Influence of Structural Defects and Chemical Functionalisation on the Mechanical Properties of Graphene

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In recent years graphene has gained significant attention. In particular, its excellent mechanical properties are an important advantage for the practical applications of graphene. These mechanical properties have extensively been investigated, and in particular, the Young's Modulus has been predicted using a range of experimental and theoretical approaches.

Many theoretical methods have been used to predict the mechanical properties of graphene. In particular, a supermolecular approach can be used, studying a finite graphene sheet. Using this approach with *ab initio* calculations has already allowed us to predict the Young's modulus of graphene as 1.11 TPa.[1] The mechanical properties of pristine graphene can also be investigated by periodic calculations on infinite graphene sheets, and a value of 1.029 TPa was calculated at 0.3% elongation.[2] Nonetheless, stress-strain curves are seldom reported, and other mechanical properties such as the bending modulus were not investigated up to now.

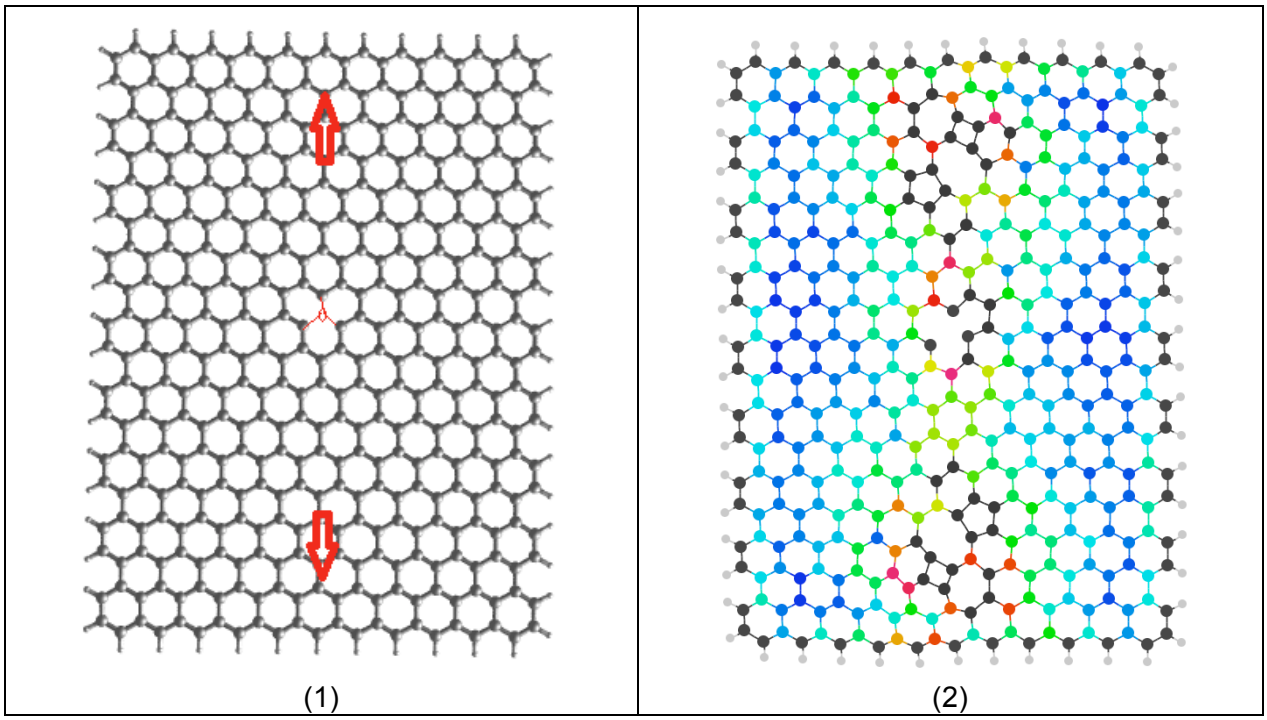
Structural defects in the graphene lattice can affect the electronic properties of graphene in unexpected ways, and harnessing the influence of these defects may be one method to control both the mechanical strength and electrical properties of a material. Defects change essentially not only the electronic properties but also the chemical properties of graphene. Real graphene systems contain structural defects and in experimental studies graphene oxides or reduced graphene oxides are often used. In addition, the influence of these defects on the mechanical properties is unclear.

In this study, structural defects occurring in real graphene systems are considered by modeling single vacancies and oxygenated vacancies, and the Young's modulus has been predicted by using semi-empirical and Density Functional Theory (DFT) methods.[3] For a finite graphene sheet within a supermolecular approach, the internal forces are calculated and the Young's modulus predicted when external strain is applied on the system. These results are in a good agreement with theoretical and experimental results from the literature. In addition, the influence of the presence of a single vacancy, as well as for oxygenation of a vacancy, on the mechanical properties of graphene has been analysed. Our results indicate that the presence of structural defects in the system will stiffen the system upon low strain, but reduces the elastic limit from about 20% strain for pristine graphene to less than 10% strain when defects are present.

References

[1] G. Van Lier, C. Van Alsenoy, V. Van Doren, P. Geerlings, Chem. Phys. Lett. **326** (2000) 181–185.
[2] K. N. Kudin, G. E. Scuseria, B. I. Yakobson, Phys. Rev. B, **64** (2001) 235406.
[3] S. Güryel, B. Hajgató, Y. Dauphin, J.-M. Blairon, H.E. Miltner, F. De Proft, P. Geerlings, G. Van Lier, submitted for publication (2012).

Figure



(1) (2)

Graphene sheet containing a single vacancy (indicated in red), and elongated at two anchor atoms on each side of the sheet in the direction of the arrows (1), together with a colour coding of the geometry, depicting the deformation of the system upon 20% induced strain.