Supplementary Material

A molecular dynamics assisted insight on damping enhancement in carbon fiber reinforced polymer composites with oriented multilayer graphene oxide coatings

Muhan Zhang[1], Yalin Yu[2], Li Li[3], Helezi Zhou[1], Luyang Gong[1], Huamin Zhou[1]

[1]State Key Laboratory of Material Processing and Die & Mold Technology, School of Materials Science and Engineering, Huazhong University of Science and Technology, Wuhan 430074, Hubei, China.

[2]Aerospace Research Institute of Materials & Processing Technology, Beijing 100076, China.

[3]State Key Laboratory of Intelligent Manufacturing Equipment and Technology, School of Mechanical Science and Engineering, Huazhong University of Science and Technology, Wuhan 430074, Hubei, China.

Correspondence to: Assoc. Prof. Helezi Zhou, School of Materials Science and Engineering, Huazhong University of Science and Technology, 1037, Luoyu Road, Hongshan District, Wuhan 430074, Hubei, China. E-mail: Helezizhou@hust.edu.cn; Prof. Huamin Zhou, School of Materials Science and Engineering, Huazhong University of Science and Technology, 1037, Luoyu Road, Hongshan District, Wuhan 430074, Hubei, China. E-mail: Hmzhou@hust.edu.cn

Structural optimization

Figure S1 shows the energy optimization results of DGEBA/TETA unit. After a series of energy minimization, the total potential energy and nonbond energy no longer exhibit significant fluctuations and tend to converge. The premature auto-kill in Newton interaction means that the molecular structure has reached its optimal state. In addition, a 500-ps NVT dynamics was further applied to eliminate residual stress inside the cell, causing relaxation of polymer segments. The stability of energy can also be observed during this stage.

