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A molecular dynamics simulation study to investigate the effect of C60 on thermo-mechanical and elastic properties of DGEBA/DETA nanocomposites

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Abstract

Molecular dynamics simulations were performed to investigate the effect of fullerenes (C60) on the thermal and mechanical properties of a cross-linked epoxy system composed of epoxy resin DGEBA and curing agent DETA. Hence, a comparative investigation was performed on the thermal and mechanical properties of DGEBA/DETA reinforced with 2.3 wt% C60 and neat epoxy systems. Properties such as glass transition temperature (GTT), coefficients of thermal expansion (CTE), and elastic properties at different cross-linking densities. Simulation results indicated that the GTT of the epoxy increased by about 25 K due to the presence of C60. The effect of C60 on the CTE was very less, and at higher crosslinking densities, an increase in CTE before the glass transition was observed. It was also observed that the effect of C60 on mechanical properties is dependent on the crosslinking density. The young's modulus of the epoxy/C60 system at a high strain rate showed a drastic decrease as compared to the neat epoxy system at higher crosslinking densities. The highest value of young's modulus of the epoxy/C60 system was observed at 65% crosslinking density.

Table S1. DFT optimized geometrical parameters of DGEBA.

Bond	Length (Å)	Bond	Length (Å)
R(C1-C2)	1.392	R(C22-H24)	1.095
R(C1-C6)	1.398	R(C22-H25)	1.095
R(C1-H7)	1.086	R(C26-H27)	1.095
R(C2-C3)	1.403	R(C26-H28)	1.095
R(C2-H8)	1.085	R(C26-H29)	1.096
R(C3-C4)	1.401	R(C30-C31)	1.408
R(C3-C21)	1.543	R(C30-C32)	1.396
R(C4-C5)	1.395	R(C31-C33)	1.387
R(C4-H9)	1.087	R(C31-H34)	1.087
R(C5-C6)	1.400	R(C32-C35)	1.401
R(C5-H10)	1.084	R(C32-H36)	1.085
R(C6-O11)	1.370	R(C33-C37)	1.403
R(O11-C12)	1.422	R(C33-H38)	1.086
R(C12-H13)	1.099	R(C35-C37)	1.395
R(C12-H14)	1.100	R(C35-H39)	1.084
R(C12-C15)	1.509	R(C37-O40)	1.369
R(C15-H16)	1.091	R(O40-C41)	1.421
R(C15-O17)	1.431	R(C41-H42)	1.100
R(C15-C18)	1.468	R(C41-H43)	1.099
R(O17-C18)	1.436	R(C41-C44)	1.509
R(C18-H19)	1.090	R(C44-H45)	1.091
R(C18-H20)	1.090	R(C44-O46)	1.431
R(C21-C22)	1.548	R(C44-C47)	1.468
R(C21-C26)	1.548	R(O46-C47)	1.436
R(C21-C30)	1.542	R(C47-H48)	1.090
R(C22-H23)	1.096	R(C47-H49)	1.090

Table S2. DFT optimized geometrical parameters of DETA.

Bond	Length (Å)	Bond	Length (Å)
R(C1-2)	1.097	R(N10-C12)	1.462
R(C1-H3)	1.096	R(C12-H13)	1.097
R(C1-N4)	1.466	R(C12-H14)	1.098
R(C1-C7)	1.540	R(C12-C15)	1.538
R(N4-H5)	1.020	R(C15-H16)	1.105
R(N4-H6)	1.020	R(C15-H17)	1.099
R(C7-H8)	1.098	R(C15-N18)	1.467
R(C7-H9)	1.107	R(N18-H19)	1.020
R(C7-N10)	1.465	R(N18-H20)	1.019
R(N10-H11)	1.017		

Table S3. Parameters for atomic interactions of C60.

Pairwise interactions	
E	Σ
0.104996656	3.851

Bond interactions		
D	A	r_o
114.3833	2.1867	1.418

Angle interactions	
K_θ	θ_o
134.2791631	120

Dihedral interactions		
K_φ	D	n
5.999809	-1	2

Table S4. Equilibrium bond length and Force constant assigned to created bonds at given steps.

Step	Equilibrium bond length assigned	Force constant assigned
1	$r_e + \left(\frac{R_{crslnk} - r_e}{5}\right)4$	$\frac{K_b}{5}$
2	$r_e + \left(\frac{R_{crslnk} - r_e}{5}\right)3$	$\frac{K_b}{4}$
3	$r_e + \left(\frac{R_{crslnk} - r_e}{5}\right)2$	$\frac{K_b}{3}$
4	$r_e + \left(\frac{R_{crslnk} - r_e}{5}\right)$	$\frac{K_b}{2}$
5	r_e	K_b

Text S1. Atom list generation.

The fix bond/create command available in the Monte-Carlo package also allows setting the atom type of the bonding atoms to a different atom type when its requirement of "max-bonds" is reached. So, the atom type of the epoxy carbon atoms which got bonded to hardener nitrogen atoms was changed to a different type. Then the atom IDs of all the atoms with this new type were listed for the C−O bond-breaking step and charge update. The list of O atoms bonded to the reacted C atoms was obtained from the list of reacted C atoms, which was required for the C−O bond-breaking step, O−H bond-forming step, and the charge update step. The list of other epoxy atoms, whose charge changes due to the C−N bond formation, was also obtained from the list of reacted C atoms. Similarly, the list of secondary amine N atoms reacted once and twice and that of primary amine N atoms was generated by assigning new atom types during the C−N bonding step. These lists of N atoms were used for breaking N−H bonds, charge update, and generating a list of H atoms to be de-bonded from N atoms. This list of H atoms was used in the N−H bond-breaking step, O−H bond-forming step, and charge update.