Supporting Information

# Resolving the Dynamic Properties of Entangled Linear Polymer in Non-equilibrium Coarse Grain Simulation with *a priori* Scaling Factor

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**S1 Structural distribution functions for the IBI, LIBI, and HIBI in 2BD and 1BD model**

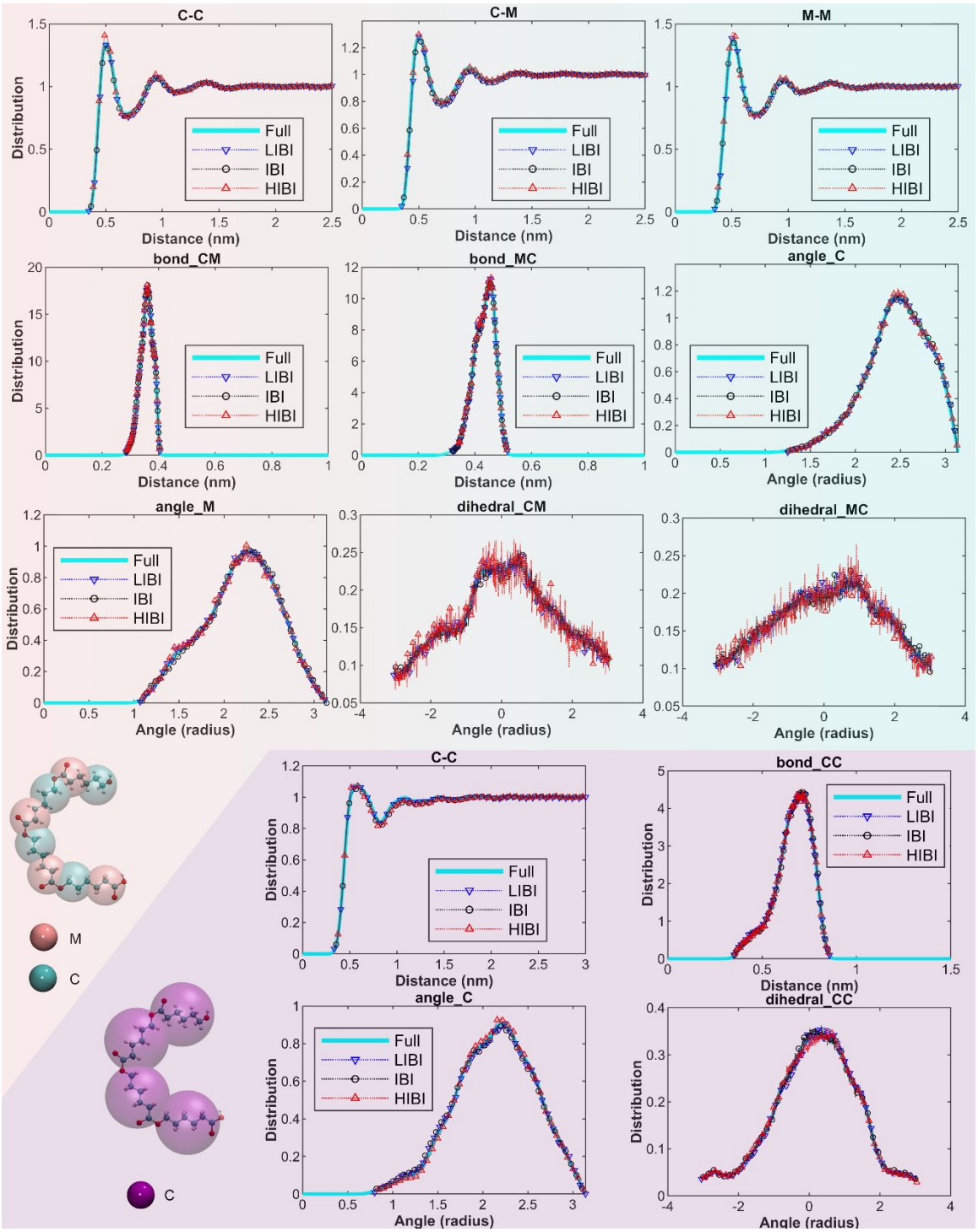


**Figure S1** The distribution functions predicted by the IBI, LIBI and HIBI can match well with the full-atomic results in 2BD and 1BD models.

