Breaking 2D Materials: A Multi-Scale Statistical Analysis of Graphene Oxide Fragmentation

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One of the main advantage for applications of graphene and related 2D materials is that they can be produced on large scales by liquid phase exfoliation. The exfoliation process shall be considered as a particular fragmentation process, where the 2D character of the exfoliated objects will influence significantly fragmentation dynamics as compared to standard materials.
The production of large quantities of 2D materials in solution with well-controlled morphological properties of the nanosheets (i.e. area, lateral size and shape) is not only a technological challenge but also a fundamental one, because several scientific aspects still need to be clarified for a detailed understanding of the fragmentation mechanisms and the control of the final products. Furthermore, it is necessary to develop fast and reliable protocols to measure and analyze a large number of 2D objects and well as to find a set of “robust” parameters to achieve an accurate multi-scale description of the system.
Here we show how these problems can be fruitful solved by using a statistical approach. In particular, the study of the distribution of the morphological parameters such as area and shape represents the key-factor i) to understand the physical mechanisms of the fragmentation in liquid,[1] ii) to test the theoretical models and iii) to explore the mechanical and the structural properties of both the starting material and the final fragments.[2] Recently, we developed a fast and automatic procedure based on topographic images to measure, one by one, the exact shape and size of thousands of nanosheets obtained by exfoliation and fragmentation in general.[3] Previously tested on low-dimension materials such as boron nitride flakes, here we used the procedure to monitor the time evolution of the area and the shape distribution of 2D single sheets of graphene oxide (GO) in water during extended sonication treatment (i.e 100 hours). Combining the analysis of images acquired with different techniques such as Fluorescence (FM), Scanning Electron (SEM) and Atomic Scanning Probe (AFM) microscopies, we monitored the distribution of the 2D fragments studying the morphological parameters from the millimeter to the nanometer scale, as shown in Figure 1. In particular, we showed that the quantitative analysis of the fragments distributions on multi-scale provides to measure the mechanical properties of the GO single sheet such as the Young’s modulus and the fracture strength. Moreover, the analysis of the fragment distributions gives detailed information on the dynamics of the 2D fragmentation providing direct evidence of different regimes given by the interplay of two breaking mechanisms, such as core fragmentation and peripheral erosion.
Finally, based on the high-skewed size-distribution of the GO sheets, we propose a new approach to parametrize the polydispersity of the 2D materials.
The capability to monitor and to control the morphological and the mechanical properties at nanoscale of large quantities of 2D materials in solution will pave the way towards using these materials as fillers for industrial-scale production of graphene- and 2D-based composites.

References

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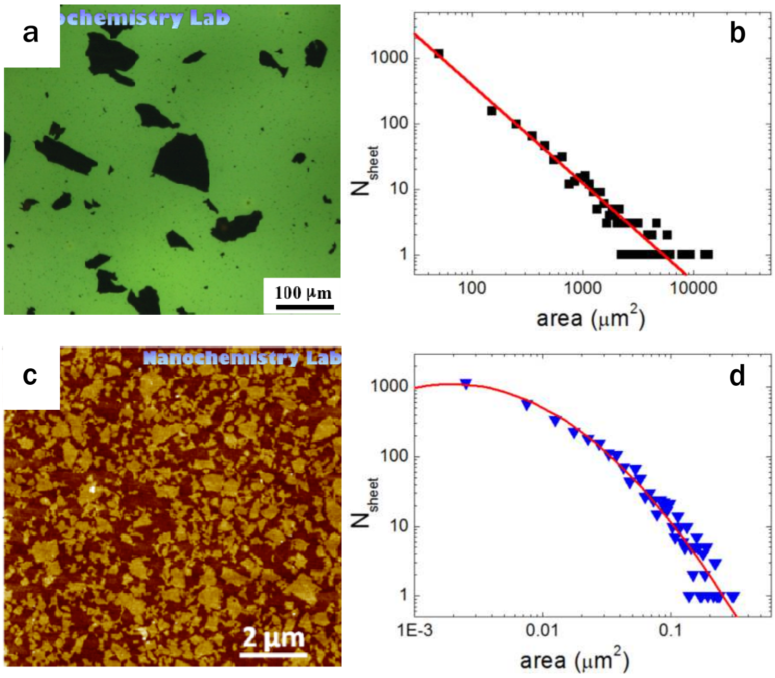

Figure 1: (a,c) FM and AFM images and (b,d) corresponding area distributions of GO sheets acquired on the pristine material (on top) and after 20 hours of sonication (on bottom side)