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Effect of Functionalization on Glass Transition Temperature of Carbon Fiber Reinforced Epoxy Nanocomposites using Md Simulation

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Abstract

As we all know that the mechanical characterization of any material plays a vital role in performance of the material throughout its life cycle. One of the major parameters in calculating the mechanical properties of carbon fiber reinforced nanocomposite is glass temperature. Understanding glass transition behaviour of polymer nanocomposites are crucial for optimizing their mechanical properties and performance. We used "Molecular dynamics simulations" to calculate sequel functionalization effect on glass transition behaviour of carbon fiber-reinforced epoxy (LY556) nanocomposites. In this investigation three distinct form of graphene that is pristine graphene, Graphene modified with amine and graphene modified with carboxyl is studied. In this simulation the glass transition temperature (Tg) of pure carbon fiber and epoxy is lower than that of graphene carbon fiber and epoxy composites (GCFEC). The Tg of pristine graphene is higher that of the functionalized graphene and the Tg of graphene functionalized with amine is much higher than that of graphene functionalized with carboxyl group. The results of this simulation are very much close to the experimental results hence this approach can be used to anticipate the glass temperature of epoxy composites. So, from this study it can be concluded that glass transition temperature of carbon fiber reinforced nanocomposites can gives better results on functionalization of graphene.

Keywords: Nanocomposites, simulation, graphene, functionalization, carbon fiber, epoxy

INTRODUCTION

In the study of material science and engineering, the development of advanced composite materials along with advanced properties has gained significant attention [1]. Among these, carbon fiber reinforced polymer (CFRP) composites came out as high-performance materials because of their good mechanical characteristics, lightweight nature, and versatility in various applications such as aerospace, automotive, and sporting goods [2, 3].

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In recent years, the incorporation of functionalized graphene into CFRP composites has emerged as a promising strategy to further enhance their mechanical, thermal, and electrical properties [4]. Functionalized graphene, with its interesting two-layered structure and excellent mechanical toughness, offers the potential to significantly improve the overall performance of CFRP composites [5, 6].

One crucial property which governs the performance of polymer-based composites is the Tg, which addresses temperature on which the polymer changes from a polished, unbending state

to a rubbery, more adaptable state [7]. Understanding and predicting Tg of functionalized GCFEC is essential for optimizing their processing conditions and execution in different applications [8].

Molecular Dynamics simulation (MD Simulation) is a tool which is used by different researchers for studying the materials behaviour at the smaller level, providing insights into their structural, thermal, and mechanical characteristics [9]. In the context of functionalization of GCFEC, MD simulations offer a unique opportunity to investigate the interactions between graphene, carbon fibres, epoxy matrix, and their collective influence on the glass transition behaviour [10]. This study aims to utilize molecular dynamics simulation techniques to investigate the glass transition temperature of Pristine graphene, -NH2 functionalization of graphene and -COOH functionalized graphene reinforced with carbon fiber and epoxy resin and compared with neat carbon fiber and epoxy resin [11].

EXPERIMENTAL PROCEDURE

Epoxy Resin Modelling

Additionally, "LY556 epoxy resins" are corrosion-resistant, thermally stable, and highly adhesion-promoting having temperature range of -80°C to 200°C. For the sub-atomic model, LY556 resin and carbon fiber incorporated as a grid are thermosetting polymers that have above one epoxide bunch for each molecule [12]. Because of their outstanding bond properties, excellent warmth security, high versatile modulus, and consumption obstruction, 10 rehashing units were chosen for each chain. Epoxy pitches are broadly used in an assortment of designing province of a polymer framework to the development of PNC (polymer nanocomposites) because of those exceptional characteristics. The H2 particle in the - NH2 get-togethers of alleviating subject matter expert (di-ethylene toluene di-amine - DETDA) epoxide social affairs answers molecule to epoxy gum [13]. The ensuing reestablished gum molecule again answers with epoxy iotas on the site of NH2 and HN, another epoxide bundle answers one easing expert particle at the site of it. Finally, a link is made among the restoring specialist and epoxy pitch [14].

