previous section, a force curve of dynamic atomic force spectroscopy experiment is analysed (Fig. 2). The investigated experimental force curve (Fig. 2a) has been acquired in ambient conditions (room temperature 296 K, relative humidity 55%, atmospheric pressure) with thermally driven rectangular Au-coated silicon cantilever. Its first free flexural eigenmode is equal to 12.5 kHz and spring constant is equal to 0.15 N/m. Spring constant has been calculated by using the thermal tune method applied to the first flexural eigenmode [14]. The experiment itself has been performed on HOPG surface with constant approach velocity 0.8 nm/ms during the entire dynamic force spectroscopy experiment. Calculated inverse optical lever sensitivity [15] in the present experiment is equal to 190.4 nm/V.
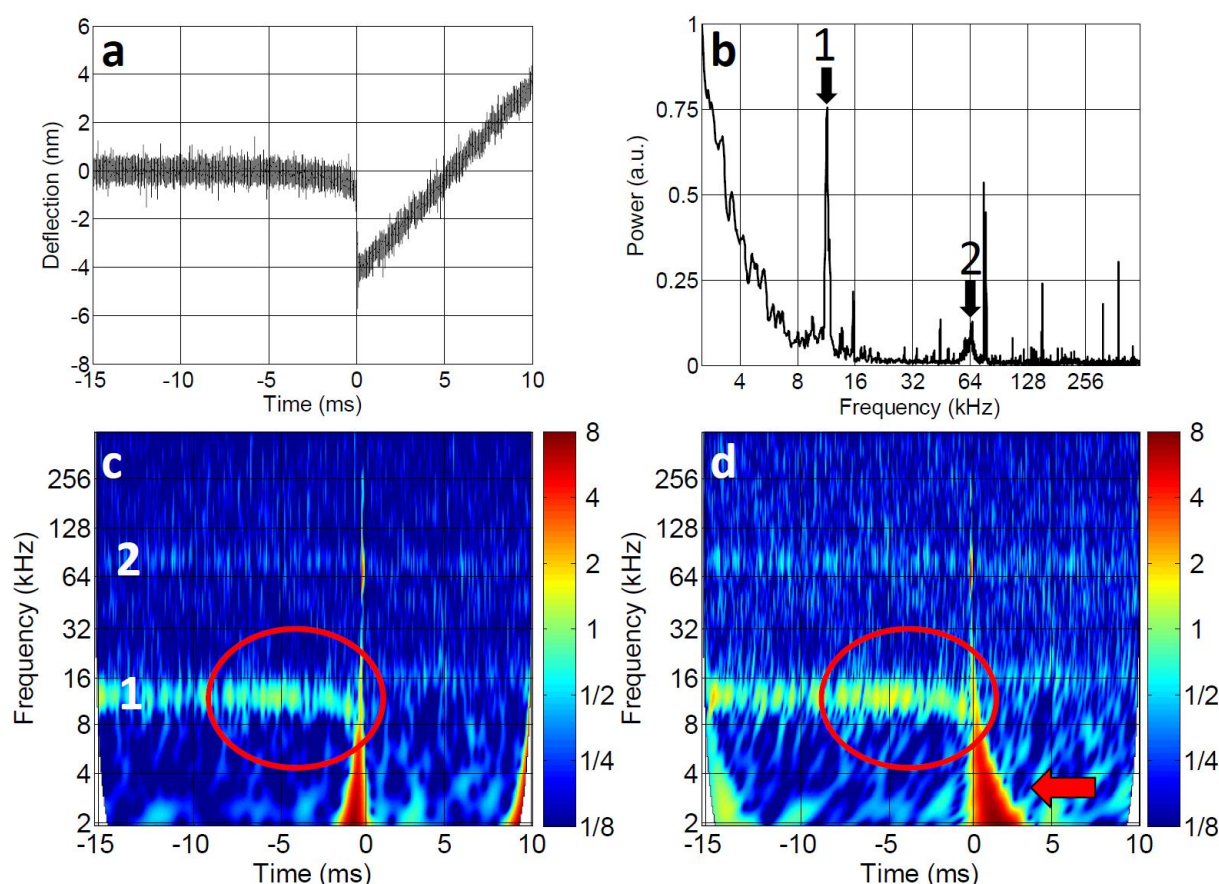
Figure 2. Analysis of the force curve obtained in dynamic atomic force spectroscopy experiment:
(a) Cantilever deflection as a function of time registered by a standard optical beam deflection
system. (b) FT of the signal (a). (c) WT of the signal (a). (d) Down-chirplet transform of the signal
(a). The first and the second flexural eigenmodes are labelled as 1 and 2. Red ellipse allocates an
area of particular interest. Red arrow indicates an area, where the applied approach causes
artificial shear in time-frequency space. (c,d) Side lobes on both sides marked by white colour are
edge effects of the applied transforms. (a,c,d) Zero time corresponds to the jump-to-contact
transition. (b,c,d) Frequency axes and colour scales are presented in base-2 logarithm scales.

