

Pull-out behavior of CNT with cap from CNT-reinforced nanocomposites

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Abstract

Systematic atomic simulations based on molecular mechanics are carried out to investigate the pull-out behavior of carbon nanotubes (CNTs) in CNT-reinforced nanocomposites. In contrast with open-ended CNT, capped CNT is incorporated into the current computational model to explore the effect of the CNT cap for the first time. Two common cases are discussed: the pull-out of a whole CNT from a polymer matrix in a CNT/Polymer nanocomposite, and the pull-out of the broken outer walls against the intact inner walls of a CNT (i.e., sword-in-sheath mode) in a CNT/Alumina nanocomposite. By analyzing the obtained relationship between energy increment and pull-out displacement, a set of simple empirical formulae is proposed to predict the corresponding pull-out force from the nanotube diameter. The obtained pull-out force agrees well with experimental measurement. Moreover, the much higher pull-out force in the case of capped CNT than that of open-ended CNT implies a great contribution of the CNT cap to the interfacial properties of CNT-reinforced nanocomposite. This finding provides valuable insight into designing nanocomposites with desirable mechanical properties.

Keywords: Carbon nanotube, Nanocomposites, Mechanical properties, Pull-out behavior