Effects of nanostructures on macroscopic physical properties of graphene layers

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The macroscopic behavior of graphene products is already determined by atomistic effects on the nano-level, which generally escape experimental observation. In order to gain insight into the effects on this level it is necessary to rely on atomistic simulation and particle dynamics, while at the same time linking the observations on this scale to macroscopic measurable properties. Such properties include for example structural stability, as it relies on the strength of inter-atomic bonds - within and between the graphene sheets. Specifically the latter may be significantly influenced by additional nanostructures or composites.

In addition to the reproduction of known effects for already existing structures this approach allows the design of novel (nano-)structures and the prediction of their characteristics prior to synthesis, such as the measure of diffusion values in dependence of specific nanostructures, saving laboratory cost by pointing experimenters in appropriate directions.

At Fraunhofer SCAI these investigations are carried out using the inhouse-developed Molecular Dynamics software package Tremolo-X. Nanostructured graphene composites are modeled using reactive potentials, such as of Tersoff or Brenner type. Simulations may be carried out in a variety of physical ensembles depending on the suitability to the task.

The presentation will encompass current molecular dynamics research on graphene and their future applications.

References

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