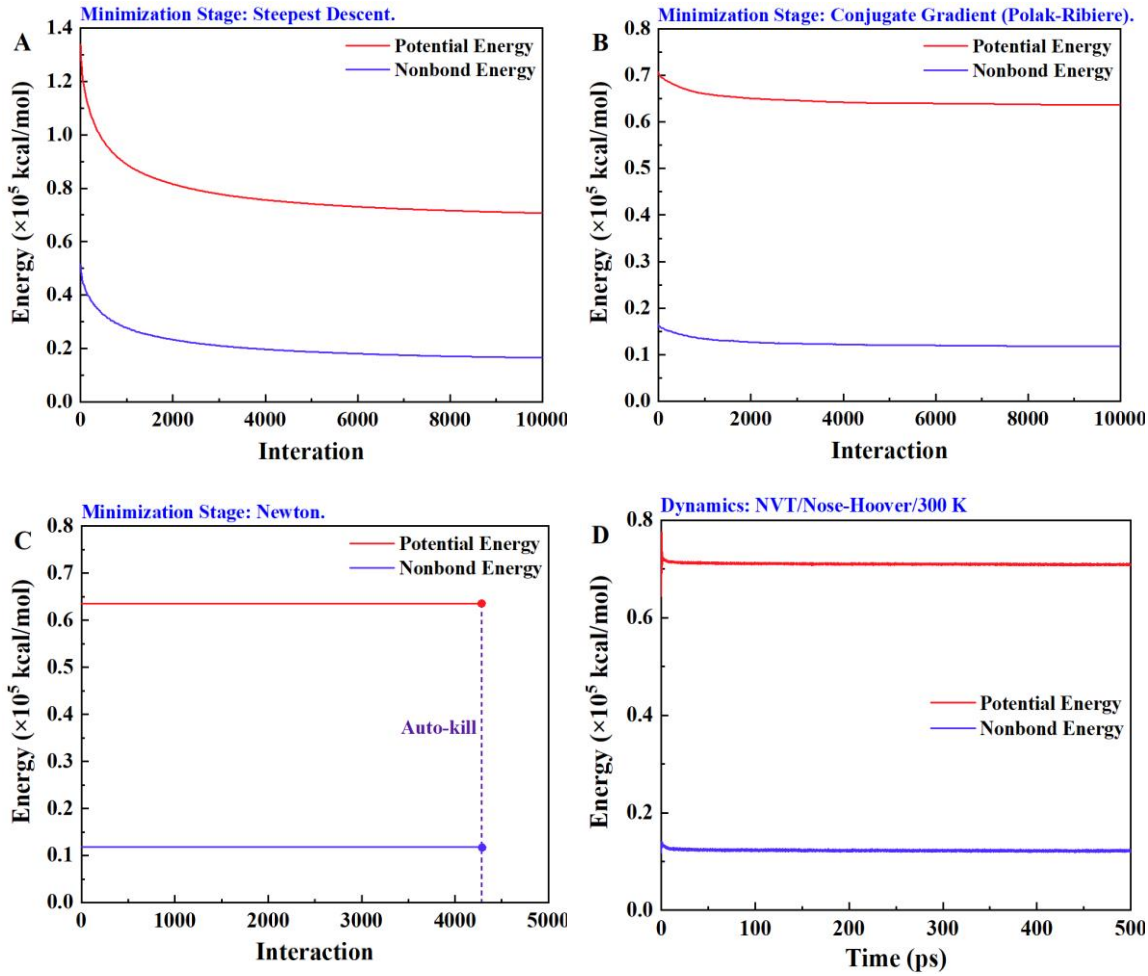


Figure S1. Structural optimization of EDGBA/TETA epoxy unit: (A) Steepest Descent method (×1000 steps), (B) Conjugate Gradient (Polak-Ribiere) method (×1000 steps), (C) Newton method (×1000 steps) and (D) a 500-ps NVT dynamics process under 300 K.

Fundamental stretching frequency

The fundamental stretching frequency of the atomistic model was investigated using a standard free vibration method. In detail, the system was initially equilibrated at 300 K using an NVT ensemble ($\Delta t = 1\,fs$). The atoms at both ends of the model along the y-axis were fixed. Subsequently, the ensemble transitioned to a micro-canonical condition (NVE), wherein the total energy of the system remained constant. Following this, a force was applied to one side of the fixed part to induce a 2% elongation of the box in the y direction. Upon removing the force, the unrestrained atoms oscillated freely. The resonant frequency of the system was determined by conducting a fast Fourier transform on the time response of the center of mass (COM).

The temporal response of the displacement of the COM (X_{com}) is monitored in **Figure S2A**, and the resonant frequency of the system was then obtained from the Fast Fourier transform of the time response of the X_{com}, as shown in **Figure S2B**. As can be seen, the values of the fundamental stretching frequency for the D-CFRP$_{0LGO}$, D-CFRP$_{4LGO}$ and D-CFRP$_{8LGO}$ groups were 2.467 THz, 2.533 THz, and 2.633 THz, respectively.

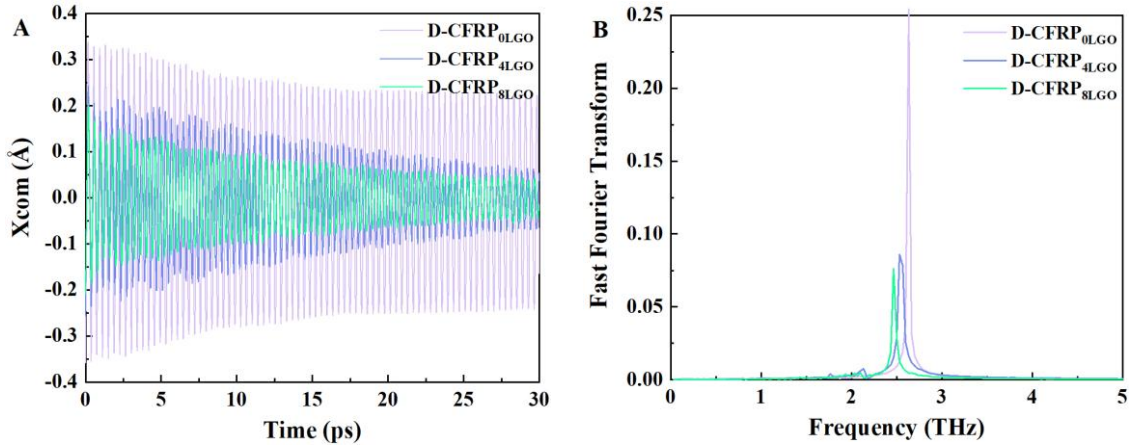


Figure S2. Simulation results obtained by free vibration method: (A) the relationship between the displacement of the centroid along the y-axis and the vibration time, (B) Fast Fourier transform of the X_{com}-time response.

