Original Article

Reinforcement of Aramid fiber with bagasse epoxy bio-degradable composite: investigations on mechanical properties and surface morphology

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A B S T R A C T
In this paper, the dynamic mechanical and tailored morphological behaviour of Aramid fiber (AF) treated with bagasse/epoxy (BG/E) resin, a bio-degradable composite, was investigated. Bio-degradable composite with homogeneous microstructures were fabricated using hand lay-up technique with untreated bagasse/epoxy matrix and treated 5% Aramid fiber with bagasse/epoxy resin (BG/E). Three different types of composites with different BG to epoxy (40:60, 50:50, and 60:40) ratios were prepared. Dynamic mechanical properties like tensile, flexural and impact strength of untreated and treated composites have been investigated. The SEM monograph of the treated surface BG/E composite has shown the enhanced fiber–matrix interaction. Nanostructures were characterized using transmission electron microscopy (TEM), and energy dispersive X-ray spectroscopy (EDS). FTIR studies confirmed the hydrogen bonding between Aramid fiber and BG/E matrix. Treated fiber composites have enhanced dynamic mechanical properties compared to those of untreated fiber-based composites. DFT studies revealed that hydrogen bonds are accountable for keeping multiple fiber strands.

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1. Introduction

The studies on the composite materials constitute a significant proportion of the engineered materials that promote various applications ranging from everyday products [1–3]. Biocomposite materials are very attractive due to the fact that a small amount of composite structure can lead to great improvement in many properties, such as mechanical and thermal [4–7]. Composite materials are the most attractive materials having properties that are not found in nature, consisting of two or more chemically different constituents forming polymeric matrix and reinforcement. The reinforcement ordinarily induces a stiffer and stronger composite with relative to the matrix, whereas the matrix holds the reinforcement in its set place [8,9]. Considerable growing awareness and issues with greener and surroundings within the society generated profound interest to use the natural fiber as reinforcements in polymer composites [10,11]. Polymeric composite materials have been used in many applications due

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to their excellent biocompatibility, satisfactory and mechanical properties [12, 13]. Doping of polymeric materials, products with low cost and light-weight may be achieved for a wide range of applications with desirable mechanical, thermal, and optical properties [14, 15].

Green composite syntheses have been intensively studied in a wide range of applications in the material science and biological science [16–20]. The green composites are developed by using partly bio-degradable composites which are barely outlined to support the properties of their constituents. An enormous change was reported on the usage of natural fibers, everywhere in the globe for the production of green composites [21–23]. Most of the studies have been focussed on reinforcing single artificial or fiber like carbon fiber, optical fiber, AF fiber, kenaf, jute, hemp, abaca, sisal, etc. with the addition of many materials to the polymer matrix.

In order to arrive polymer composites with new properties, many research works have been made on crossbreeding fibers into polymer matrix. Fibers are often hybridized between artificial fibers like glass/graphite fibers [24], AF/glass fibers [25–28], carbon/glass fibers [28–30], and natural fibers like banana/sisal fibers [31] or fruit bunch/jute fibers [32]. Studies have been additionally conducted on crossbreeding man-made fiber with fiber like short banana/glass fibers [33], basalt/carbon fibers [34] and coconut/glass/AF fibers. AF/glass fiber reinforced hybrid composites are frequently used as light-weight materials in marine applications, sporting equipment and military structures [35].

The present study deals with bagasse fiber as filling material, which is a residue fiber remaining when sugar cane is pushed to extract the sugar. This material is easily available and low cost. The bagasse fiber was incorporated at different ratios in discontinuous AF material system. AF is employed as reinforcement filler for epoxy based compound composites. The mechanical properties and surface morphology of bio-degradable AF/BG/E/composites have been investigated by various performance studies.

2. Experimental

2.1. Materials and methods

Epoxy resin LY 556 is used as polymer matrix owing to its high strength, mechanically adhering properties and good resistant to solvent and high temperature. Table 1 shows the technical specifications of this resin. In the present investigation, 8% by weight, hardener HY951 was used as curing agent [36]. The bagasse fiber was collected from Salem Co-operative sugar mill. It was dried in sunlight for a week and then cut into small size in ball mill and washed with water to remove the pulps. Aramid (AF) was synthesized by simple condensation reaction between para-phenylenediamine (PPDA) and terephthaloylchloride (TPC) in which the by product is HCl. These two compounds are dissolved in N-methyl-2-pyrorilide and the polymerization reaction was carried out in the presence of CaCl2 for safety reasons.

