Graphene reinforced nanocomposites: 3D simulation of damage and fracture - DTU Orbit (30/12/2018)

Graphene reinforced nanocomposites: 3D simulation of damage and fracture

3D computational model of graphene reinforced polymer composites is developed and applied to the analysis of damage and fracture mechanisms in the composites. The graphene/polymer interface properties are determined using the inverse modeling approach. The effect of composite structure, in particular, of the aspect ratio, shape, clustering, orientation and volume fraction of graphene platelets on the mechanical behavior and damage mechanisms of nanocomposites are studied in computational experiments. It was shown that the Young modulus of the nanocomposites increases with increasing aspect ratio, volume content, elastic properties of graphene/polymer interface layer, and decreasing the degree of intercalation. The tensile strength follows similar tendencies, except for the aspect ratio and clustering degree, where the opposite effects are observed. Nanocomposites with randomly oriented sheets of graphene demonstrate much lower Young modulus and strength as compared with the composites with the aligned graphene sheet reinforcement. It was further concluded that the structural imperfections of graphene reinforcement (like crumpling shape or random misalignment) have considerable effect on the composite performances.

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