Simulation models

In current study, “LY556” is cross connected with a curing agent in polymer lattice with Hyosung 951. One layer sheet of graphene having 162 molecules of Carbon with it, used as the nano-filler in this composite as described in Diagram 1. Crosslinking can raise a polymer's Tg value because it restricts molecular motion and makes the polymer more rigid [4].

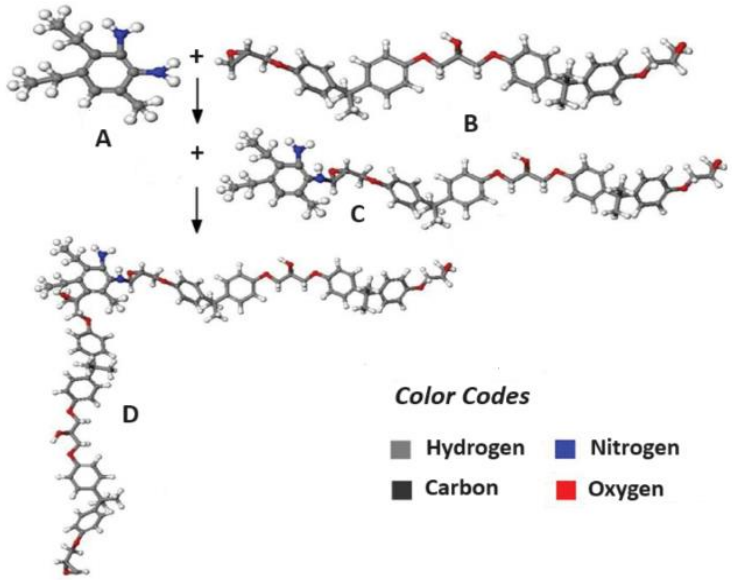

Diagram 1. Molecular modelling under minimum energy o1f (A) curing agent detda, (B) the epoxy resin ly556, (C) cured epoxy resin, (D) cross-linked epoxy resin

Engineered functionalization relies upon covalent linking of serviceable social affairs into carbon field of graphene. Many problems are there that can to be locked in upon to use graphene as strong contributing nano filler in PMC (Polymer Matrix composites). The dispersing of graphene is maybe of the most by and large pondered inconvenience [15]. Synthetic covalent connections among the functionalized graphene in the composites and the chains of polymer can bring about development of a portion of natural particles, for example, - NHN, - CHN, - Goodness, and - COOH [16]. The difficulty of graphene scattering and epoxy agglomeration framework might be solved by this. Consequently, the substance covalent bond part of viable social events to the graphene's external layer which is more meaningful in staying aware of the consistent associations among epoxy and functionalized graphene

Modelling of representative single cell systems

DGEBA cross-connected with DETDA fills in as the polymer grid in this examination. The nanofiller in the composites was a single-layer graphene sheet with 162 carbon atoms, as depicted in Diagram 2. To circumvent unsaturated boundary effects, hydrogen atoms were added to the ends of graphene sheets in order to end-graft them [17]. Chemical functionalization may be an option for achieving strong adhesive contact between graphene and the surrounding polymer chains in adding to good dispersion. The covalent bonding of functional groups to the graphene carbon scaffold is the foundation of chemical functionalization [18]. Before graphene can be used as a good reinforcement in polymer composites, many barriers must be overcome.