2.2. Fabrication of epoxy composites

The fabrication of composite specimens was done by incorporating AF in bagasse epoxy polymer resin by hand layup process. A light steel mould was used to fabricate composite panels by maintaining the required thickness panels. Wax was used between mould surface and composite specimen. The mould was tightened by bolts and allowed to cure for 24 h at room temperature (30 °C). Specimens of appropriate dimensions are cut for mechanical testing as per ASTM standards. Table 2 shows the fabric specifications.

2.3. Fourier transform-infrared spectroscopy (FTIR)

The Fourier transform infrared spectroscopy (FTIR) analysis was carried out using Perkin-Elemer 783 to examine the chemical structures of the AF obtained from treated composites, in the range of 4000–400 cm−1 by using KBr pellets.

2.4. Nuclear magnetic resonance spectroscopy (NMR)

1H and 13C NMR spectra were recorded to examine molecular identities and structures of Aramid fiber on a Bruker spectrometer shield at 300 MHz using CDCl3 as solvent and TMS as an internal standard.

2.5. X-ray diffraction (XRD)

Powdered X-ray diffraction (XRD) analysis was used to know the degree of crystallinity of Aramid sample by using Shimadzu XRD 6000 X-ray diffractometer having Ni-filtered CuKa radiation at angle range 2θ (angular incidence of 0–80°).

2.6. Scanning electron microscopy (SEM)

The morphological and microstructure characterization of the untreated and treated composites have been analysed using

<table>
<thead>
<tr>
<th>Table 1 – Technical specifications of resin.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Epoxy resin specifications</td>
</tr>
<tr>
<td>Density at 25 °C (g/cm²)</td>
</tr>
<tr>
<td>Boiling point (°C)</td>
</tr>
<tr>
<td>Specific gravity</td>
</tr>
<tr>
<td>Coefficient of thermal expansion (°C)</td>
</tr>
<tr>
<td>Properties of the resin-hardener system</td>
</tr>
<tr>
<td>Mix ratio</td>
</tr>
<tr>
<td>Full cure time at 30 °C</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2 – Fabric specifications.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fabric properties</td>
</tr>
<tr>
<td>40%, 50% and 60% by weight</td>
</tr>
<tr>
<td>5% by weight</td>
</tr>
<tr>
<td>Moulds of size</td>
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<table>
<thead>
<tr>
<th>Fiber properties</th>
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</thead>
<tbody>
<tr>
<td>Fiber type</td>
</tr>
<tr>
<td>Fiber diameter (mm)</td>
</tr>
<tr>
<td>Relative density</td>
</tr>
<tr>
<td>Tensile modulus (GPa)</td>
</tr>
<tr>
<td>Tensile strength (MPa)</td>
</tr>
</tbody>
</table>
scanning electronic microscopy (SEM) with JEOL JSM 6390 Scanning Electron Microscope.

2.7. Transmission electron microscopy (TEM)

Characterization of nanostructures of the treated composite was performed by transmission electron microscopy (TEM) (FEI Technai Basic at 100 kV).

2.8. Energy dispersive X-ray spectroscopy (EDS)

Chemical purity of treated composite was analysed by EDS with JEOL JSM 6390 energy dispersive X-ray spectroscopy.

2.9. Thermogravimetric analysis

Thermogravimetric analysis (TGA) study was carried out for AF/BG/E composites at a heating rate of 5 °C/min in nitrogen atmosphere using Thermogravimetric Analyzer (NETZSCH Germany & STA 449 F3 Jupiter, DIN 51006). Thermal decomposition of all specimens occurred in a programmed temperature range of 30–800 °C.

2.10. Tensile strength (ASTM D 638)

The specimens for tensile strength analysis were prepared in line with the ASTM D 638 standard. ASTM dimensions are presented in Table 3. The tensile strength analysis was carried out on the universal testing machine. The dimension of fabricated specimen was 165 mm × 19 mm × 3 mm.

2.11. Impact strength (ASTM D-256)

The impact strength was performed on AF strengthened composite samples to determine the impact strength. ASTM D-256 standard was adapted to prepare specimens. The dimension of specimen was 64 mm × 12.7 mm × 3 mm.

