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Molecular Dynamics Simulation Of Carbon Nanotube Pull-Out From Polyethylene Matrix

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Abstract

The objective of this study is to examine the influence of carbon nanotube (CNT) pull-out from polyethylene (PE) matrix on the mechanical properties of CNT/PE composite. Materials Studio 8.0 has been used for carrying out the molecular dynamics (MD) simulation. The mechanical properties predicted are the Young's modulus and the interfacial shear stress (ISS). The effect of increase in strain on the Young's modulus of CNT has also been studied. A (5,5) armchair single walled carbon nanotube (SWCNT) of diameter 6.78 Å and length of 49.2 Å has been used. When the SWCNT was pulled out from the PE matrix by 10 Å, there was 14.30% reduction in the longitudinal modulus (E33). When the displacement was increased to 50 Å, E33 was reduced by 43.79% with respect to a fully embedded CNT. ISS was mainly distributed over the first and final 10 Å of pull-out, in the stage I and stage III where the energy increments see a large change.

Keywords: Single-walled carbon nanotubes; Molecular Dynamics; Interfacial shear stress; Mechanical properties.

1. Introduction

Single walled carbon nanotubes (SWCNTs) have exceptional mechanical properties. The Young's modulus of SWCNT varies from 600-1000 GPa whereas the tensile strength is about 200 GPa [1]. Thus, these are the preferred reinforcements for various polymer based

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