DYNAMICS OF CNT AEROGEL FORMATION: A HYBRID LANGAVIN AND MOLECULAR DYNAMICS APPROACH

Boies, A[1], Chao, M, Kateris, N, Hoecker, C[1], Bhalerao, A[1], Kloza, P[2] and Elliot, J[2]

Presenting author's e-mail: a.boies@eng.cam.ac.uk

[1]*Department of Engineering, University of Cambridge, Cambridge, United Kingdom*
[2]*Department of Material Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom*

ABSTRACT TEXT

Aerogel formation within carbon nanotube (CNT) reactors enables continuous production of a self-assembled material with hierarchical structure which is of significant academic and industrial interest. Despite the discovery of the phenomenon over a decade ago, there remains no detailed description of the criteria for aerogel onset or dynamics of formation. The aggregation of spherical particles in dense particle systems is well studied. While it has been shown that for certain conditions an aerosol of spherical particles can form a macro structure, *i.e.* gel, little is known about the agglomeration of 1-D CNT materials. To investigate the dynamics of aerogel formation both the rate of collision and CNT reorientation must be determined to find the critical aerogel criterion in which CNT collisions that lead to bundling cease and long-range structure begin to form.

In this presentation we report on the dynamics of 1-D materials undergoing Brownian motion, collisions and re-orientation. By employing both molecular dynamic and Langevin dynamic modelling, we demonstrate that under typical conditions the time-scale for collision is much longer than the time-scale for re-orientation of individual CNTs. The results of simultaneous modelling of both long-range CNT collisions and short-range bundling dynamics enables the timescale of each process to be investigated in detail. These findings are applied to the continuous gas phase process for the bulk production of CNTs, to identify the critical length and number concentration of CNTs required for gelation.

Our results show that CNT bundle formation occurs at time scales typical of CNT aerogel reactors for CNT lengths and mass densities found experimentally. Ongoing work suggests that as the number of CNTs per bundle grows, the bundle stiffness increases, thus decreasing the rate of reorientation. As the rate of reorientation slows, the likelihood of a successive collision prior to reorientation increases. These findings underpin efforts to determine the mechanisms for aerogel formation within any 1-D system and are broadly applicable to comparable systems of nanorods, nanotubes or fiberous systems.