2.12. Flexural strength (ASTM D-790)

The specimen for the analysis of flexural strength was prepared in accordance with ASTM D-790 standard. The dimension of the tested samples was 127 mm × 12.70 mm × 3 mm.

| Table 3 – ASTM dimensions of the samples for tensile, flexural and impact strength. |
|---------------------------------|-----------------|-------------------|-------------------|
| Tensile strength | D638 | 165 mm × 19 mm × 3 mm | |
| Flexural strength | D790 | 127 mm × 12.7 mm × 3 mm | |
| Impact strength | D256 | 64 mm × 12.7 mm × 3 mm | |

Three point flexural strengths were performed on the specimens. In three point flexural strength method, the cross-head position was used to verify the deflection in specimens. The experiments were performed at 30 ± 1 °C with 40% humidity level.

2.13. Quantum chemical studies

Quantum chemical studies have been carried without any symmetry constraints by means of various basis sets using Gaussian code Becke3-Lee-Yang-parr (B3LYP) with 6-311+G(d,p). The studies have been performed after geometrical optimization. The resulting geometry was checked with respect to true minima of Molecular Electrostatic Potential that have been indicated in Fig. 1. The quantum chemical parameters are derived from Gaussian 09W program software using the optimized structure shown in Fig. 2.

| Table 4 – FTIR analyses of Aramid/treated AF composite. |
|---------------------------------|-----------------|-------------------|-------------------|
| Wave number (cm⁻¹) | Vibration mode |
| AF | Treated AF composite |
| 793 | 725 | Ring vibration |
| 1179 | 1178 | C-C-ring stretch (C-phenyl-C) |
| 1263 | 1235 | C-C-ring stretch (n-phenyl-n) |
| 1516 | 1506 | C=O-ring (C-phenyl-C) |
| 1649 | 1606 | 80% N-H bond10% C=O stretch |

3. Results and discussion

3.1. FTIR analyses of AF and AF/BG/E composite

Table 4 shows the important absorption bands observed in the FTIR spectrum of AF and treated (AF/BG/E) composites. The FTIR spectrum shown in Fig. 3(a) confirms the construction of amide linkage in the main chain of AF. The N–H bond stretching appears at 1649 cm⁻¹, whereas the peaks at 1516 cm⁻¹ and
1263 cm$^{-1}$ are due to $\equiv C$ stretching vibrations of aromatic rings. From the FTIR spectrum, Fig. 3(b) of AF treated with BG/E composite, it is clear that the stretching frequency of this peak was decreased to 1506 cm$^{-1}$ [37–39]. It was observed that stacking of AF in the BG/E composite brings an interaction between AF chain and the BG/E composite. The amide linkage is more stretchable compared to AF. It is due to more intensive hydrogen bonding between the AF chain and BG/E composite compared to free AF.

### 3.2. Nuclear magnetic resonance spectroscopy (NMR)

Fig. 4 shows $^1$H NMR spectrum of the AF, the peak appeared around at 8.78 ppm was associated with NH group, and the peak appeared around 7.73–7.89 ppm due to aromatic protons. The synthesized AF structure was additionally established by $^{13}$C proton magnetic resonance spectrum. From Fig. 5, it is clear that the peaks observed at 173.31, 137.98 and 133.56 ppm, respectively represent the carbon of $\equiv O$, $\equiv N$, and $\equiv C$. The aromatic ring carbon peak appeared around 120–130 ppm.

### 3.3. XRD of AF and AF/BG/E composite

The value of wide angle XRD confirms the structural regularity of AF. Fig. 6 shows that synthesized AF exhibited two sharp optical phenomenon peaks at $2\theta$ (°) = 20.07 and 23.01 that are sharp and slender. Such peaks indicate the high crystalline nature of AF. It is noted that the value of $2\theta$ (°) is closely associated with the layer like arrangement of polymer chains within the crystal [40]. The distance between adjacent layers, held together by Vander Waals forces and to some extent by $\pi$-electron overlap, was allotted by the value of $2\theta$ (°) = 23.01 [41], whereas the value of $2\theta$ (°) = 20.07 was associated with the gap between adjacent polymer chains on the crystallographic planes, that were distinguished by a prominent concentration of non-bonded, building block interactions [42]. XRD patterns of Aramid fiber and AF treated/BG/E composite are identical at the same location, as shown in Figs. 6 and 7. The $2\theta$ of 20.03°, 23.0°, and 34.5°, respectively, represents 101, 002, and 040 crystal planes, such peaks indicated the cellulose-crystalline behaviour [43]. The crystallinity indices of Aramid fiber and AF treated/BG/E composite are 30.0% and 56.3%, respectively. The XRD data suggested that the crystalline morphology of cellulose does not change during the treatment and the crystallinity of AF treated/BG/E composite is improved due to the removal of hemicellulose and lignin, which is inconsistent with the results obtained from the FTIR spectra.