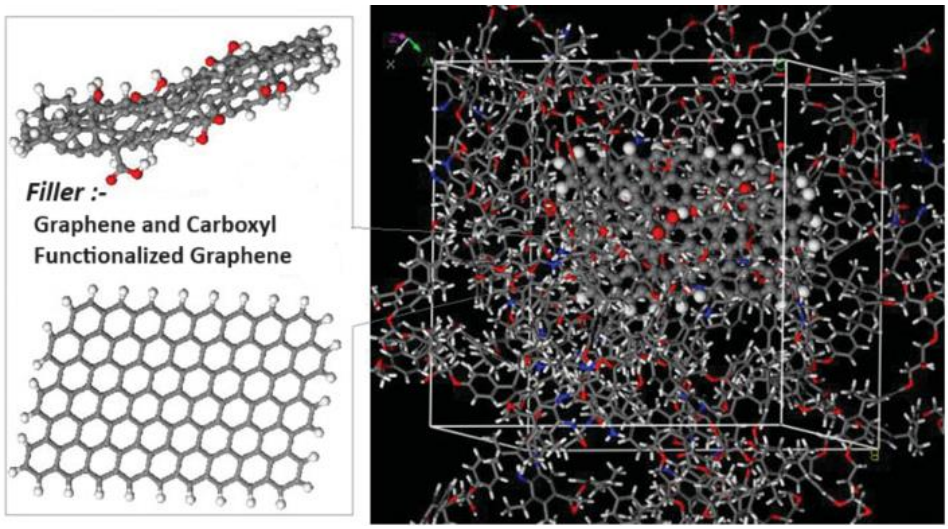

Diagram 2. Cross-linked LY556 epoxy resin forms the basis of the molecular model of a nanocomposite with graphene and adjusted graphene as filler.

Graphene dispersion is the most commonly discussed challenges. In composites, chemical covalent interactions between functionalized graphene and chains of polymer can reaction in the production of several organic compounds., including -NHn, -CHn, -OH, and -COOH. Various functional groups are examined, including the -NH2 group, having great reactivity which can be immediately integrated to the resin, as described by Shen et al. [19]. This may address the problem of graphene mixing with accumulation in surface of EPC (epoxy matrix), which is critical for establishing stable links among epoxy and functionalized graphene [20].

Force field and criteria for simulation

In this study, Material Studio 6.0's COMPASS force field. The confirmation of the valence parameters was based on the COMPASS force field, ab-initio parameterization approaches, condensed phase characteristics, and empirical evidence from isolated molecules [21]. Energy terms used in COMPASS are: (i) Reinforced terms, (ii) Cross-terms and (iii) non-reinforced terms, a Coulombic

capability for electro-static cooperations, and for Vander Walls connections 6-9 Lennard-Jones potential is used, which are discussed in Condition 1 [22].

$$E_{total} = E_b + E_\theta + E_\varphi + E_\chi + E_{b,\,b'} + E_{b,\,\theta} + E_{b,\,\varphi} + E_{\theta,\,\varphi} + E_{\theta,\,\theta'} + E_{\theta,\,\theta',\,\varphi} + E_q + E_{vdW} \quad (1)$$

Where,

E_b = "covalent bond-stretching energy"

$E\theta$ = "bond-angle bending energy"

E_φ = "torsion-angle rotation energy"

$E\chi$ = "out-of-plane energy"

E_q = "electrostatic energy"

E_{vdW} = "van der Walls energy and"

$E_{b,\,b'}, E_{b,\theta}, E_{b,\varphi}, E_{\theta,\varphi}, E_{\theta,\theta'}, E_{\theta,\theta',\varphi}$ = " The cross terms mirror the energy coming about because of bond stretch-bond stretch", "bond stretch-bond twist", "bond stretch-bond twist", "bond twist bond curve", and "bond twist bond twist bond twist communications".

The solidity of epoxy resin LY556 is set to 1.2 g/cc by adjusting the dimension of simulation cell. After using Material Studio's Discover tool to minimize energy and create a more relaxed configuration, we carried out a "anneal cycle" at 50-K intervals, ranging from 300 to 550 K, to eliminate any adverse interactions from the original structure [23].

For the system's equilibration, the conjugate gradient reduction procedure with a large convergence rootmean square force "1×10−3 Kcal/mol ^ A" was used. the simulation cell is immediately cooled after minimization [24]. At a temperature of 2073 K, a simulated annealing dynamics technique is employed. During the thermal annealing process, the system is heated in increments of 25 K from 300 to 2073 K. The duration and reproduction run were set to 1.00 and 17.80 ps, individually. The NVT ensemble was used in all MD simulations, pressure of 0.10 MPa was used [25].

OUTCOMES AND DISCUSSION

Glass Transition Temperature (T_g) of functionalized graphene carbon fiber epoxy composites

Freezing of chain segment motion is the primary cause of the glass transition.

For example, local chain movement. Therefore, two elements that directly impact a polymer when taken into account are (i) Free volume and (ii) Mobility of chained segments.