Frequency/Temperature dependence of Q factors

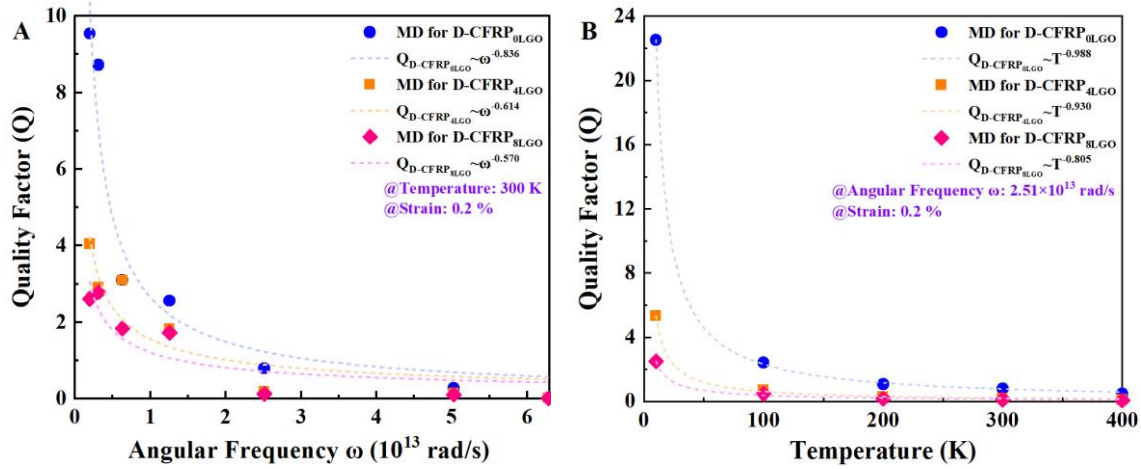


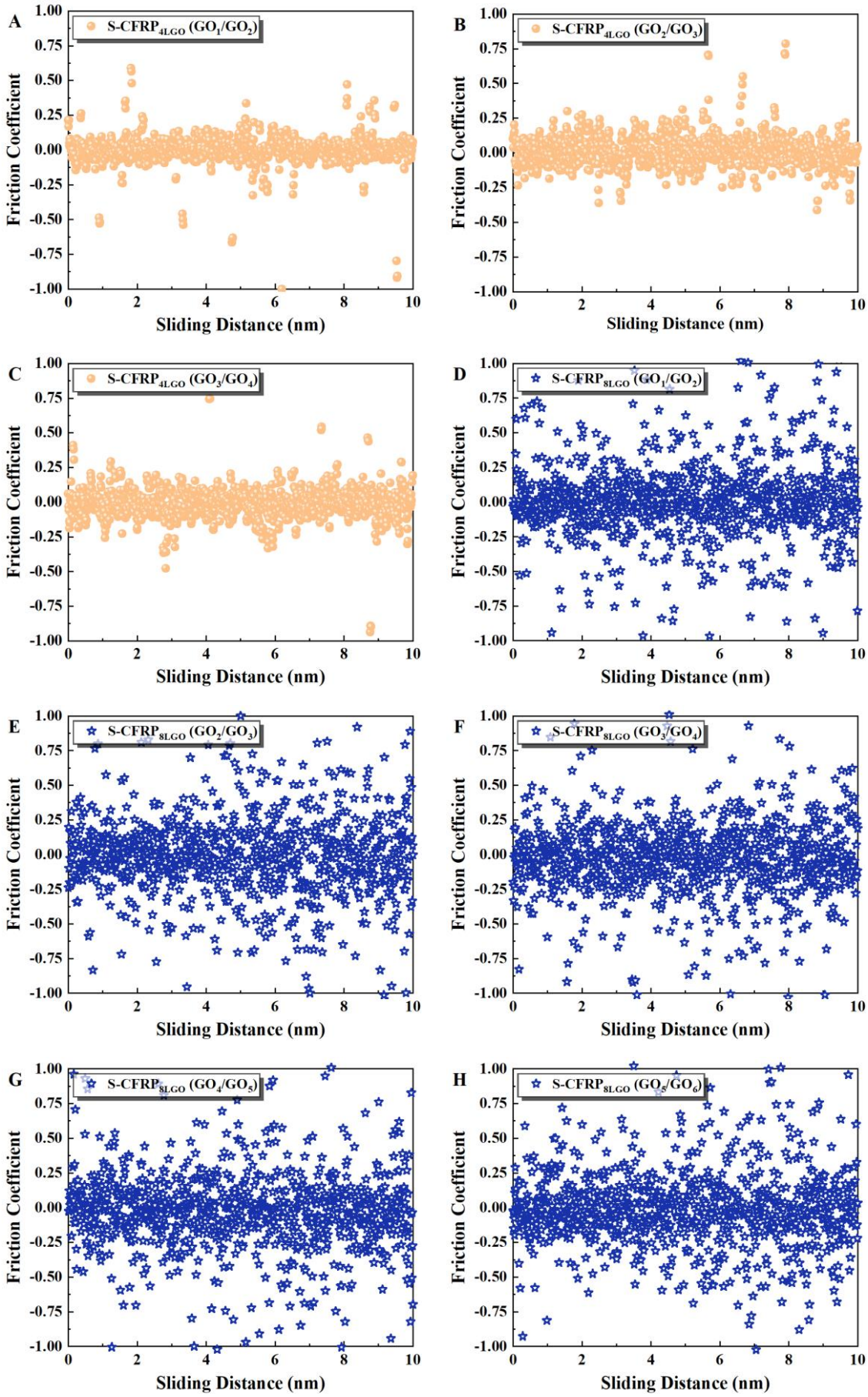
Figure S3. (A) Frequency dependence and (B) Temperature dependence of Q factors for the CFRP systems.

