Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Grain-boundary unzipping by oxidation in polycrystalline graphene[1] SIMONE ALEXANDRE, UFMG-Brazil, ALINE LUCIO, UFLA-Brazil, RICARDO NUNES, UFMG-Brazil — The need for large-scale production of graphene will inevitably lead to synthesis of the polycrystalline material [1,2]. Understanding the chemical, mechanical, and electronic properties of grain boundaries in graphene polycrystals will be crucial for the development of graphene-based electronics. Oxidation of this material has been suggested to lead to graphene ribbons, by the oxygen-driven unzipping mechanism [3]. A cooperative-strain mechanism, based on the formation of epoxy groups along lines of parallel bonds in the hexagons of graphene's honeycomb lattice, was proposed to explain the unzipping effect in bulk graphene [3] In this work we employ *ab initio* calculations to study the oxidation of polycrystalline graphene by chemisorption of oxygen at the grain boundaries. Our results indicate that oxygen tends to segregate at the boundaries, and that the unzipping mechanism is also operative along the grain boundaries, despite the lack of the parallel bonds due to the presence of fivefold and sevenfold carbon rings along the boundary core.

[1] J. Cervenka et al., PRB 79, 195429 (2009).
[2] J. da Silva-Araújo and R. W. Nunes, PRB 81, 073408 (2010).
[3] J-L. Li *et al.*, PRL 96, 176101 (2006).

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

Simone Alexandre
UFMG-Brazil

Date submitted: 28 Dec 2010 Electronic form version 1.4