Supporting Information

for

Enhancing Mechanical Properties of Epoxy with Graphene Quantum Dots: A Molecular Dynamics Study

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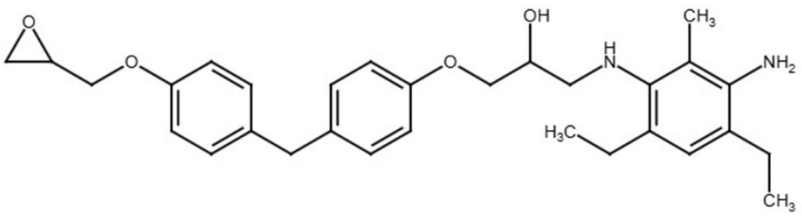
S1: Crosslinking of Epoxy

a)



b)

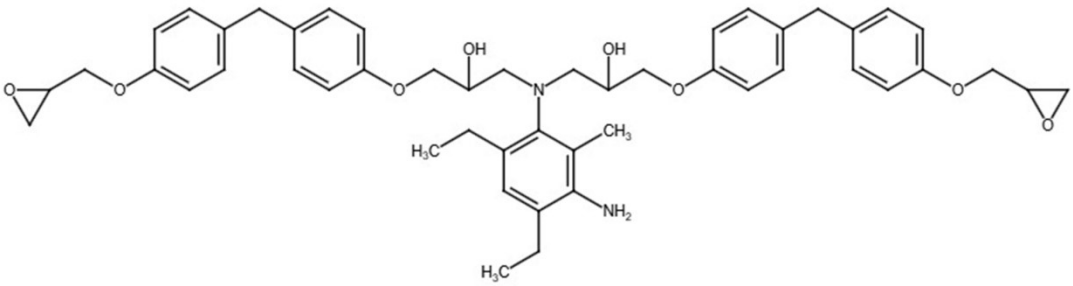


Figure S1: Crosslinking mechanism of bisphenol-A epoxy a) step-1 illustrating epoxide-primary amine reaction product b) step-2 epoxide-secondary amine reaction product.

Crosslinking of epoxy was simulated using the REACTER[1, 2] algorithm in LAMMPS[3]. Using the fix bond/react command in LAMMPS the reaction input files such as pre-rection template, post-reaction template and reaction map file were assigned to simulate the new bond formation. The epoxy undergoes two-step crosslinking reaction as shown in Figure S1. In the 1st step, the epoxide rings of the DGEBF monomer reacts with the nitrogen from the primary amine functional group of the DETDA monomer. As a result, the hydroxyl group and a secondary amine group is formed as shown in Figure S1(a). In the

second step, the newly formed secondary amine group reacts with the epoxide group of the another DGEBF molecule to form the tertiary amine and another hydroxyl group as shown in Figure S1(b). This reaction continues to form the crosslinks withing the epoxy until all the epoxide molecules are reacted within the cut-off radius.

S2: Analysis of Stress-Strain Plots

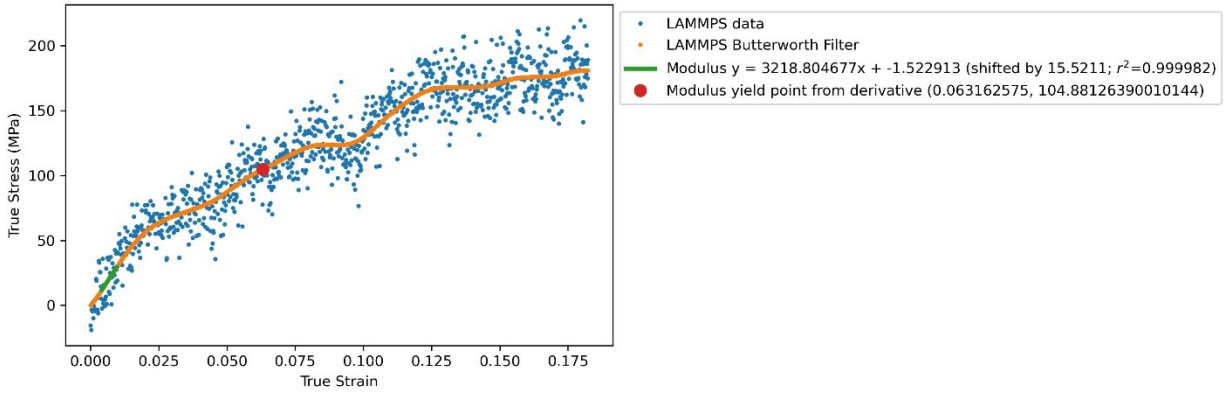


Figure S2: Plot of true stress against true strain for a representative e6N-GQD-Epoxy nanocomposite model in x-direction tensile test.

