polymers

MDPI

Supplementary Materials

Molecular Dynamics Simulation on the Interfacial Behavior of Over-molded Hybrid Fiber Reinforced Thermoplastic Composites

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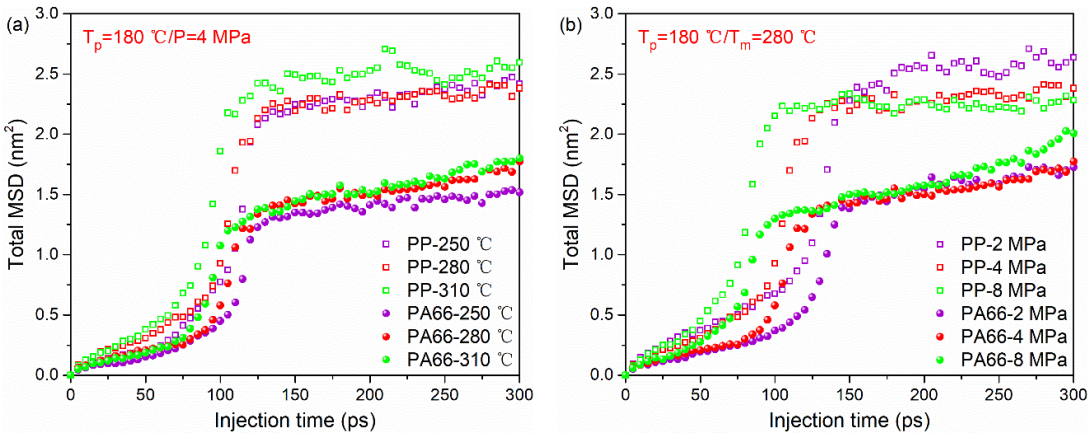
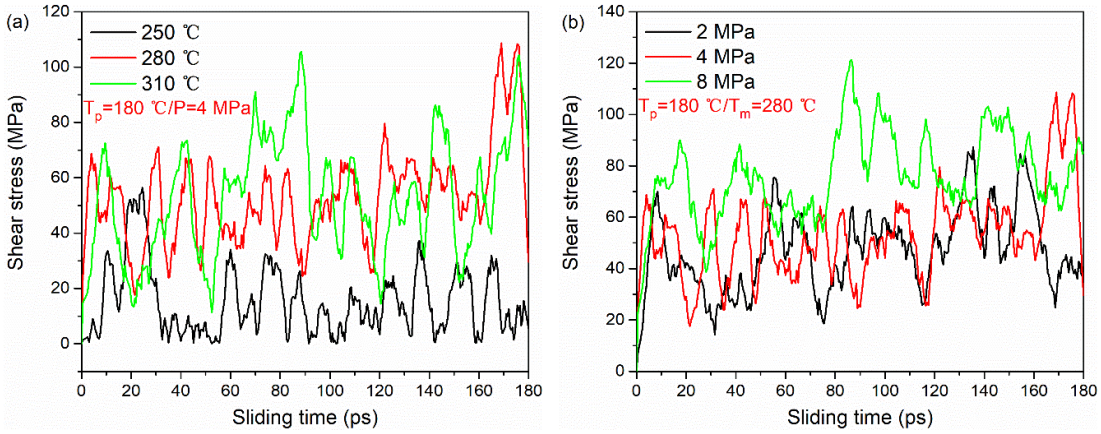


(**a**) (**b**)

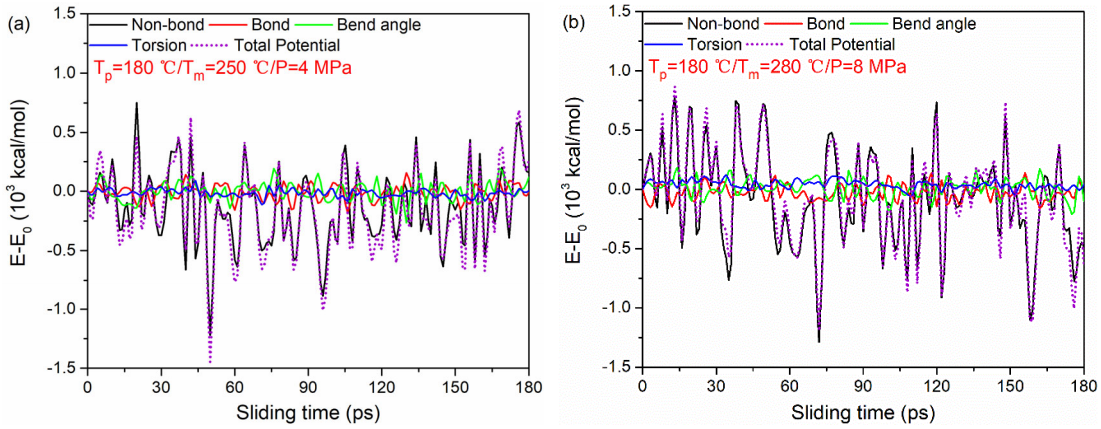
Figure S1. The MSD–time curve of PP and PA66 layer separately under various processing parameters: (**a**) melting temperatures and (**b**) injection pressure.

The MSD–time curves of PP and PA66 layers during simulations under various processing parameters are given in **Figure S1**. As seen, the fluctuation trend of the curves of the two materials is basically consistent with the general trend of the whole system (**Figure 6** in the Article). The motions of PP molecules are significantly stronger than that of PA66 molecules due to their shorter chain length and lower stiffness.



(**a**) (**b**)

Figure S2. Shear stress versus sliding time curves for PA66–PP interface under various processing parameters: (**a**) melting temperatures and (**b**) injection pressure.



(**a**) (**b**)

Figure S3. Potential energy decompositions of sliding deformation process for PA66–PP interface under processing parameters: (**a**) T_p= 180 ℃, T_m= 250 ℃, P= 4 MPa and (**b**) T_p= 180 ℃, T_m= 280 ℃, P= 8 MPa.