The analysis of the force curve obtained in dynamic atomic force spectroscopy experiment is carried
out in several consecutive steps, namely FT, WT, and chirplet transform (Fig. 2).

The first transform that is applied to the acquired signal is FT, which gives an overall understanding
of the signal spectrum (Fig. 2b). The system dynamics is not available from the Fourier power spectrum,
since it shows spectrum integrated over 25 ms. Obtained Fourier power spectrum allows observing few
resonance peaks, and in order to properly attribute these spectral components to the eigenmodes of the
cantilever, the WT analysis can be carried out.

The WT analysis of the force curve shown in Figure 2a is presented in Figure 2c. In this case, the
mother wavelet is Morlet wavelet (see section 2). On the WT spectrum, the behaviour of the cantilever
during the experiment is unfolded in time. It is clearly seen that the behaviour of the cantilever before
and after the jump-to-contact (JTC) transition is different and while interacting with the sample surface
the evident spectral broadening around the first flexural mode and short-term excitations of the higher
flexural modes appear. The detailed description of these phenomena could be found here [6, 8].

Comparing both FT and WT spectra of the signal, it is possible to confidently identify flexural
eigenmodes of the cantilever. For the given system, the value of the first flexural mode is equal to
12.5 kHz and the second flexural mode is equal to 77.8 kHz, in Figure 2b,c they are labelled as 1 and 2.

In most research tasks, such joint FT and WT analysis provides enough information about the studied system; however, in some cases additional information is required or it is necessary to enhance visibility of particular area on wavelet transform spectrum. In such cases, it is useful to apply a complementary analysis. One of such analyses is up-chirplet/down-chirplet transform (see section 2).

As an example, consider the area within the red ellipse in Figure 2c. In the allocated area the down shifting of the first flexural eigenmode is clearly visible. This phenomenon appears due to the acting of the tip-sample force gradient on a cantilever when its tip approaches the sample surface. The data from this time-frequency range could be used to calculate instantaneous values of the tip-sample force gradient acting on a cantilever. Since the frequency is down shifting in the encircled area, it is reasonable to apply (D)CT analysis to improve the frequency resolution. Down-chirplet transform of the signal is shown in Figure 2d. The improvement of the frequency resolution, and thus visibility of the spectrum, is obvious in the allocated area.

(D)CT/(U)CT analysis could be very useful in particular tasks, but it should be applied carefully. For example, consider area in Figure 2d indicated by a red arrow pointing left. In this time-frequency range, the spectral broadening around the first flexural mode due to the JTC appears, but since no frequency down shifting takes place in this region (Fig. 2c), the down-chirplet of the applied (D)CT does not resemble this part of the analysed signal, and thus application of the (D)CT causes artificial shear in time-frequency space. This effect is particularly evident at low frequencies and should be taken into account every time while applying (U)CT/(D)CT to avoid possible misinterpretation of the spectrum.

4. Conclusion

AFM experimental data analysis is not a trivial task; thus, its solution requires a signal analysis method that can be adaptive to allow detail representing of the signal spectral response. Approach proposed in the present work implies a joint use of a few consistently applied data analysis techniques. It is worth to begin with application of the Fourier transform to the signal under investigation, which gives a range of frequencies for the given system and a general understanding about the spectral content of the signal. Then, to correctly attribute the spectral components of the obtained Fourier spectrum, the wavelet transform analysis is applied to the observed range of frequencies. This analysis displays evolution of each spectral component of the signal in time, which allows registering distinctive nonlinearities of the signal to be studied in details. However, it often happens that such signal parts have poor visibility due to the fact that they are usually changing their properties in a very short time interval. To enhance the resolution of these signal parts on a time-frequency plane, it could be beneficial to additionally use a complementary analysis based on the up-chirplet or down-chirplet transform described in the present work. If duly executed, such approach to the signal analysis gives the most comprehensive understanding about the system behaviour in the time-frequency space.

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