Tomography through Points applied to accurate 3D reconstruction of Graphene-like structures

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Abstract

At atomic scale, classical tomography reconstruction can be replaced by tomography through points (TTP) reconstruction[1], that is, the 3D information can be obtained by using geometrical models instead of the classical integral approach. It offers the advantages of a fast but accurate reconstruction and its behavior is robust in the presence of noise as well as in the use of few projections, especially with low noise levels. In this work, TTP technique has been applied to the study of corrugated graphene with errors in 3D location in the range of pm.

In order to investigate the corrugation of suspended graphene, the length scale may vary from angstroms to a hundred nanometers. Scanning tunneling microscopy is one of the candidate techniques, but tip–sample interaction makes the application to suspended graphene quite a complex task. Tomography can be a suitable approach for the study of graphene, as it provides a variety of models and techniques by which it is possible to characterize the material. The peculiarity of graphene-like materials having a monolayer structure has been exploited to develop a new methodology for the analysis of monoatomic layers, such as graphene. In order to show quantitatively the results of the technique, five equally spaced projections(Fig.1) of a grapheme corrugated sample between +10º and -10º using a Nion Ultrastem microscopy (Voltage=100 KV; Cs=7.47x10^{-6} m; C5=1.5x10^{-3} m; C7=0; aperture =30x10^{-3} rad; Defocus=0m; resolution 100 pixel/nm; and Debye-Waller factor=0.01) in HAADF mode has been simulated using SICSTEM software[2], each having 498x493 pixels. Four different tomography series at different noise levels σ=(1.12, 1.51, 2.24 and 3.16)x10^{-5} were simulated. It must be remarked that the intensity of the simulated images ranges from 5.97x10^{-5} to 5.97x10^{-4}.

The proposed approach is based in the following steps: (i) Each atom will be considered as a marker and will be obtained from projections after a filtering stage (Fig.2); (ii) Using a small angles range to obtain the tomography. In this way, radiation damage and sample focusing problems are reduced; (iii) Exploiting an algebraic approach, the reconstruction speed can be improved without loss of precision and (iv) Using the positions of the atomic positions in the projections instead of using the whole image, as it is done in classical tomography, reduces the impact of problems such as the missing wedge or the presence of noise in the projections (Fig. 3).

We first compared the effect of noise with respect to the number of projections (Table 1). The descendent trend of the error with respect to the increasing number of projections is confirmed. Still in the presence of a high level noise, the error is lower than 0.02 nm when five projections are used. From another point of view, it seems that with a sufficiently high number of projections the effect of the noise is almost negligible, being between 0.3688$\pm$0.27 and 1.1452$\pm$0.79 pixels when using five projections.

This approach greatly reduces the influence of the noise in the reconstruction. Moreover, it overcomes the setbacks coming up from the missing wedge problems and focusing at high tilt angles. It offers the advantages of a fast but accurate reconstruction and its behavior is robust in the presence of noise as well as in the use of few projections, especially with low noise levels. We consider that the TTP approach is useful for the study of the corrugation, and can be considered an effective method in graphene structural analysis. It can be easily extended to other grapheme-like laminar materials and single molecules.

References

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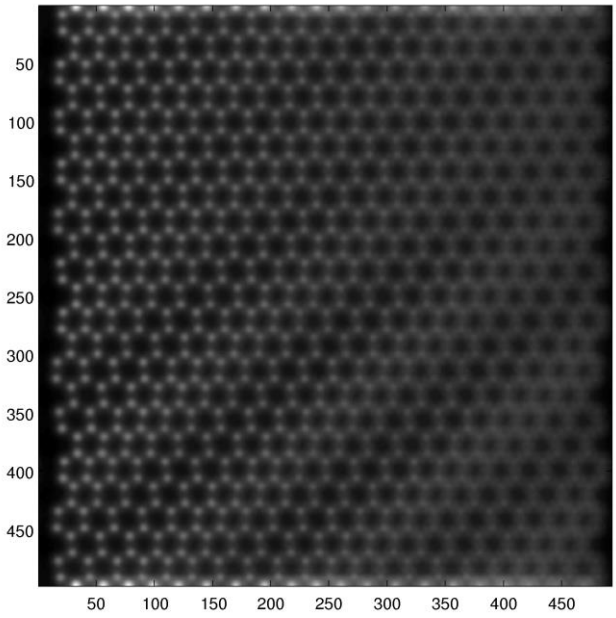

Fig 1. HAADF electron microscopy simulated image of a corrugated graphene sheet obtained with the SICSTEM software simulating a Nion UltraStem (V=100 keV), where corrugation may be appreciated due to changes in the defocus

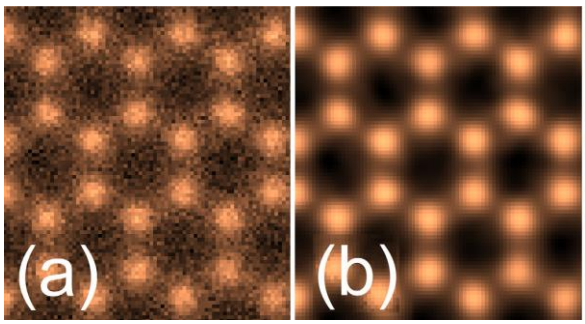

Fig. 2 (a) Simulated image with gaussian noise added (σ=2.23607x10^{-5}). (b) Filtered image, obtained after applying a Wiener filter followed by a low-pass filter. Atom positions are calculated by detecting eight-neighbor maxima in the image followed by local interpolation

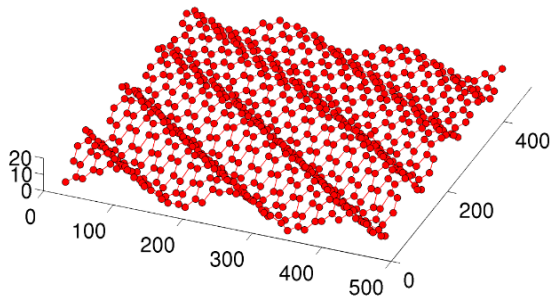

Figure 3. Reconstructed graphene corrugated structure using five projections and noise level σ= 2.24x10^{-5} nm

		Noise standard deviation (x10^{-5})			
		1.12	1.58	2.24	3.16
Number of projections	2	0.13591	0.20100	0.21318	0.30044
	3	0.10922	0.12051	0.17120	0.17746
	4	0.06674	0.08532	0.09762	0.12796
	5	0.03688	0.04658	0.06968	0.11452

Table 1. Mean absolute error in angstroms for the reconstruction in z coordinate calculated by varying the number of projections and different levels of noise in order to test the robustness of the method