### 3.4. Scanning electron microscopy (SEM) analysis

The state of dispersion of 5% AF treated BG/E resin matrix is primarily important to decide the dynamic mechanical properties of the composite which are compared with untreated composite. The fiber dispersion on the surface is assessed using SEM in the treated and untreated composites. The treated 5% AF composite containing various weight percent of BG/E and also untreated composite containing various weight percent of BG/E resin matrix were investigated using SEM analysis. Fig. 8(a and b) shows the SEM monographs of untreated composite which shows the surface having no uniform dispersion in the resin. The presence of several voids around the fiber indicated that there will be a poor adhesion between fibers and epoxy matrix. There is no pullout of fiber, rather fibers are broken uniformly. Fig. 8(c and d) shows that SEM
Fig. 4 – $^1$H NMR spectra of Aramid.

Fig. 5 – $^{13}$C NMR spectra of Aramid.
micrographs of treated 5% AF to BG/E fiber composite which indicates the surface with good dispersion. Hence the effect of DMA is remarkably high and that may be due to uniform dispersion of AF in BG/E composite. The fiber and matrix interaction can also be seen from SEM images. There is pull-out of fiber, rather fibers are broken uniformly. The treated composite surface showed closely packed interfacial bonding between fiber and matrix. The AF treated composite has adhesion between fibers and epoxy matrix indicating that there are no any voids around the fiber. Fig. 9 shows the SEM observation of synthesized Aramid fiber surface which has good uniform dispersion.

3.5. Transmission electron microscopy (TEM) analysis

TEM image of AF treated composite, after introducing the Aramid into the bagasse epoxy composite by pep stacking, is shown in Fig. 10. The TEM image clearly shows that Aramid is adsorbed and attached on the surface of BG/E composite. This also demonstrates that the composite surface of bagasse epoxy could interact with the aromatic area of Aramid through pep stacking interaction. In other words, the TEM image of AF/BG/E composite indicated the successful functionalization of the BG/E with the Aramid.

3.6. Energy dispersive X-ray spectroscopy (EDS)

EDS analysis of the Aramid and AFs treated composite is shown in Fig. 11(a and b). The percentage of nitrogen in the EDS analysis confirmed the presence of Aramid in the Aramid fiber and AF treated/BG/E composite sample. The rest components carbon and oxygen are common for both epoxy and bagasse composites.
Temperature–weight loss data was analysed to determine the thermal stability of the samples. The continuous records of temperature and weight loss were found out and analysed to determine the following TGA indices: thermal degradation rate (% weight loss/min), initial degradation temperature and residual weight. Fig. 12 shows the weight loss curves for pure, 40, 50 and 60 wt% of AF/BG/E composites, respectively. From Fig. 12 it can be seen that 40 wt% of AF/BG/E composites had much higher thermal stability than other wt% composites. There was no major variation in thermal stability between 50 and 60 wt% of AF/BG/E. All the samples showed thermal stability up to 60–70 °C. The experiential thermal stability is quite higher than other bagasse fiber reinforced biocomposites reported in literature [44]. It was noticed that all samples showed a moderate weight loss at 160 °C. The next weight loss of all the samples started roughly 220 °C, due to the initial decomposition of cellulose and hemicellulose and the heat of evaporation of moisture in the sample. The cruel weight loss from 220 to 470 °C for 40 wt% AF/BG/E is due to the major components of hemicelluloses, cellulose and lignin [45]. It was noticed in all the samples in 510 °C temperature region could be viewed as the complete decomposition of all flammable materials and the formation of char. It is also clear that the total weight losses from the decompositions were 82, 85 and 89% in 40, 50 and 60 wt% of AF/BG/E composites, respectively.

