Interferometric TEM characterization of graphene materials

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Abstract:

Graphene-based materials emerged as one of the most important research areas of material science and nano-technology [1]. Knowing the morphology and atomic structure of graphene is essential, since its electronic, optical and chemical properties depend on the three-dimensional folds and buckles of the 2D lattice [2], and upon the stacking geometry of the layers [3]. Transmission electron microscopy (TEM), combining high-resolution imaging and spectroscopy, represents a unique technique to resolve the structure as well as the composition of nano-materials with atomic resolution. In this contribution, we will review the potentialities provided by interferometric TEM techniques, like Geometric Phase Analysis (GPA) [4] and electron holography [5], to resolve the 3D shape of folds and buckles in graphene membranes [6] and to probe interlayer charges in graphene stacks [7].

Combining high-resolution TEM imaging and GPA with continuum elasticity theory and tight-binding atomistic simulations [8,9] allows us for a complete nano-scale geometrical and physical picture on the edge curvature and topography of folded graphene membranes, with different crystalline orientations. Theoretical predictions were validated by experimentally recovering the 3D topography of the folded graphene with sub-nanometre lateral resolution and height precision, analysing apparent strains in the high-resolution TEM images [6].

Using transmission electron holography [5], we further investigate the redistribution of electronic crystal charges in few graphene crystals [7] and individual monolayers, mapping the effect of the Van der Waals interaction between graphene layers as the distance between the layers varies close to folded edges. We show that electronic density and internal electrostatic potential energy experienced by an electron passing through the crystal can be computed by *ab-initio* approaches based on Density Functional Theory, with high accuracy on single and multiple graphene layers. The computed phase-shift values are in very good agreement with the ones measured experimentally, strengthening the perspectives of the application of the technique, as well as of the computational approach, to more complicated and interesting systems, like doped and functionalized graphene layers.

References

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