It has cooled and solidified into a glassy form. Our predicted outcome demonstrates that Tg can be increased by the epoxy matrix including functionalized graphene. The Tg values of the Carboxyl functionalized graphene and Amine functionalized graphene epoxy composites, as displayed in Diagram 3, are 457.2 K and 462.9 K, respectively, greater than the Tg values of the neat bulky pristine graphene carbon fiber epoxy resin by 40 K and 45 K. The findings of the simulation indicate that Tg can be raised by the matrix of epoxy augmented with functionalized graphene. The primary cause of Tg's significant increase is the modified groups strengthened the interaction between graphene and epoxy molecules.

In another research article by Ramanathan et al. done the comparative study about the effect of nanofillers on glass transition temperature (T_g) using expanded graphite, Single walled nanotubes and functionalized graphene sheets and concluded that there is a great increment of 30K in the T_g on functionalized graphene sheets and minimal change in single walled nanotubes both the comparative results are in good agreement, so from the above study we can say that MD simulation is the effective way to predict the glass transition temperature (T_g) of graphene based epoxy nanocomposites [26].

Radial distribution function

The radial distribution function, is derived from MD simulation by forcite examination in MS software. g(r) is the chance of getting a particle in a spherical shell at a span of r from an arbitrary atom

[27]. This value measures likelihood and is used to analyse how filler, cross-linking density, and additives affect the local structure of the epoxy nanocomposites system [28]. Equation 2 is used to determine the RDF.

$$g_{(a-b)}(r) = \frac{V\left(\sum_{i \neq j} \delta(r - |r_{Ai} - r_{Bj}|)\right) 4\pi r^2 dr}{N_A N_B - N_{AB}} \quad (2)$$

In this situation, I and J address ith and jth particles of gatherings An of N_A molecules and B of N_B particles, independently [29]. The number of atoms that belong to both groups is called N_{AB}. The RDF curve, which was calculated for each of the three simulated models, is shown in Diagram 4. The chemical bond span among hydrogen and different atoms is indicated by the first peak around 2.1 A and 2.32 A. The span among bound and unbound carbon atoms is the subject of the second peak, which occurs between 2.4 and 2.5 A.

