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Interfacial Property in Nanocomposites due to van der Waals Interactions and Pull-out Force Predictions

***N. Hu[1], Y. Li[2] and H.M. Ning[1]**

[1]Department of Mechanical Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba, Japan.
[2]Department of Nanomechanics, Tohoku University, 6-6-01, Aramaki-Aza-Aoba, Aoba-ku, Sendai 980-8579, Japan.

*Corresponding author: huning@faculty.chiba-u.jp

Systematic atomic simulations based on molecular mechanics are carried out to investigate the pull-out behavior of a capped carbon nanotubes (CNTs) in CNT-reinforced nanocomposite. 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 (Al_2O_3) 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 desirably mechanical properties.

Keywords: Molecular mechanics, Interfacial property, Nanocomposites, Pull-out force prediction.