T716: Modeling and simulation of nanoscale materials, structures and devices

Simulations in graphene oxide: Benefits of molecular dynamics in nanotechnology

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The better understanding of nanomaterial properties will be a key factor to tailor and enhance properties of new materials. Graphene oxide in particular can be synthesized with different oxidation levels in order so gain similar properties to its deoxidized counterpart, graphene. Through the molecular dynamic simulations, the atomistic behavior of a tri-layer graphene membrane under mechanical indentation, highlighting the importance of molecular dynamics in the analysis.

This work will study a highly oxidized graphene oxide tri-layer that will be indented with a repulsive spherical indentator. The modeling of the membrane will generate single layer graphene oxide candidates to pick the lowest energy configuration and later stack this layer over itself. The simulations were performed using the software LAMMPS [1] along with the REAXFF [2] interatomic potential. Thanks to this approach, atomic positions of graphene oxide can be analyzed along the whole process.

These thin membranes have a known behavior when the indentation force is strong enough. In that regime the reaction force grows along the cube of the penetration magnitude [3]. For these simulations the behavior followed the membrane behavior with some differences which can be attributed to geometrical or intrinsic non-itineraries [4]. A deeper analysis in atomic configuration allow to recognize suggest an important role of epoxide groups in the mechanical deformation of the membrane. All these results, show the relevance of computational simulations to connect theoretical approaches and material characteristics.

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