J Material Sci Eng 2012, 1:3
http://dx.doi.org/10.4172/2169-0022.S1.008

OMICS Group Conferences
Accelerating Scientific Discovery

International Conference and Expo on
Materials Science & Engineering

October 22-24, 2012 DoubleTree by Hilton Chicago-North Shore, USA

Molecular modeling of mechanical behavior of amine functionalized MWCNT-Epoxy composites

Kamal Sharma[1] and Mukul Shukla[1,2]
[1]Motilal Nehru National Institute of Technology Allahabad, India
[2]University of Johannesburg, South Africa

The exceptional physical and mechanical properties have made multi-walled carbon nanotubes (MWCNTs) an ideal reinforcement for a new generation of multi-functional, high performance engineering composites. Three-phase polymer composites containing carbon fiber, CNTs and metals alongwith the matrix are promising materials for use in military platforms for improved stealth response and reduced weight, corrosion and operational costs. In this paper molecular dynamics (MD) siulation of three-phase carbon fiber-MWCNT-epoxy composite is presented to parametrically describe the mechanical behavior. Amine functionalized MWCNTs (1.5 %) have been used as the main reinforcing element in the mid-plane of a uni-directional carbon fiber-epoxy laminate. The carbon fibers are coated with chemical surface functionalized MWCNTs to improve the dispersibility and interfacial adhesion. MD simulations have been carried out using Materials Studio, a commercially available software. The COMPASS force field is used to model the inter-atomic interactions. Within the MD model the carbon fiber volume fraction has been fixed at 60% and CNT volume fraction varied from 0.25-5%. Stress-strain curves of the three-phase composites containing different % CNT have been generated. The Young's modulus and tensile strength along the carbon fiber direction were found to vary from 92 GPa to 224.4 GPa and 1.35 to 2.85 GPa respectively for different MWCNT volume fractions. Poisson's ratio values ranging from 0.42 to 0.51 were also calculated. The values calculated above are in good agreement with the experimental results available in open literature.

Biography

Mukul Shukla holds a PhD in Mechanical Engineering from the Indian Institute of Technology, Kanpur, India. Currently, he is an Associate Professor in the Department of Mechanical Engineering Technology at the University of Johannesburg, South Africa. He is also an Associate Professor in the Department of Mechanical Engineering at Motilal Nehru National Institute of Technology (MNNIT), Allahabad, India. His research interests include polymer composites, nanocomposites, natural fiber composites, FEM, modeling and simulation. He has over 21 years of experience in research and teaching and has published over 75 papers in refereed journals and international conferences.

mukulshukla2k@gmail.com

Synthesis and characterization of N-(triethoxysilylmethyl) phthalimide, N-((2,8,9-trioxa-5-aza-1-sila-bicyclo[3.3.3.0]undecan-1-yloxy) methyl) phthalimide, N-((sila-2,10,11-trioxa-6-aza-3,4;8,9;12,13-tris (4,6-dimethylbenzo) [4.4.4.0] tricyclotetradecane) methyl)) phthalimide

Satinderpal Singh Mangat and Gurjaspreet Singh
Panjab University, Chandigarh, India

Most of the known organosilicon compounds contain a tetracoordinate silicon atom. However, the coordination number of silicon can increase to 5 or 6, especially when the silicon atom is surrounded by electronegative substituents. In the second half of the 20th century, the attention of scientists was attracted by intramolecular complexes of pentacoordinate silicon. Of particular interest among these are silatranes studied in detail by Academician M. G Voronkov and his co-workers1. Silatranes are a challenging target for scientists from the point of view of their structural features and applications[2-3], some of them have attracted extensive interest due to their medical use to heal wounds or stimulate hair-growth (pilotropic activity), biological properties, pharmacological properties e.g. antitumor, anticancer, antibacterial, anti-inflammatory, fungicidal activities, stimulating effect in animal production and seed germination effects. In recent years a number of authors have evinced interest in intramolecular heterocyclic inorganicesters of tripaodal ligands of the type $R\text{-}Si(OCH_2CH_2)_3N$ where R is a heterocyclic radical. The aim of present work is to synthesize the various novel silatranes bearing N-methylphthalimide functionality. The procedure for the synthesis starts with the N-(triethoxysilylmethyl)phthalimide(1) which is synthesized by the reaction of N-hydroxymethylphthalimide with chlorotriethoxysilane. In the presence of a base the resulting silane undergo transesterification reaction with triethanolamine and tris(2-hydroxy-3-tert-butyl-5-methyl benzyl)amine thus forming the corresponding silatranes, N-((2,8,9-trioxa-5-aza-1-sila-bicyclo[3.3.3]undecan-1-yloxy)methyl)phthalimide(2), N-((sila-2,10,11-trioxa-6-aza-3,4;8,9; 12,13-tris(4,6-dimethylbenzo) [4.4.4.0]tricyclotetradecane)methyl))phthalimide(3) respectively. These three are novel compounds which were characterized by elemental analysis, IR, multinuclear (^1H, ^{13}C and ^{29}Si) NMR and mass spectroscopy.

mangat.satinder@gmail.com