Experimental and Numerical Characterization of Interlaminar Properties of SWCNTs Doped PAN Nanomats Strengthened Multiscale-Hybrid Composites

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Abstract

Polymer composite reinforced with conventional macro size fibres have taken a major role in various modern engineering applications and their demand is ever increasing due to their light weight and design flexibility. Various improvements in manufacturing methods, fabrication techniques and composite constituents have been made over the years to produce better polymer composites. However, the major challenge of the conventional polymer composites is that failure at the matrix rich interlaminar region still remains and limits their performance resulting in unreliable usage of these composites. A number of research attempts had little success due to various limiting factors have been carried out to rectify this problem. One of the potential methods expected to improve the strength of the interlaminar region is the incorporation of nanosize fillers, such as electrospun Polyacrylonitrile (PAN) nanofibres mat as an interalia into the matrix rich interlaminar region of the conventional polymer composite. However, controlling the alignment and distribution of the PAN nanofibres during the chaotic electrospinning process is a major hurdle for improving the interlaminor regions. The random orientation of electrospun PAN nanofibres mat reduces their strengthening effect and also the required material properties.

Hence, the current study has focused on the design of electrospinning process for improving the orientation and distribution of the PAN nanofibre mats. The developed electrospinning process was used to produce random and aligned PAN nanofibres mat and also used for producing both pristine and functionalized single walled carbon nanotubes (SWCNTs) doped PAN nanofibres mat. These nanomats were then sandwiched with the glass fibre-epoxy matrix to produce nano strengthened multiscale hybrid composites.

As part of the electrospinning procedure, electric fields of general electrospinning technique were manipulated using two position adjustable auxiliary vertical electrodes (AVEs) to produce aligned nanofibres mat along with reduced diameter. So as to optimise the electrospinning parameters, the effect of AVEs on the PAN nanofibres mat orientation, distribution and diameter were experimentally matrixed and analysed. The fractographic study showed that auxiliary vertical electrodes (AVEs) added to the electrospinning process reduced the diameter, enhanced the alignment of the nanofibres and improved molecular orientation. Among four different volume fractions of 0.1%, 0.2%, 0.5% and 1% randomly oriented PAN nanofibre

mats, the volume fraction of 0.5% PAN polymer was selected to manufacture aligned PAN nanofibres mat strengthened hybrid composite based on the improved experimental randomly oriented PAN nanofibre mats strengthened hybrid composites.

A series of tests showed that glass fibre composites (GFC) reinforced with the volume fraction of 0.5% aligned nanofibre mats were better than those of 0.5% randomly distributed nanofibre mats. The aligned nanofibre mat with reduced diameter increased the tensile, flexural, and impact properties of glass fibre composite by 68.91%, 95.32% and 45.30% respectively.

Aligned nanofibres mat was further utilised to align and disperse the pristine and functionalized SWCNTs into the interlaminar region of fibreglass composite. Alignment and a nano-range diameter of nanofibres helped in improved distribution and alignment of pristine SWCNTs (p-SWCNTs), which was reflected in an increase in tensile, flexural and impact resistance by 89.30%, 105.48% and 107.17% respectively. A nondestructive functionalization method (Friedel craft alkylation) was used to improve the interface bonding of SWCNTs with the host PAN polymer nanofibre. PVA chains crafted to the surface of the SWCNTs without damaging the wall was confirmed using FTIR and Raman spectroscopy. The effect of functionalized SWCNTs (f-SWCNTs) doped aligned PAN nanofibre mats improved the properties of nano-hybrid multiscale composite up to 111.34%, 117.11% and 180.03% in tensile, flexural and impact resistance respectively.

A multiscale model was used to determine the properties of the multiscale nanohybrid composite strengthened with random and aligned PAN nanofibre mats, PAN doped with p-SWCNTs and f-SWCNTs aligned nanofibre mats. Three length scales, such as nano, micro and macro scales were modelled. At first, a numerical model was developed to determine the elastic properties of different carbon nanotubes (CNTs) i.e. Pristine and defective single wall (SWCNTs), double wall (DWCNTs), and multiwall (MWCNTs) for zigzag and armchair configurations. CNTs atomic geometry was replicated with an equivalent space frame structure (SFS). Co-ordinates definition of SFS of CNTs was developed in MATLAB code and transferred to the finite element analysis (FEA) software 'ANSYS'. The basic entity of SFS, C-C chemical bond was designed as a circular beam of orthotropic properties. The properties were determined by linking the energy equation of molecular mechanics to structural mechanics along with the parametric study. The van der Waals forces between inter-shell of DWCNTs and MWCNTs were modelled as linear elastic springs in a simplified way. The simplified model avoided the problems due to the nonlinear behaviour of van der Waals forces and improved the performance of the FEA software by computational resources. The effect of chirality, vacancy defects, different diameters and numbers of walls on elastic properties of CNTs were calculated, tabulated and compared with each other. The result of the proposed SFS model with orthotropic properties was compared with others result. The SFS model is found better than the equivalent shell model as the defects can be placed at the exact location and a more realistic behaviour could be predicted. The SFS models could be developed with any type of defects, a number of walls, van der Waals and agglomerated forms with variable geometries.

Using the space frame structures (SFS) of SWCNTs, the nanoscale RVE of PAN nanofibre doped with SWCNTs was modelled. Simulated results of nanoscale RVEs were used to determine the equivalent properties of p-SWCNTs and f-SWCNTs doped nanofibres, which were further used in microscale RVE models. Four micro scale RVEs were developed to represent the random and aligned PAN nanofibres mats, PAN nanofibres mat doped with p-SWCNTs and f-SWCNTs aligned PAN nanofibres mat in epoxy matrix. Analysed micro scale RVEs provided equivalent properties of interlaminar regions developed with random and aligned PAN nanofibres mat, PAN doped with p-SWCNTs and f-SWCNTs aligned nanofibres mat. At the macro scale, MNHCs were developed with equivalent interlaminar regions and analysed. The results of the simulated MNHCs were compared with experimentally obtained results.

The results of the experimental study suggested that aligned nanofibres with reduced diameter improved the properties of interlaminar region noticeably than the random nanofibres mat of the same volume fraction. Aligned nanofibres successfully placed the pristine and functionalized SWCNTs within the multiscale hybrid composites which significantly improved the properties of the multiscale hybrid composite. Results of the multiscale modelling were in line with the experimental results, which could be useful in extending the small-scale theoretical results to the real-life applications.