Probing Local Distortions in Graphene Grain Boundaries with Sub-Ångstrom Precision

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Defects in 2D materials have a fundamental impact on their properties, modifying electrical, mechanical, and magnetic properties [1]. However, the study of these defects is usually done by considering their ideal structure, assuming that the system is perfectly relaxed. In this work, we show how cantilever-based nc-AFM can resolve the real structure of defects, atom by atom. Focusing on graphene grain boundaries, we demonstrate the existence of metastable grain boundaries whose structure differs from the ideal model [2] due to various factors such as substrate, growth, and local stresses. We introduce local energy using AFM to allow the grain boundaries to reach their minimum energy structure. Our unprecedented resolution allows us to quantify the change in atomic positions between the two configurations of the grain boundary. AFM simulations perfectly matched the experimental images, allowing us to reveal that the distortion of the grain boundary with respect to its ideal structure is concentrated in a few atoms. We attribute this to the independent growth of graphene domains during sample preparation.

References

[1] Huang, P. et al. Nature 469, 389–392 (2011)
[2] Yazyev, O. V. and Louie, S. G., Phys. Rev. B 81, 195420 (2010)

Figures

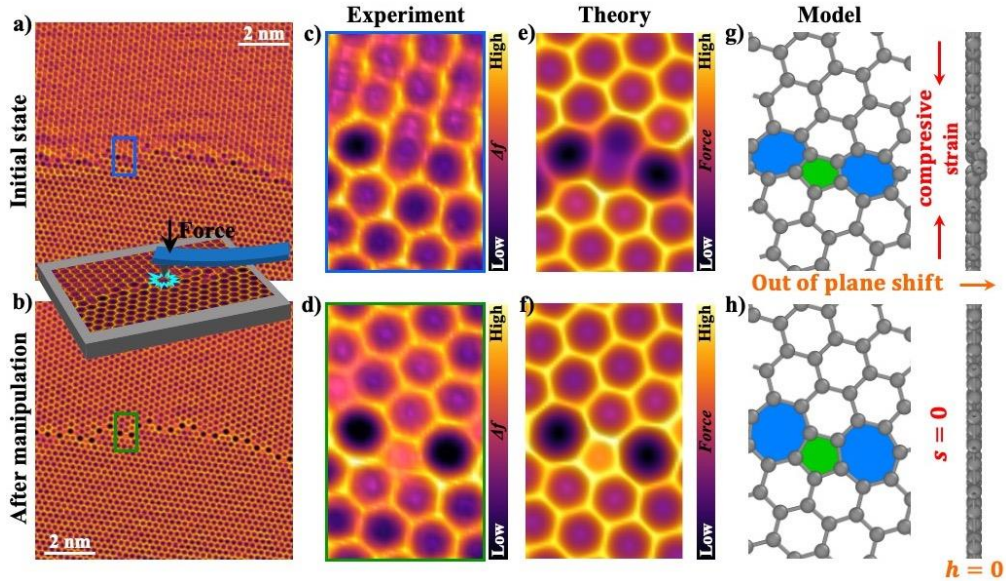

Figure 1: Strain manipulation on graphene grain boundary. a,b) Corresponding ncAFM images acquired on the same region before and after manipulating the GB with the tip. c,d) Magnified view within the region delimited by the blue and green rectangle highlighted in (a,b), respectively. e,f) Theoretical simulated ncAFM images that reproduce the feature of the grain boundary shown in the experimental images. g,h) Grain boundary model used to simulate the theoretical ncAFM images. In (g), we considered a GB under the effect of a compressive strain that induces an out of plane corrugation. In (h), we considered an ideal GB, which does not present any strain and it is fully

planar. A FFT filtering process and 3D effect have been applied to all images, except for the theoretical images, which only has a 3D effect.