# Micromechanical Modeling of Semi-Crystalline Polymer Nanocomposites

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**Abstract**

This study provides an insight into the mechanical properties of semi-crystalline nanocomposites. Semi-crystalline polymers are the most used thermoplastic polymers and their mechanical properties have been of interest to researchers. These polymers consist of two phases, the randomly oriented chains called amorphous and the other one with ordered parallel chains called crystalline phase. The amorphous phase is isotropic while the crystalline phase has directional properties. In semi-crystalline polymers the stiffness of the crystalline phase in the direction of chains is several times higher than that in the transverse direction. The formation of the crystalline phase, crystallization, starts from seeding points in the polymer melt and propagates radially from these points. This phenomenon generates voronoi cells. The properties in each voronoi cell are radially directional but the properties of polymer in macro scale, containing a number of voronoi calls, is isotropic. For a pure Semi-crystalline polymer, these seeding points are located at random. However, in polymer nanocomposite the nanoparticles themselves act as seeding points therefore there is a higher chance for formation of voronoi cells in nanocomposites. Therefore, voronoi cells in nanocomposites are smaller than those in pure polymer. In addition, the average size of cells decrease by increasing the number of nanoparticles, i.e. seeding points in the polymer melts (Fig. 1). The smaller size of

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the voronoi cells changes the deformation mechanism of the material. To study the effect of adding nanoparticles to the polymer matrix, nanoparticles are randomly distributed in a representative volume element (RVE) and the voronoi structure has been generated based on the location of nanoparticles using an available code in MATLAB. Importing the voronoi structures generated into a finite element package (ABAQUS), associated with a local coordinate system defined for each cell, yields the geometry of RVE in FEM model. The directional properties of the polymer are set based on the local coordinate system in each cell and compressive and tensile loading is applied to the RVE. To extrapolate the simulation results to the behavior in macro scale, periodic boundary conditions are considered for the RVE through the model generation. The stress strain behavior of the RVE is extracted and compared with the experimental results.

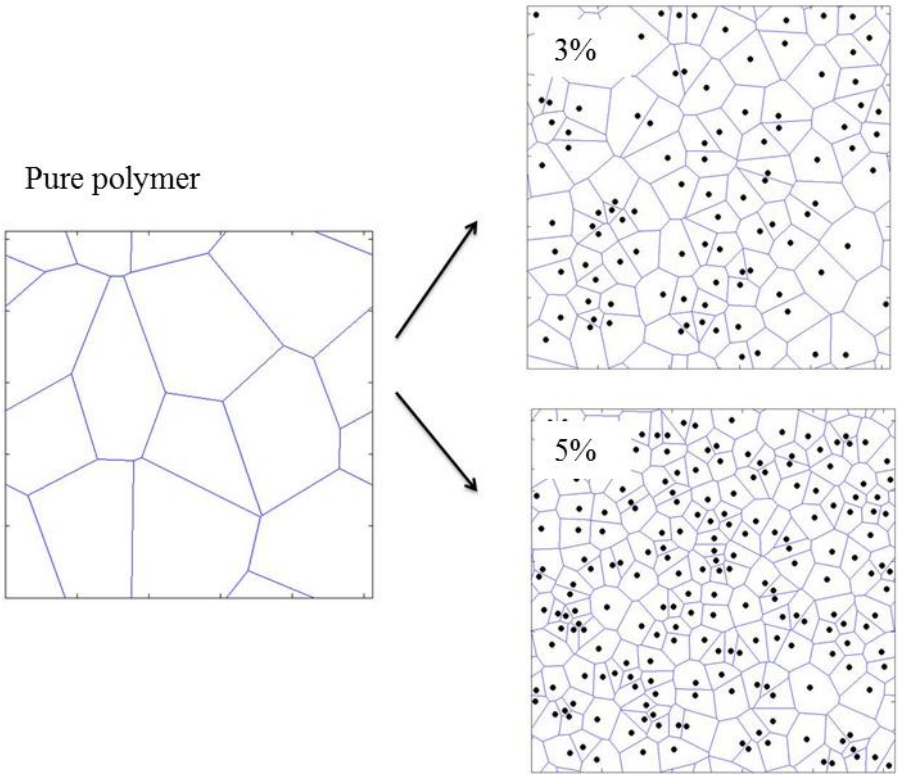


**Figure 1. Schematic illustration of change in voronoi size after adding nanoparticles to Semicrystalline polymer (RVE models generated using MATLAB)**