

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Topological defect clustering and plastic deformation mechanisms in functionalized graphene¹ RICARDO NUNES, JOICE ARAUJO, HELIO CHACHAM, UFMG-Brazil — We present ab initio results suggesting that strain plays a central role in the clustering of topological defects in strained and functionalized graphene models. We apply strain onto the topological-defect graphene networks from our previous work [1], and obtain topological-defect clustering patterns which are in excellent agreement with recent observations in samples of reduced graphene oxide [2]. In our models, the graphene layer, containing an initial concentration of isolated topological defects, is covered by hydrogen or hydroxyl groups. Our results also suggest a rich variety of plastic deformation mechanism in functionalized graphene systems.

[1] Joice da Silva-Araujo, H. Chacham, and R. W. Nunes, Phys. Rev. B 81, 193405 (2010).

[2] C. Gomez-Navarro et al., Nano Lett. 10, 1144 (2010).

¹We acknowledge support from the Brazilian agencies: CNPq, Fapemig, and INCT-Materiais de Carbono.

Ricardo Nunes
UFMG-Brazil

Date submitted: 28 Dec 2010

Electronic form version 1.4