Hybrid Multiscale simulation of Carbon Nanotube Reinforced Composites

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Description

A hybrid computational multiscale strategy is introduced, based on a combination of sequential and semi-concurrent (FE2) approaches and was used to investigate the behavior of a benchmark cantilever beam-type structure consisting of a polymer reinforced with CNTs. Specifically, the combined influence of the Interfacial Shear Strength (ISS) and CNT weight fraction on the overall structural behavior is assessed. Due to the well-known difficulties in establishing experimentally a rigorous quantification of the interfacial constitutive law, a sensitivity analysis was considered with respect to various values of a so-called ISS parameter, in order to simulate different bonding conditions between the CNTs and the polymer and evaluate their relative influence on the overall structural behavior. The analysis is performed on the following three levels: a) the atomic one, where a lattice of carbon atoms representing a CNT was analyzed as an equivalent continuum, b) the microscopic one, where a representative volume element (RVE) of the carbon-nanotube reinforced polymer was analyzed using Finite Elements and, finally, c) the macroscopic one, where cantilever beam consisting of the polymer was analyzed using again finite elements. For the transition from the atomic to the microscopic level a sequential (hierarchical) multiscale technique was implemented. On the other hand, in order to minimize the loss of information when transitioning from the microscopic to the macroscopic level, the semi-concurrent FE2 multiscale technique was preferred. For the CNT model at the atomic level the modified molecular structural mechanics approach (mMSM) was used, according to which, the bond between a carbon atom and each one of its three nearest atoms is represented by a beam element with rectangular cross-section. For the purposes of the analysis at the subsequent level, the behavior of the resulting space frame CNT model was projected to an equivalent beam finite element (EBE). At the microscopic level, a structure consisting of an EBE, representing a single CNT inside the polymer matrix was analyzed using the embedded finite element method coupled to a bond slip mathematical description of the interface between the CNT and the matrix. The microscopic level is linked to the macroscopic one using a first-order homogenization scheme pertaining to displacement type boundary conditions in conjunction with a nested FE2 multiscale solution. The numerical experiments conducted showcase the applicability of the proposed multiscale strategy, while useful conclusions have been extracted from a detailed sensitivity analysis with respect to various scenarios of the ISS parameter.