True stress values in x-direction are plotted against the true strain values for a e6N-GQD-Epoxy model using LUNAR[4] as shown in Figure S2. The stress values were computed during the unidirectional tensile test simulation in x-direction. The raw LAMMPS data was filtered using Butterworth filter option in LAMMPS. Further, the Young's modulus and yield strength were determined using RFR method developed by Kemppainen[5] et.al. RFR method identifies the linear region in the stress-strain plots for Young's modulus prediction by fringe slope method, and further evaluates yield strength by analyzing the second derivative of the fringe slope[5].

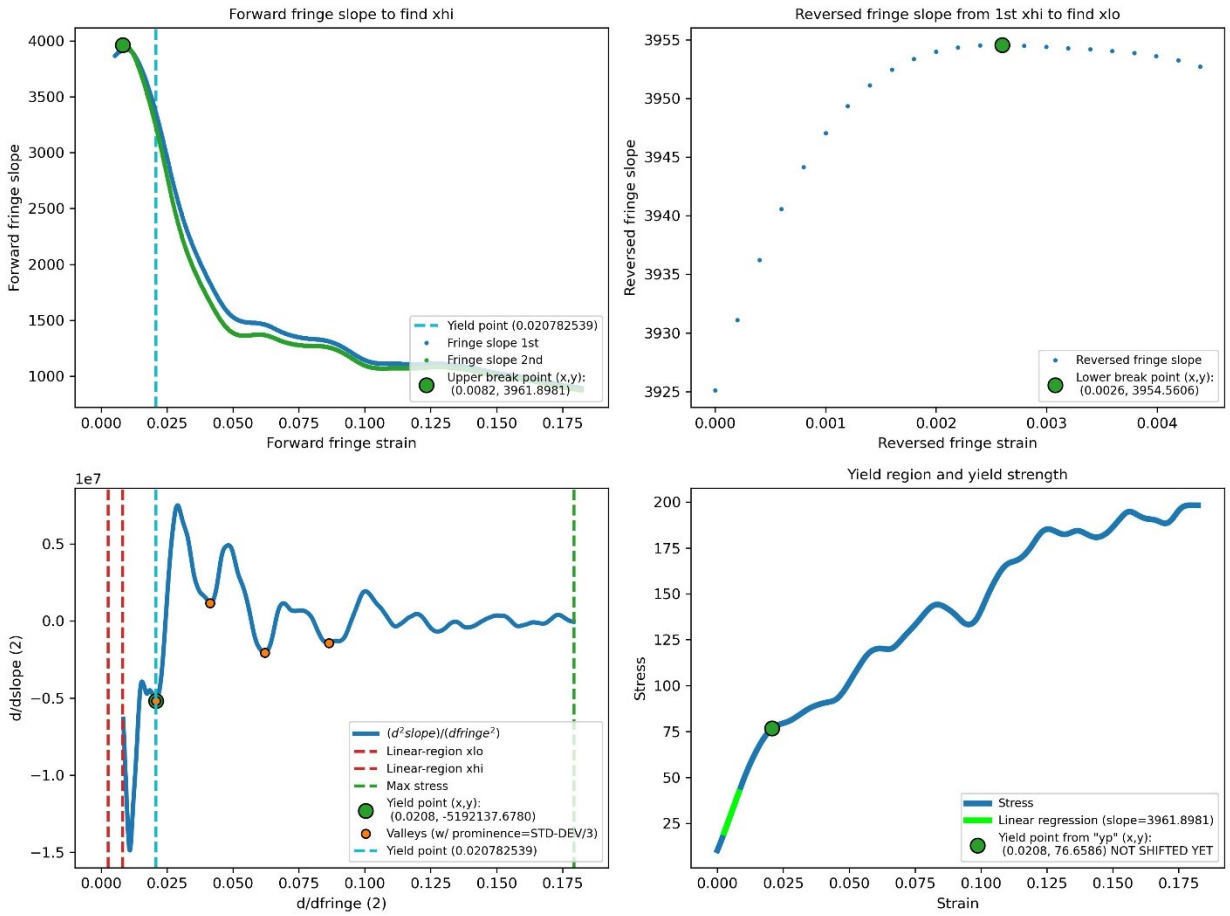


Figure S3: RFR method analysis to determine yield point

Figure S3 shows the chart of forward and reverse fringe slope of the stress-strain data in the top charts. The peaks of these curves are used to identify the start and the end point of the identified