3.8. Tensile strength

Tensile strength of 5% AF treated composites and untreated composites were determined to check their capability to oppose breaking under tensile stress. The various ratio of bagasse reinforced in epoxy matrix (40%, 50%, and 60% by weight), respectively incorporation of AF fillers at 5% by weight loadings for the samples. The DMA of the BG/E untreated/AF treated composites is presented in Table 5. It was observed the tensile strength increases with the addition of AF filler in the BG/E composites as compared with the untreated BG/E composites by transmitting and distributing the applied stress.
The stiffness of the BG/E composites increases with the addition of AF filler by minimizing the free spaces, which also results in the improvement in tensile strength of the treated bio-degradable composites. The untreated BG/E composite is shown in Fig. 13. The treated composite surfaces are AF filler interaction between the reinforced fibers and matrix, this indicates better bonding between the matrix and fiber as the result to increase the tensile strength. The tensile strength of the many filled polymers is improved by compatibilizers, that enhance the adhesion between fiber and matrix interface. These results showed that (5 wt%) NaOH treated bagasse fibers have better interface with polymer matrix, permitting an increased stiffness, higher distribution of tension and thus, increased tensile testing results. As the result, it was observed that untreated 40% BG/E composites have tensile strength of 4.55 MPa. It shows that lower dynamic mechanical analysis compared to those of AF treated fiber-based composite (19.84 MPa). As prepared AF/BG/E composites have higher tensile strength than that of previous report of 5% glass fiber filled with 30% bagasse composites [46] and also bagasse fiber-reinforced cardanol composites [47].

### 3.9. Impact strength

The impact strength of composite shows its ability below plastic deformation. The hybrid composite impact strength has tendency to high energy impact without breaking or fracturing. The AF treated BG/E non-breakable epoxy composite or hybrid composites impact properties depend upon the properties of AF treatment which is used for cross, inter-laminar and surface adhesion between the fiber and the matrix. Fig. 14 presents the impact strength of untreated BG/E composites compared to AF treated BG/E composites. The lowest impact properties of the untreated BG/E composite but increased impact strength of AF treated BG/E composites may be due to the assimilation of AF filler. The enhanced impact properties for 5% AF treated with 40% by weight of BG/E composites is seen from the results. The higher surface interactions and bonding of the AF particles with the BG/E matrix makes them to resist the high impact stress/load. The rise within the impact strength was jointly accomplished by the addition of 5% of AF to the BG/E because of the uniform dispersion and high ratio of the AF. 40% BG/E (untreated) composite has impact strength of 0.337 J, whereas incorporation of 5% AF filler to 40% BG/E treated composites increase in the impact strength 0.7538 J. From the results of dynamic mechanical testing it is clear that the combination of AF filler and 40% by weight BG/E reinforcements in the polymer can be perfectly used to fabricate composites of high strength and light-weight with enhanced mechanical properties.

### 3.10. Flexural strength

It is evident from Fig. 15 that adding AF to BG/E matrix enhanced flexural strength when compared to the untreated BG/E composites. It was explained with the support of upper rigidity, higher interface space and stiffness of the additional AF packing, which directly governs the enhanced

---

**Table 5 – DMA of untreated BG/E/treated AF composites.**

<table>
<thead>
<tr>
<th>Untreated/treated composite</th>
<th>Tensile strength (MPa)</th>
<th>Flexural strength (MPa)</th>
<th>Impact strength (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Untreated 40% BG/E</td>
<td>4.55</td>
<td>810.62</td>
<td>0.337</td>
</tr>
<tr>
<td>Treated AF</td>
<td>19.84</td>
<td>8516.78</td>
<td>0.7538</td>
</tr>
<tr>
<td>Untreated 50% BG/E</td>
<td>3.96</td>
<td>695.78</td>
<td>0.252</td>
</tr>
<tr>
<td>Treated AF</td>
<td>14.13</td>
<td>7865.72</td>
<td>0.578</td>
</tr>
<tr>
<td>Untreated 60% BG/E</td>
<td>3.58</td>
<td>587.91</td>
<td>0.191</td>
</tr>
<tr>
<td>Treated AF</td>
<td>10.28</td>
<td>7361.85</td>
<td>0.420</td>
</tr>
</tbody>
</table>

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**Fig. 10 – TEM images of AF treated composite.**
flexural strength. The enhanced flexural strength is due to the stress that gets expeditiously transferred via the interface in addition to the outstanding enhancements. These were noted in 5% AF treated BG/E in comparison to untreated BG/E composites. This outstanding enhancement is attributed to the efficient dispersion of 5% AF within the 40% by weight BG/E matrix. It was observed that the untreated 40% BG/E composite has a flexural strength 810.68 MPa which is lower than that of AF treated fiber-based composite (8516.78 MPa). AF treated 40% BG/E fiber composite shows higher flexural strength than the composites already reported [46,47].

