

EDGE ENGINEERING OF GRAPHENE NANORIBBONS

Ph. Wagner¹, C. P. Ewels¹, V. V. Ivanovskaya¹, P. R. Briddon², A. Pateau¹, and B. Humbert¹

¹Institut des Matériaux Jean Rouxel (IMN),
Université de Nantes, CNRS UMR 6502, 44322 Nantes, France

²School of Electrical, Electronic and Computer Engineering,
University of Newcastle, Newcastle upon Tyne, NE 1 7RU, United Kingdom

Today it is possible to produce graphene nanoribbons (GNRs) in the lab with atomically defined widths [1]. GNRs, one-dimensional strips of graphene, offer many opportunities for electronic devices and composites. If we can additionally control the width, and establish the link between edge structure and functionalization, we can design specific GNR properties. The simplest way to saturate GNR edge dangling bonds is via hydrogen termination, which is the standard approach in GNR modelling [2, 3]. However other terminating heteroatoms can be imagined (e.g. N, O). However to develop a more realistic picture of the possibilities of GNR edge chemistry, more complex termination groups have to be investigated. A good example are hydroxyl groups (OH), which as well as being bulkier than simple heteroatoms also show more complex chemical interaction between themselves.

In addition two dimensional layered materials such as graphene have alternative mechanisms for relieving edge-induced strain, namely structural deformation into the third dimension via rippling or buckling [4, 5, 6]. This additional degree of freedom adds significant richness to graphene edge chemistry, which we investigate here for armchair graphene nanoribbons (AGNRs) using the example of hydroxyl functionalisation (see Fig.1). We show how -OH termination of different width armchair GNRs modifies their structure, strain and stability. We show that such functionalisation can drastically alter their band gap, chemical reactivity to metal deposition, and Young's Modulus [6] (see Fig.2). This study points the way towards “edge termination engineering” as a way to create GNRs with custom designed properties.

References

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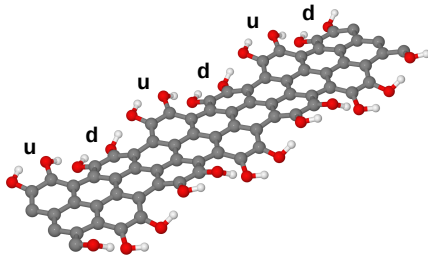


Figure 1: Perspective view of OH-terminated armchair GNR edge structure. u stands for “up” and d for “down” as guide to the eye for the rippled edge structure.

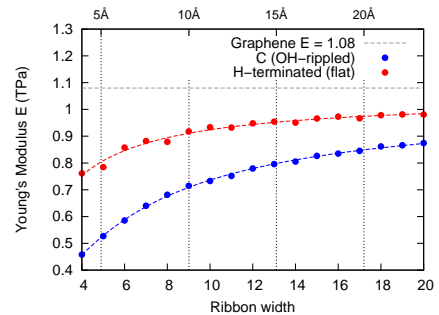


Figure 2: Young's Modulus E along the AGNRs. E fitted with $E = ax + bx^2 + c$ as guide to the eye.

¹philipp.wagner@cnrs-imn.fr