Mechanical Properties of Graphene and Boron Nitride sheets and ribbons

S. Alexandri[1 *], G. Kalosakas[2,3], N. N. Lathiotakis[4], C. Galiotis[2,3] and K. Papagelis[2, 3]

[1]*Interdepartmental Programme in Polymer Science and Technology, University of Patras, Patras (Greece)*

[2] *Foundation of Research and Technology Hellas, Institute of Chemical Engineering Sciences, P.O. Box 1414, GR-26504 Patras (Greece)*

[3] *Department of Materials Science, University of Patras, 26504 Patras (Greece)*

[4]*Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, Athens GR-11635, Greece*

The study of atomically thin 2D crystals is expected to remain one of the hottest fields in nanomaterials for many years [1]. Among the 2D materials, graphene is an ideal one to model its mechanical properties. In particular, the elastic modulus of single layer graphene and its elastic response have been a subject of intensive theoretical research [2]. Hexagonal boron nitride (BN) is a structural analogue of graphene exhibiting large band gap (5.5eV) and partially ionic sp^2 hybridized bonds which are responsible from its notably different properties compared to graphene.

In this work, we have calculated and compared the mechanical properties of graphene and boron nitride sheets and ribbons. We have used empirical force fields derived from first principles' calculations to describe the bond stretching and angle bending interactions between the atoms in graphene and BN. By using molecular dynamics simulations, Young modulus, fracture stress, fracture strain and Poisson ratio for zigzag and armchair directions of graphene and boron nitride nanoribbons are determined.

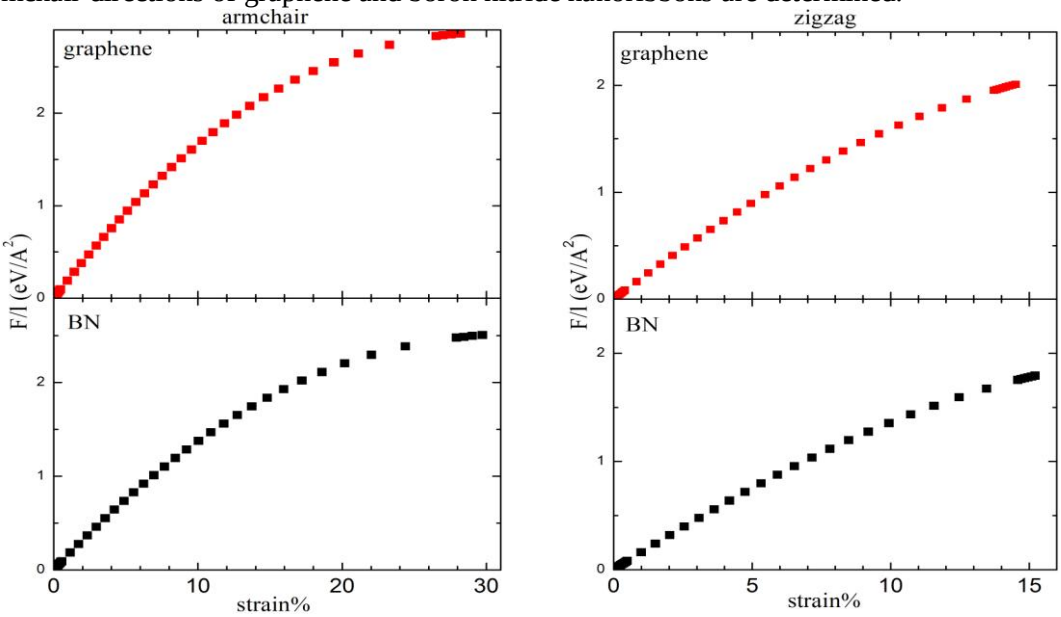

Figure 1: Stress-strain relation of bulk graphene and BN under uniaxial tensile loading along the armchair and zigzag directions.

References

[1] A. K. Geim and I. V. Grigorieva, Nature **499**, 419 (2013).

[2] G. Kalosakas, N. N. Lathiotakis, C. Galiotis and K. Papagelis, Journal of Applied Physics **113**, 134307 (2013).

* sotiria.th.al@gmail.com

Acknowledgements: This work has been supported by the Thales project GRAPHENCOMP, co-financed by the European Union (ESF) and Greek national funds (ΕΣΠΑ).