An-all atom investigation on morphological stability and transport properties of Reduced Graphene Oxide

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Reduced Graphene Oxide (RGO) is a material resulting from the (chemical or thermal) reduction of Graphene Oxide. There is general consensus that RGO can be described as a random distribution of oxidized areas bearing the oxygenated functional groups, separated by nonoxidized regions wherein most of the carbon atoms preserve sp^2 hybridization [1]. Despite numerous spectroscopic studies, poor information on the density and types of defects generated during the reduction process together with their spatial distribution is yet available.

Hence, a detailed study of the atomistic structure of RGO represents a crucial step toward understanding the properties of this material and its effect on thermal and electronic properties.

In this study, we use molecular dynamics simulations to mimic the process of high-temperature thermal reduction of an oxidized graphene sheet by simulating the structural evolution of defects and impurities. Starting from several sheets differing for oxidation level and impurity composition, we examine the concentration of carbon atoms sp-2 hybridized, and hence the integrity of the resulting material.

Moreover, the effect of the annealing temperature and of the spatial distibution of functionalizing agents (epoxy and hydroxyl groups) on the overall sample morphology is also investigated.

The corresponding thermal and electron conductivities are then calculated, highlighting the strong dependence of on the application performance on the fabrication parameters.

References

[1]   Gómez-Navarro, Meyer et al. *NanoLetters*, 2010, 10.
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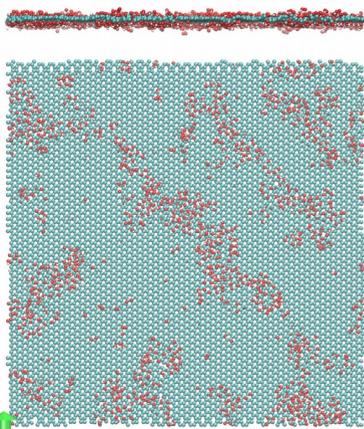
Figures

Figure 1: Side and top view of a GO sample before thermal reduction.

Figure 2: Evolution of the functionalizing groups on a GO sample during thermal annealing (T=1000K).