In recent years, polymer nano-composites (PNCs) have increasingly gained more attention due to their improved mechanical, barrier, thermal, optical, electrical and biodegradable properties in comparison with the conventional micro-composites or pristine polymers. With a modest addition of nanoparticles (usually less than 5wt. %), PNCs offer a wide range of improvements in moduli, strength, heat resistance, biodegradability, as well as decrease in gas permeability and flammability. Although PNCs offer enormous opportunities to design novel material systems, development of an effective numerical modeling approach to predict their properties based on their complex multi-phase and multiscale structure is still at an early stage. In this research, I have focused on establishing a computational framework to predict the mechanical properties of PNC. I have developed a microstructure inspired material model based on a statistical technique to reconstruct the microstructure of polymer nanocomposite. The model was able to successfully predict the material behavior obtained experimentally.

This 3D microstructure model was later incorporated in a damage modeling problem in nanocomposite where damage initiation and damage progression have been modeled using cohesive-zone and modified Gurson-Tvergaard-Needleman (GTN) material models. There is a significant difference between the properties of inclusion and the host polymer in polymer nanocomposite, which leads to the damage evolution during deformation due to a huge stress concentration between nanofiller and polymer. The finite element model of progressive debonding in nano-reinforced composite has been proposed based on the cohesive-zone model of the interface. In order to model cohesive-zone, a cohesive zone traction displacement relation is needed. This curve may be obtained either through a fiber pullout experiment or by simulating the test using molecular dynamics. In the case of nano-fillers, conducting fiber pullout test is very difficult and result is often not reproducible. Using our newly developed framework based on molecular dynamics simulation, fiber-matrix pullout test has been conducted in order to obtain traction-displacement curve for cohesive zone model. This damage model was implemented in our 3D model to predict the material response more accurately.