Dynamic friction coefficient between GO layers

Interlayer slip behavior of GO film by external vibration is highly correlated with the improvement of damping performance. The interface friction of graphene nanomaterials has been proposed as an important energy dissipation pathway[1-2]. Herein, the trajectory of atoms and forces generated in the sliding direction have been recorded and used for calculating the dynamic friction coefficient (μ), which is expressed as follow:

$$\mu = \frac{f}{F_n} \tag{S1}$$

where the friction force f is obtained by summing the force acting on the adjacent GO layers along the sliding direction and F_n is the normal force acting on the adjacent GO layers along the z direction. **Figure S4** shows the calculated μ for each CFRP system. In details, as the thickness of the coating increases, μ between the sheets gradually diverging during the sliding process. It means that the dynamic friction force inside the multi-layer GO is higher, which can consume more mechanical energy.


A
S-CFRP4LGO (GO1/GO2)
B
S-CFRP4LGO (GO2/GO3)
C
S-CFRP4LGO (GO3/GO4)
D
S-CFRP8LGO (GO1/GO2)
E
S-CFRP8LGO (GO2/GO3)
F
S-CFRP8LGO (GO3/GO4)
G
S-CFRP8LGO (GO4/GO5)
H
S-CFRP8LGO (GO5/GO6)
Friction Coefficient
Sliding Distance (nm)
1.00
0.75
0.50
0.25
0.00
-0.25
-0.50
-0.75
-1.00
0
2
4
6
8
10

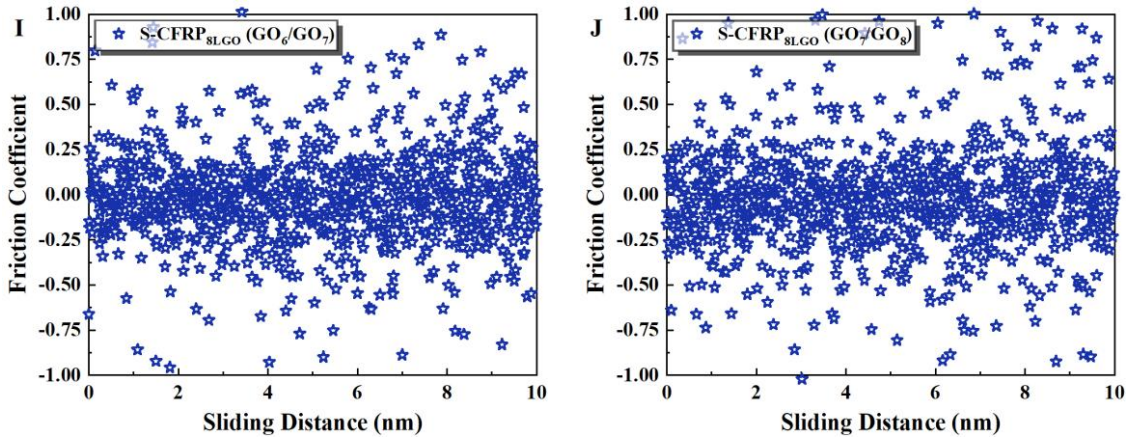


Figure S4. Dynamic friction coefficient of various adjacent GO layers from two CFRP models (A-C) S-CFRP$_{4LGO}$ and (D-J) S-CFRP$_{8LGO}$. The schematic diagrams of GO_1, GO_2, GO_3, GO_4 in S-CFRP$_{4LGO}$ and GO_1, GO_2, GO_3, GO_4, GO_5, GO_6, GO_7, GO_8 in S-CFRP$_{8LGO}$ have been shown in **Figure 9A**.

REFERENCES

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