MULTI SCALE MODELLING OF SELF-ASSEMBLY AND MECHANICS OF SINGLE WALL CARBON NANOTUBE AEROGELS

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ABSTRACT

Single wall carbon nanotubes (SWCNTs) show a variety of unparalleled properties such as high electrical and thermal conductivity, high specific surface area (SSA) and a low density. SWCNTs provide very high stiffness under axial loads or small bending deformations. One of the major challenges in tapping the vast potential of SWCNTs is to fabricate nanotube-based macrostructures that retain the unique properties of nanotubes. Pristine SWCNT aerogels are highly porous, isotropic structures with random filamentous networks of nanotubes cross-linked via van der Waals (VDW) interactions at junctions. The junction properties can be tailored via number of different ways such as covalent cross-linking, graphene coating and junction welding. These aerogels form electrically percolating networks at very low volume fractions of nanotubes, have high stiffness compared to other kinds of aerogels, and high specific surface area. They can be made super-elastic by coating nanotubes with graphene.

In order to realize the vast potential of SWCNT aerogels, a rigorous understanding of their mechanical behaviour is required. The mechanical behaviour of such aerogels is examined in several experimental studies. However, these studies generally measure the properties of the bulk. This is partly due to the absence of an in-situ characterization technique during mechanical testing that can offer insight into the deformation process unfolding at nano-scale. Therefore, it is necessary to adjunct these experimental studies with insights from simulations in order to develop a fundamental understanding of deformation of SWCNT aerogels.

The mechanical behaviour of an individual nanotube and interactions between few nanotubes can be accurately modelled using molecular dynamics (MD) simulations. However, the atomistic modelling becomes computationally expensive for large group of nanotubes. In several studies, results from atomistic simulations are fed into continuum scale finite element based models. These models are comparatively faster. Although the mechanical behaviour of individual nanotubes can be accurately modelled using continuum scale beam theory, such models perform badly while capturing several phenomena such as VDW interactions in limit of large strains and entanglements between nanotubes observed in SWCNT aerogels.

This study focuses on developing a meso-scale modelling approach that captures the complex physics associated with the mechanical deformation of SWCNT aerogels while avoiding the large computational cost of traditional MD. In essence, this is a coarse graining approach in which bunch of atoms are grouped together in order to reduce the total number of degrees of freedom (DOFs) of the system. The self-assembly and mechanics of SWCNT aerogels are studied. It involves observing the evolution of network structure under strain and quantifying the governing deformation mechanism.