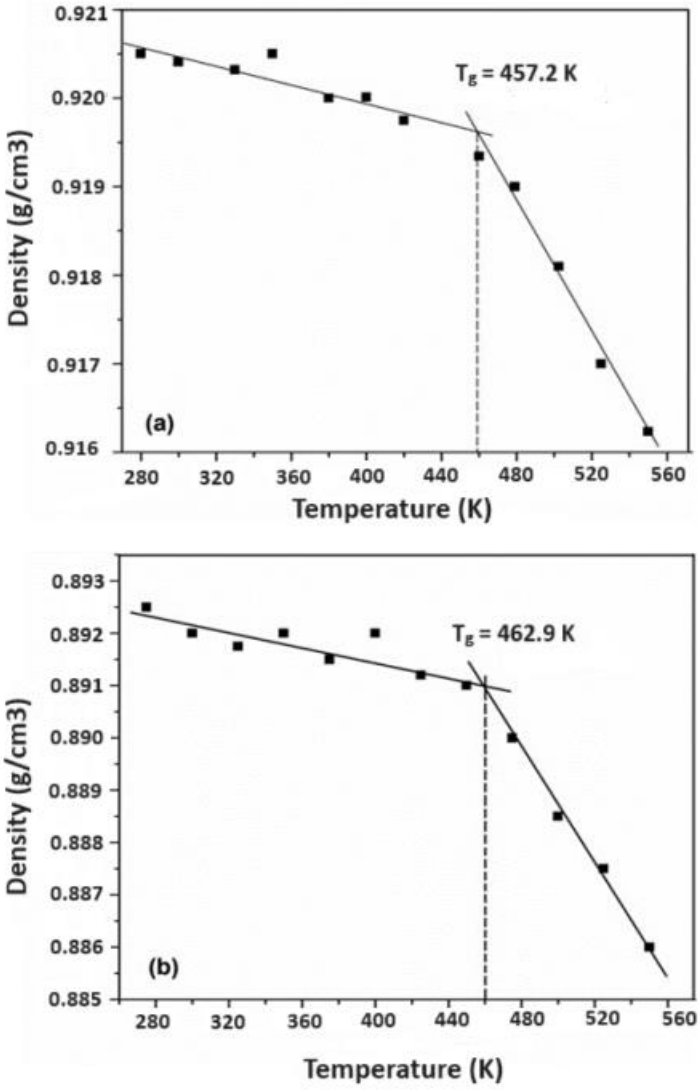

Diagram 3. Density vs temperature chart for functionalized graphene reinforced epoxy framework: (a) Carboxyl functionalized graphene (b) Amine Functionalized graphene.

The intra-molecular peaks are caused by the displacement among atoms, such as H2 and C in H−C−C series (r = 2.161˚A) and C atoms in C−C−C series (r = 2.430˚A) [30]. Increasing graphene content reduces the number of direct chemical bonds among H2 and other atoms [31]. Although, the behaviour of RDFs varies with different ties [32].

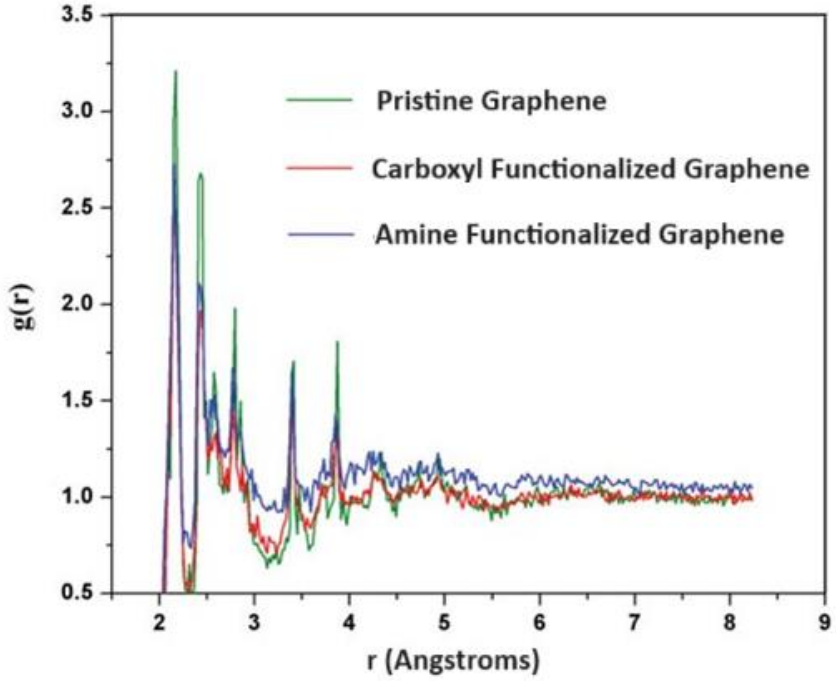

Diagram 4. Total RDF at room Temperature for three various epoxy composites.

CONCLUSIONS

In this study the effect glass transition Temperature (Tg) on the performance of polymer-based composites is calculated using MD Simulation, which addresses temperature on which the polymer changes from a polished, unbending state to a rubbery, more adaptable state. Understanding and predicting Tg of functionalized GCFEC is essential for optimizing their processing conditions and execution in different applications.

Using MD modelling, this study looked at how functionalized graphene affected the cross-linked epoxy resin LY556. One with pure graphene and two with distinct functional groups "-NH2 graphene and -COOH graphene" were the three cross-linked epoxy systems analysed. When compared to plain bulk epoxy resin, simulation indicates the following outcomes-

1. The Glass Transition Temperature (T_g) Value neat pristine graphene carbon fiber epoxy composite is 416.3K which is approximately 40K and 45K less than that of the functionalized graphene carbon fiber epoxy.
2. The Glass Transition Temperature (T_g) Value is higher for -NH2 Functionalized graphene and it is approximately 462.9 K.
3. Similarly, for -COOH Modified graphene" the value of Glass Transition Temperature is 457.2K which is lower than that of -NH2 Functionalized Graphene. The effects of graphene on nearby design were examined utilizing RDFs.

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