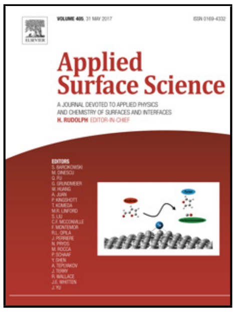

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Investigation of the interfacial properties of polyurethane/carbon nanotube hybrid composites: A molecular dynamics study

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Abstract

Considering the varied applications of hybrid polymer/carbon nanotube composites and the constant progress in the synthesis methods of such materials, we report a theoretical study of interfacial layer formation between pristine single-wall carbon nanotubes (SWCNTs) and polyurethane (PU) using molecular dynamic simulations. We vary the SWCNT diameter and the number of PU chains to examine various PU–SWCNT interaction patterns. Our simulations indicate the important role of intra-chain forces in PU. No regular polymeric structures could be identified on the carbon nanotube surface during the simulations. We find that increasing the SWCNT diameter results in stronger polymer binding. However, higher surface loadings of PU lead to stronger interpenetration by the polymeric segments; this effect is more apparent for SWCNTs with small diameters. Our core finding is that the attached PU binds most strongly to the carbon nanotubes with the largest diameters. Polymer dynamics reveal the loose distribution of PU chains in these systems.

Key words:
4,4’-methylene diphenyl diisocyanate, MDI, carbon nanotubes, poly(tetramethylene ether) glycol, PTMEG, polytetrahydrofuran, molecular dynamics simulations, noncovalent functionalisation, LAMMPS, AIREBO

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1. Introduction

Hybrid synthesis methods are increasingly focusing on pushing the limits of the properties of advanced materials. Natural and synthetic polymers reinforced with carbon nanotubes (CNTs) play an important role in these efforts. [1, 2, 3] Because of their extraordinary physical and chemical properties, carbon nanotubes [4, 5] have also been used as a reinforcing agent. CNTs have a combination of high strength, large surface area and high aspect ratio, making them ideal candidates for reinforcing many hybrid composites. However, a high-quality molecular dispersion of CNTs in polymer matrices or solutions is essential to obtain polymer nanocomposites with desirable properties, and can be realised using several techniques. [6, 7, 8] One such widely used technique is noncovalent functionalisation promoted by the interaction of polymers with the sidewalls of CNTs. [6, 8]

Various experimental procedures for wrapping CNTs with polymers, as well as applications of such systems, have recently been reported by Fujigaya and Nakashima. [1] When commercially available poly(vinyl alcohol) is combined with well-dispersed single-wall carbon nanotubes (SWCNTs), the tensile strength and modulus are significantly improved compare to those of the polymer alone. [9] SWCNTs have been successfully solubilized in water by wrapping them with a polyvinyl pyrrolidone (PVP) and polystyrene sulfonate (PSS). [10] Various composites containing various percentages of MWCNTs and polymers such as polybutadiene, polyisoprene, polystyrene, poly(methyl methacrylate) (PMMA), and poly(ethylene oxide) have also been found to dissolve homogeneously in organic solvents. [11] Conjugated polymers were used to selectively separate semiconducting SWCNTs from metallic ones, and the ability to sort CNTs by chirality and diameter holds promise for future applications of SWCNTs in electronic devices. [12]

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