Multiscale modelling of thermal transport in polymer nanocomposites

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Background

Industrial components (e.g. in electronics), which can 'sense' released excessive heat, capture it and 'guide' it to relevant storage, or powering devices require development of advanced engineering materials. Combination of light-weight polymeric materials with nanoparticles of extreme thermal conductivities (e.g. carbon nanotubes or graphene) offers promising means for achieving light-weight materials with superior effective thermal conductivities. However, this requires an optimisation of the interfacial thermal conductance, which is governed by the nanoparticle surface functionalisation, polymer crystallinity in the vicinity of the nanoparticle, nanoparticle loading, nanoparticle dispersion and orientation. The ultimate aim of this work is to develop a general multiscale molecular-continuum computational approach to predict the most optimum combination of the aforementioned parameters that enhance thermal transport properties in polymer nanocomposites. This particular MSc project will focus on developing the approach that predicts thermal transport across the nanoparticle-polymer interface, and it enables identification of near-nanoparticle thermal conductance arising from the nanoparticle surface modification. The approach will combine sequentially coarse-grained (C-G) molecular and Finite Element (FE) (continuum) approaches, where the C-G model will be used to determine the values of continuum law parameters (e.g. describing near-nanoparticle thermal conductance - see Fig. 1), which will then be applied in the FE model to predict the overall (effective) thermal conductivity of the nanocomposite.

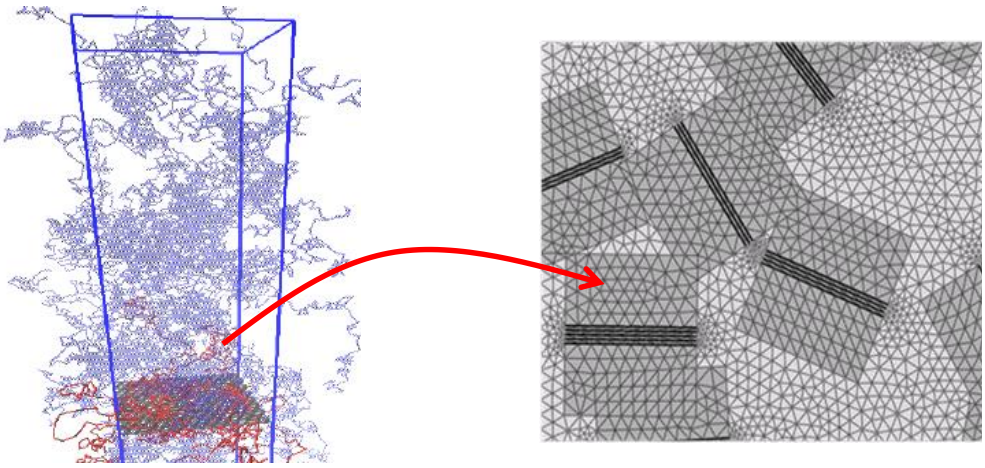

Figure 1. Molecular and continuum (2D) models of polymer-graphene nanocomposites

Programme of work

This project will involve the following work activities:

- Development of coarse-grained (C-G) molecular models of the nanocomposites accounting for different degrees of surface modification of graphene embedded in an amorphous polymer and simulating these in existing codes

- Prediction of thermal transport across the interface, and identification of continuum parameters describing near-nanoparticle thermal conductivity
- Comparison of simulations with available experimental data

Possible extensions into a PhD project would include extending the model to crystallising polymers, using non-equilibrium simulation data to parameterise analytically solvable models of heat and impurity transport, and rare event simulations methods. The overall project would suit a student interested in multiscale numerical methods, software development, molecular modelling, non-equilibrium statistical mechanics, machine learning and materials science.