## S2 Structural distribution functions for EIBI.

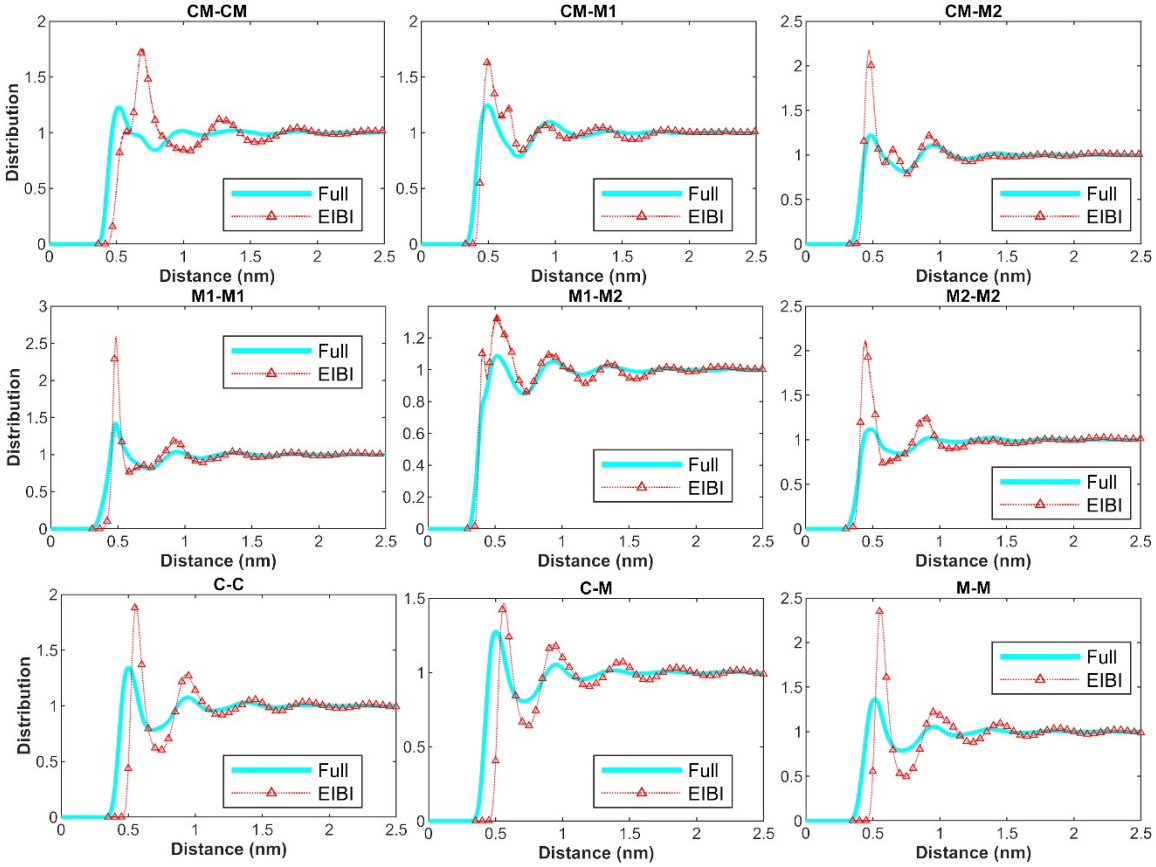


**Figure S2** The structural distribution functions in 2BD and 3BD models with EIBI potential.

## S3 Structural distribution functions for the DPD thermostat