Quantitative study of corrugated graphene by tomography and simulation

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Abstract

Graphene has been proved to be one of the most versatile materials for nanotechnologies. It is a matter of fact that its properties, such as conductivity or catalytic behaviour, are strongly affected by the lattice configuration of the layer [1]. A non-invasive methodology for the study of the 3D distribution of C atoms in corrugated graphene has been developed and tested on simulated images. The objective is to show how to adapt tomographic techniques to the study of the corrugations in a graphene layer.
Electron tomography (ET) is widely used to determine the shape of an object. It deals with the reconstruction of a 3D volume from a set of 2D projections of the object under study. Its application to nanomaterials is relatively recent, because of the limitations of the electron microscopes (resolution, aberration, etc). At atomic scale, classical tomography approaches must be replaced by ad hoc techniques. The 3D information can be obtained by processing the projections and by using geometrical models instead of the classical integral one.
In the classical model, the object to be reconstructed is represented by a volume in a 3D space. The 3D reconstruction problem can be afforded by solving a system of linear equations of the type $\vec{p} = \boldsymbol{W}\,\vec{f}$.
To obtain the solution, algebraic reconstruction methods can be used [2]. Usually, in the field of electron tomography, particles are put onto the specimen during the preparation steps such that they are clearly detectable in the series. These particles are used as markers for alignment purposes [3]. Generally, a marker is a part of the specimen that can be easily traced along the whole series.
To use a tomographic approach for the quantification of the corrugation, the characteristics of the material can help to develop special-purpose methodologies. For example, a single graphene layer has a simple geometric configuration (honeycomb regular structure) and atomic thickness. Such features can be exploited to simplify the problem and optimize the reconstruction process. In this case, each atom can be considered as a marker.
The proposed approach offers many advantages over the classical one

- By considering each atom as a marker, it is possible to obtain a direct atomic reconstruction of the structure
- By using a small angles range to obtain the images, the obtained series does not suffer from focusing problems (figure 1).
- By applying a geometric approach, the reconstruction is faster and the precision is not affected.
- By calculating straightforwardly the positions of the atoms in 3D space, the missing wedge problem is greatly alleviated and the effect of the noise reduced (figure 2 a, b).

To validate the methodology, a simulated tomography series has been obtained using SICSTEM [4] (figure 1), a parallel software that allows the simulation of high resolution images from large nanostructures. A Nion Ultrastem set up has been used with equally spaced angles from -10° to 10° and a resolution of 100 px/nm.

An original approach is proposed for corrugation mapping in graphene monolayers. It is based on tomographic series taken at a very low range angles, locating atoms along the series by exploiting the monolayer feature. It has been proved that this approach minimize the influence of the noise on the reconstructed structure. Moreover, it avoids the drawbacks coming up from the missing wedge and the focusing at high tilt angles. The advantage is a fast but accurate reconstruction and the results are robust with respect to the noise as well as in the use of few projections, especially with low noise levels (figure 3). We consider that the Tomography Through Point approach is useful for the study of the corrugation, and can be considered an effective method in graphene structural analysis [5].

References
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Figures

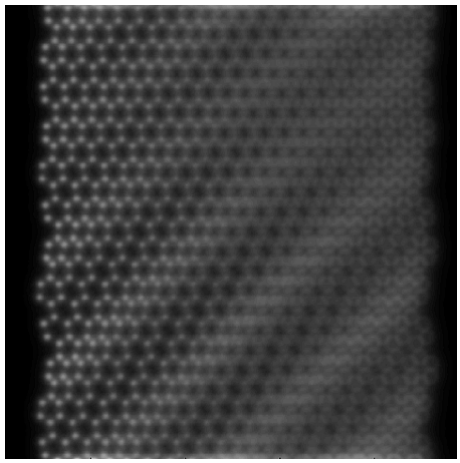
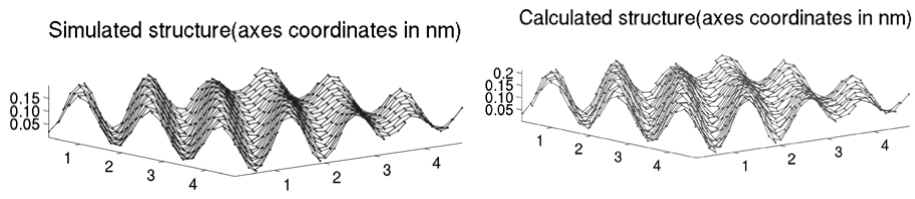


Figure 1: Corrugated graphene monolayer simulated at high tilt angle



a **b**

Figure 2: (a) Atoms' positions of the simulated structure (b) and atoms' positions of the reconstructed structure

Projections	σ			
	1.118e-05	**1.5811e-05**	**2.2361e-05**	**3.1623e-05**
2	0.013591	0.0201	0.021318	0.030044
3	0.010922	0.012051	0.01712	0.017746
4	0.0066735	0.0085323	0.009762	0.012796
5	0.0036876	0.0046581	0.0069685	0.011452

Figure 3: Quantification of the error in nm, with respect to the noise standard variation and the number of projections used for the reconstruction of the simulated structures. For more details see [5].