Determining Volume of 2D nanomaterials and Hydrogenated Reconstructed Klein edges

Chris Ewels[1], Philipp Wagner[1], Bernard Humbert[1],
Viktoria Ivanovskaya[1,2], Jean-Joseph Adjizian[1], Patrick Briddon[1,3]

[1]Institute of Materials (IMN), CNRS, Université de Nantes, BP32229, Nantes, France
[2] Thales-CNRS, 1 Av. A.Fresnel, 91767 Palaiseau & Université Paris-Sud, 91405 Orsay, France
[3] University of Newcastle, Newcastle upon Tyne, NE1 7RU, United Kingdom
chris.ewels@cnrs-imn.fr and philipp.wagner@cnrs-imn.fr

Abstract
Materials mechanical constants such as Young's Modulus, Poisson's ratio or bulk modulus rely on knowledge of applied force and the precise dimensions of a material. However the concept of cross-sectional area (e.g. wall thickness of CNTs) and volume (e.g. graphene sheet) become difficult to define as material size decreases towards the atomic scale. In the current study we propose to define material volume based on an isosurface of the electron density, such that the average nano-object electron density matches that of a related parent bulk system [1]. This new approach is universal, valid for a wide range of different geometries (tubes, sheets, …), and accurately reproduces previous geometry specific studies [2]. It also leads to surprising new physics. While Young's Modulus is often considered purely a function of bond strength we demonstrate with this approach the importance of changing volume. As an example we show that shifting the Fermi level directly modifies the graphene mechanical constants, showing doping-tunable mechanical response.

Via density functional calculations we show that the zigzag edge is **not the most stable** hydrogenated edge in the <$2\bar{1}\bar{1}0$> orientation. Instead a parallel cut results in a Klein edge structure (Figure 1), which when reconstructed [3] and hydrogenated is significantly more stable than the zigzag (Figure 2). The resultant structure, and its associated structural variants, have stabilities approaching that of the armchair edge [4,5].

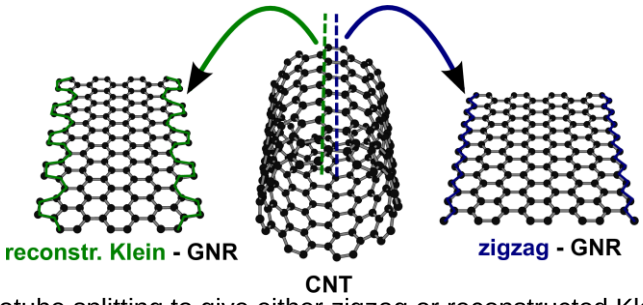

Figure 1: Nanotube splitting to give either zigzag or reconstructed Klein edges [2,3]. A hydrogenated reconstructed Klein nanoribbon is **more stable** by at least 0.027 eV/Å.

References

[1] Ph. Wagner, V. V. Ivanovskaya, M. J.Rayson, P. R. Briddon, C. P. Ewels, J. Phys. Cond. Matt., in press (2013)
[2] J. P. Lu, "Elastic Properties of Carbon Nanotubes and Nanoropes", Phys. Rev. Lett., **79**, (1997) 1297.
[3] V. V. Ivanovskaya, A. Zobelli, Ph. Wagner, M. Heggie, P. R. Briddon, M. J. Rayson, C. P. Ewels, Phys. Rev. Lett., **107** (2011) 065502
[4] Ph. Wagner, PhD Thesis, Université de Nantes, April 2013 *(interested in any postdoc positions!)*
[5] Ph. Wagner, V. V. Ivanovskaya, J. J. Adjizian, P. R. Briddon, B. Humbert, C. P. Ewels, submitted (2013)
[6] T. Wassmann, A. P. Seitsonen, A. M. Saitta, M. Lazzeri, F. Mauri, Phys. Rev. Lett., **101** (2008) 096402
[7] Ph. Wagner, C. P. Ewels, V. V. Ivanovskaya, P. R. Briddon, A. Pateau, B. Humbert Phys. Rev. B**, 84** (2011) 134110
[8] Full references can be found at www.ewels.info or via email at chris.ewels@cnrs-imn.fr