linear region. Further, the chart of second derivative of the fringe slope is shown and the first minima is identified as a yield point in the stress-strain curve. Identified yield point is shown as a green circle in the stress-strain plot.

S3: Determination of Poisson's Ratio

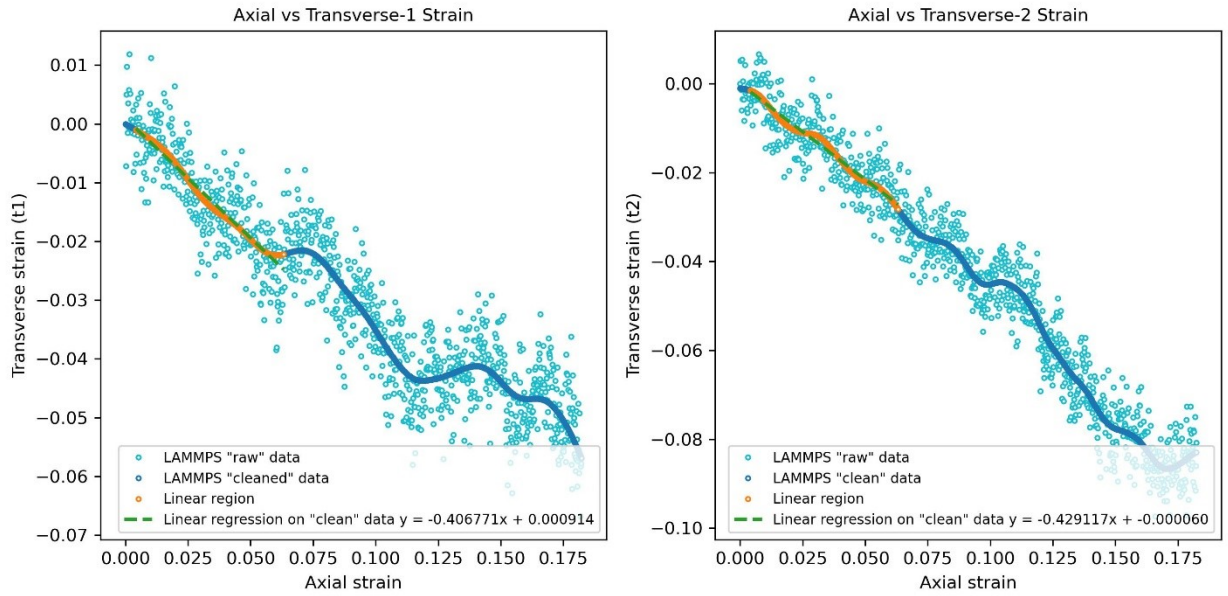


Figure S4: Plot of transverse strain vs axial strain for a representative e6N-GQD-Epoxy nanocomposite model in x-direction tensile test.

Figure S3 illustrates the transverse strains as a function of axial strains in y and z-directions respectively for e6N-GQD-Epoxy nanocomposite model. The linear elastic region and non-linear elastic regions from stress-strain plots were utilized to determine the Poisson's ratio. The linear fit was performed in the identified region as shown in Figure S3. The average negative slope of the two directions was reported as a final Poisson's ratio for this test case, that is 0.4185 ± 0.01.