3.11. Frontier molecular orbitals (FMO)

A DFT study of compounds is of interest in order to gain a deeper insight on their action and thus helping in the design of new materials [48–56]. The chemical parameters of Aramid calculated using various basis sets using DFT are presented in Table 6. Frontier molecular orbitals (FMOs) exhibit a vital rule to calculate the electronic and optical properties as well as the possible chemical reactions through the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The molecular polarizability would be exposed through $E_{HOMO} - E_{LUMO}$ energy gap, chemical hardness, chemical softness, kinetic stability and the reactivity of molecules [55–58]. The lower energy gap between the FMO molecules could be attributed to higher reactivity, low kinetic stability and high inter-molecular actions, thus the molecule is called a soft molecule. The molecule possesses greater energy gap between the FMOs of molecule processes higher thermal and kinetic stabilities and thus the molecule is called hard molecule. Table 7 shows the $E_{HOMO} - E_{LUMO}$ energy gaps for Aramid. These were computed in different functional levels and indicate that the molecule is highly reactive. The lower value of energy gap has more inter-molecular forces, hydrogen bonds in AF. The HOMO–LUMO energy gap implies the kinetic energy is higher
and high chemical reactivity. Fig. 16 shows the orbital involved in the electronic transition of Aramid.

3.12. The global chemical reactivity descriptors (GCRD)

The GCRD obtained using DFT could be an important analytical tool to understand the relationship among the structure, stability and reactivity of molecules. GCRD parameters such as chemical hardness (\( \eta \)), softness (\( S \)), chemical potential (\( \mu \)), electronegativity (\( \chi \)) and electrophilicity (\( \omega \)) were calculated for Aramid by taking the \(-E_{\text{HOMO}}\) as ionization energy (I) and \(-E_{\text{LUMO}}\) as electron affinity (A). Koopman’s theorem might even be used to assume the ionization energy furthermore as electron affinity of chemical species. This theorem
Fig. 14 – Impact strength of untreated BG/E and treated AF composites.

Fig. 15 – Flexural strength of BG/E and treated AF composites.

Fig. 16 – Representation of the orbital involved in the electronic transition of Aramid.
describes that ionization energy and lepton affinity values of molecules represent to the negative of its $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$ values. Inconsistent with Koopman’s theorem [52], hardness and electronegativity of a molecule can be calculated by following formula:

\[
\chi = -\mu = \frac{I + A}{2}
\]

(1)

\[
\eta = \frac{I - A}{2}
\]

(2)

\[
\chi = \frac{E_{\text{HOMO}} + E_{\text{LUMO}}}{2}
\]

(3)

\[
\eta = \frac{E_{\text{HOMO}} - E_{\text{LUMO}}}{2}
\]

(4)

Softness ($\sigma$) that could be a magnitude of the polarizability of chemical species is outlined because the inverse of multiplicity chemical hardness ($\sigma = 1/\chi$). Electrophilicity ($\omega$) and nucleophilicity are the two important chemical reactivity indices. Parr [55] derived the subsequent formula to calculate the electrophilicity index related to electronegativity and hardness of molecules [53,54]. Further, the nucleophilicity ($\epsilon$) because the inverse of electrophilicity ($\omega = 1/\chi$):

\[
\omega = \frac{\chi^2}{2\eta}
\]

(5)

