SM13L_10244

XXI International Congress of Theoretical and Applied Mechanics
Warsaw, Poland, August 15–21, 2004

Interfacial Properties of Nanowire-Polymer Composites

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Nanocomposites with elongated structural fillers have recently attracted many investigations. A focus is exclusively on nanocomposites with carbon nanotubes due to carbon nanotubes unique physical properties, including mechanical, thermal, optical and electrical. However, after nearly a decade of research, their potential as reinforcement for polymers has not been fully realized; the mechanical properties of derived composites have fallen short of expectations. Nanowires, having a diameter comparable to carbon nanotubes, aspect ratio close or above 1000 and a few hundred times more surface area per volume than a classical fiber reinforcement, may be considered as a new family of a reinforcing phase for nanocomposites. The mechanical performance of composite materials is critically controlled by the interfacial characteristics of the reinforcing phase and the matrix material. Her we report a study on the interfacial properties of a silicon nanowire-reinforced polystyrene nanocomposite system through molecular mechanics simulations. Results of a nanowire pullout simulation suggest that the interfacial shear transfer stress of this novel system is significantly higher than for many traditional fiber reinforced composite systems. The adhesion energy and the interfacial shear stress has been determined indicating significant bonding quality. Further improvement of the shear stress transfer could be achieved with functionalization of silicon nanowires with coupling agents.

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