S4: Density Distribution Analysis

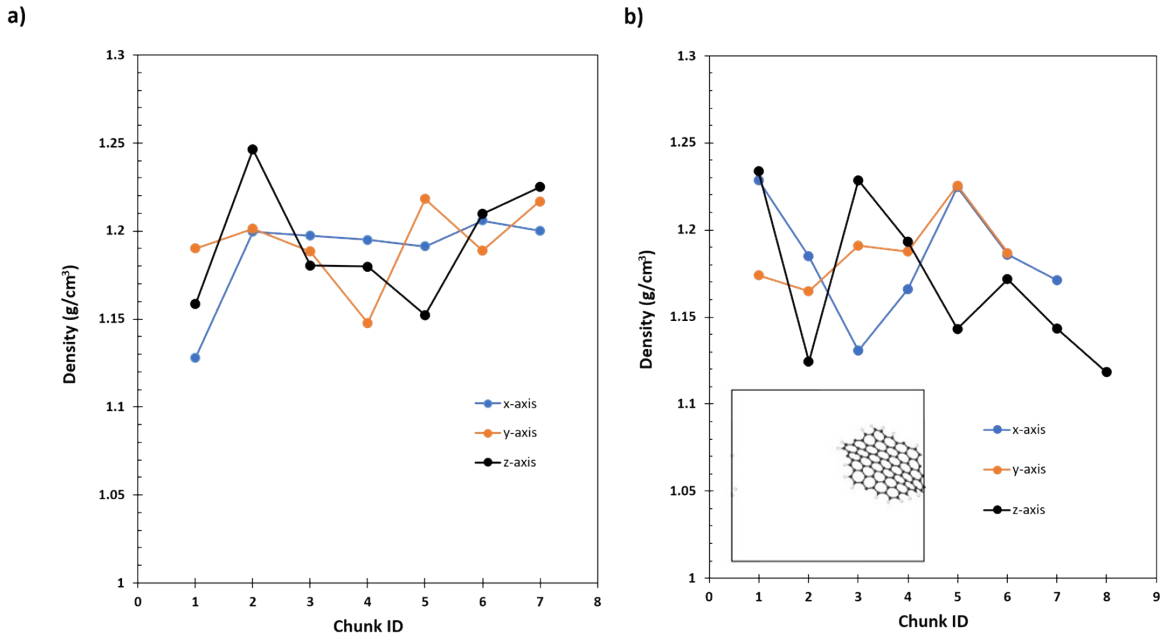


Figure S5: Plot of density distributions along *x*-, *y*- and, *z*-directions of a representative MD model for (a) neat epoxy, and (b) e6N-GQD-epoxy nanocomposite.

Figure S4 shows the comparison of density distributions of a representative neat epoxy and e6N-GQD-epoxy models. Figure S4(a) shows the density distribution along x-, y- and, z-directions of neat epoxy MD model is uniform. However, Figure S4(b) illustrates that the density distribution in e6N-GQD-epoxy nanocomposite model is not uniform compared to the neat epoxy model in any direction. These variations in the density distributions of the e6N-GQD epoxy are observed due to the planar GQD molecule and functionalized covalent bonds between epoxy with GQD, causing rearrangement of the epoxy network. The snapshot of MD model in the Figure S4(b) shows the placement of GQD in *xy* plane in the representative e6N-GQD-epoxy nanocomposite.

References:

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2. Gissinger, J. R.; Jensen, B. D.; Wise, K. E., Molecular modeling of reactive systems with REACTER. *Computer Physics Communications* **2024,** *304*, 109287.

3. Thompson, A. P.; Aktulga, H. M.; Berger, R.; Bolintineanu, D. S.; Brown, W. M.; Crozier, P. S.; in 't Veld, P. J.; Kohlmeyer, A.; Moore, S. G.; Nguyen, T. D.; Shan, R.; Stevens, M. J.; Tranchida, J.; Trott, C.; Plimpton, S. J., LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications* **2022,** *271*, 108171.

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5. Kemppainen, J.; Odegard, G.; Muzzy, T.; Wavrunek, T., Understanding and Interpreting Stress-Strain Curves from Molecular Dynamics Simulation of Amorphous Polymers. In *ChemRxiv*, 2025.