**Table 7** - Absolute hardness values of nucleophile drawn from Eigen values of HOMO and LUMO by DFT method.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\epsilon$ HOMO</th>
<th>$\epsilon$ LUMO</th>
<th>LUMO–HOMO</th>
<th>$\eta$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF/6-31(G)</td>
<td>−9.895</td>
<td>−3.026</td>
<td>−1.869</td>
<td>0.935</td>
</tr>
<tr>
<td>HF/6-311G(d,p)</td>
<td>−6.574</td>
<td>−3.292</td>
<td>−3.282</td>
<td>1.641</td>
</tr>
<tr>
<td>B3LYP/6-31(G)</td>
<td>−6.095</td>
<td>−2.581</td>
<td>−3.515</td>
<td>1.757</td>
</tr>
<tr>
<td>B3LYP/6-311G(d,p)</td>
<td>−6.563</td>
<td>−2.860</td>
<td>−3.703</td>
<td>1.852</td>
</tr>
</tbody>
</table>

Table 7 shows the hardness and softness values of molecules are 1.85 eV and 0.94 eV, respectively. The molecule with larger values of hardness is low toxicity and vice versa. The calculated GCRD parameters viz., chemical potential, electronegativity, and electrophilicity suggested AF has highly reactive strong molecule.

### 3.13. Water absorption

Water absorption examination was carried out to find out the absorptive of the composites. As per the ASTM D570 standard, water absorption test is done. Test specimens of 76 mm × 25 mm × 3 mm are prepared for the water absorption test. The specimens were weighed by digital weighing machine to get the weight of the specimens before immersed in distilled water and noted. Then they were immersed in the beaker containing distilled water to evaluate the water absorption up to attaining equilibrium condition by the samples. After attaining equilibrium (10 days), the specimens were weighed again to record the weight of water absorption. The percentage of water absorption was calculated using the expression:

\[
W(\%) = \frac{W_w - W_d}{W_d} \times 100\%
\]

where $W_w$ and $W_d$ were wet and dry weight of specimens, respectively.

**Fig. 17** shows the difference in % water absorption with different wt% filler content of the AF treated BG/E composites. For the composites, the water absorption increased with increasing wt% fiber reinforcement. In general natural fiber content possesses water absorption nature. Along with the natural fibers, bagasse fiber has more water absorption tendency relatively, and also this is due to the presence of hydroxyl group and hydrophilic characteristics of the bagasse fiber [59,60]. 40 wt% of AF/BG/E composite had less water absorption.

**Fig. 17** - Effect of AF/BG wt% on water absorption.
compared to other wt% of composites. It indicates better fiber matrix adhesion, thereby considerably increasing the strength of the composite, and improving its thermal stability [61]. Mechanical strength and thermogravimetric analyses (TGA) data supported these results.

4. Conclusions

The reinforcement of Aramid fiber (AF) with bagasse epoxy bio-degradable composite has been successfully fabricated and characterized. AF composites were successfully prepared with different volume fraction of (40%, 50% and 60%) bagasse/epoxy (BG/E). Incorporation of 5% AF filler into 40% treated composite showed enhanced dynamic mechanical properties like tensile strength (19.84 MPa), impact strength (0.7538 J) and flexural strength (8516.78). SEM analysis of the treated composite resulted in a closed packed interfacial bonding between fiber and matrix and also fiber end reflects the non-appearance of fiber pullout and ensures better interfacial adhesion. The TEM analysis of bagasse epoxy fibers was successfully modified by Aramid through non-covalent modification with π–π stacking interaction between the aromatic area of Aramid and the bagasse epoxy fiber surface of Aramid. After modification, the Aramid fiber can be well dispersed in the bagasse and epoxy matrices and exhibited a strong interaction between them with the help of Aramid. As a result, the mechanical properties of the treated composite show significant improvement. Thermogravimetric analysis of the three samples showed in, 40 wt% of AF/BG/E indicated with least weight losses. The 40 wt% of AF/BG/E composite had less water absorption compared to other wt% of composites. It indicates better fiber matrix adhesion, thereby considerably increasing the strength of the composite and improving its thermal stability. Mechanical strength and thermogravimetric analyses (TGA) data supported these results.

This suggests that sample 40 wt% of AF/BG/E was a better optimized level of fiber incorporation. The FTIR tests proved that there is an interaction between AF chain and 40% of BG/E composite. It comes from AF π–π stacking interaction. These properties are ascribed to the better reinforcing effects of rigid AF filler and the formation of interfacial interaction by hydrogen bonds between AF and the BG/E matrix. It was observed 5% AF loaded with 40% by weight of BG/E composites has considerably higher and better dynamic mechanical properties. The DFT study has lower value of energy gap and it has more inter-molecular forces.

Conflicts of interest

The authors declare no conflicts of interest.

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