in 3BD model

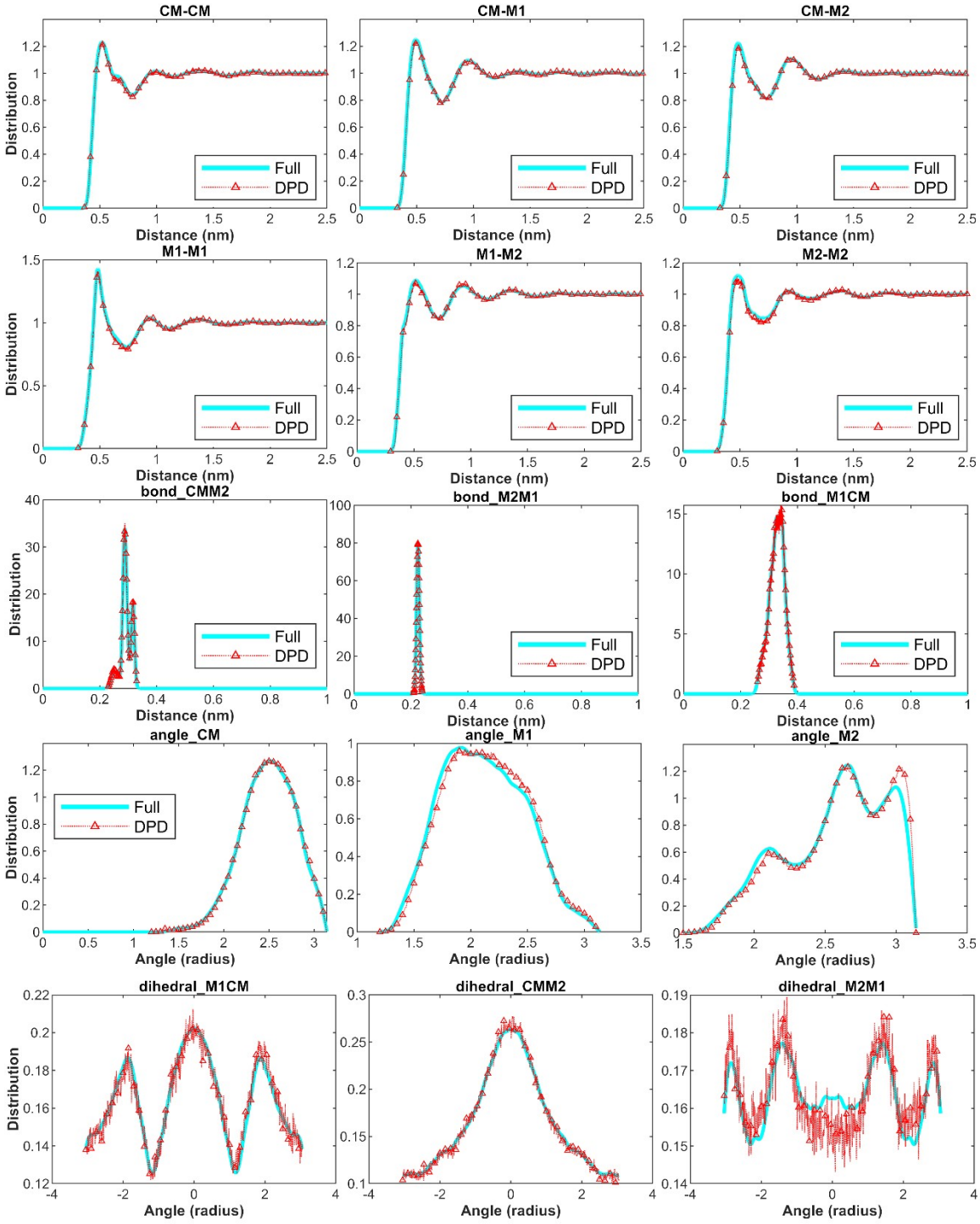


**Figure S3** The structural distribution functions in 3BD model with IBI potential and DPD thermostat.

**S4 Structural distribution functions for the DPD thermostat in 2BD and 1BD model**

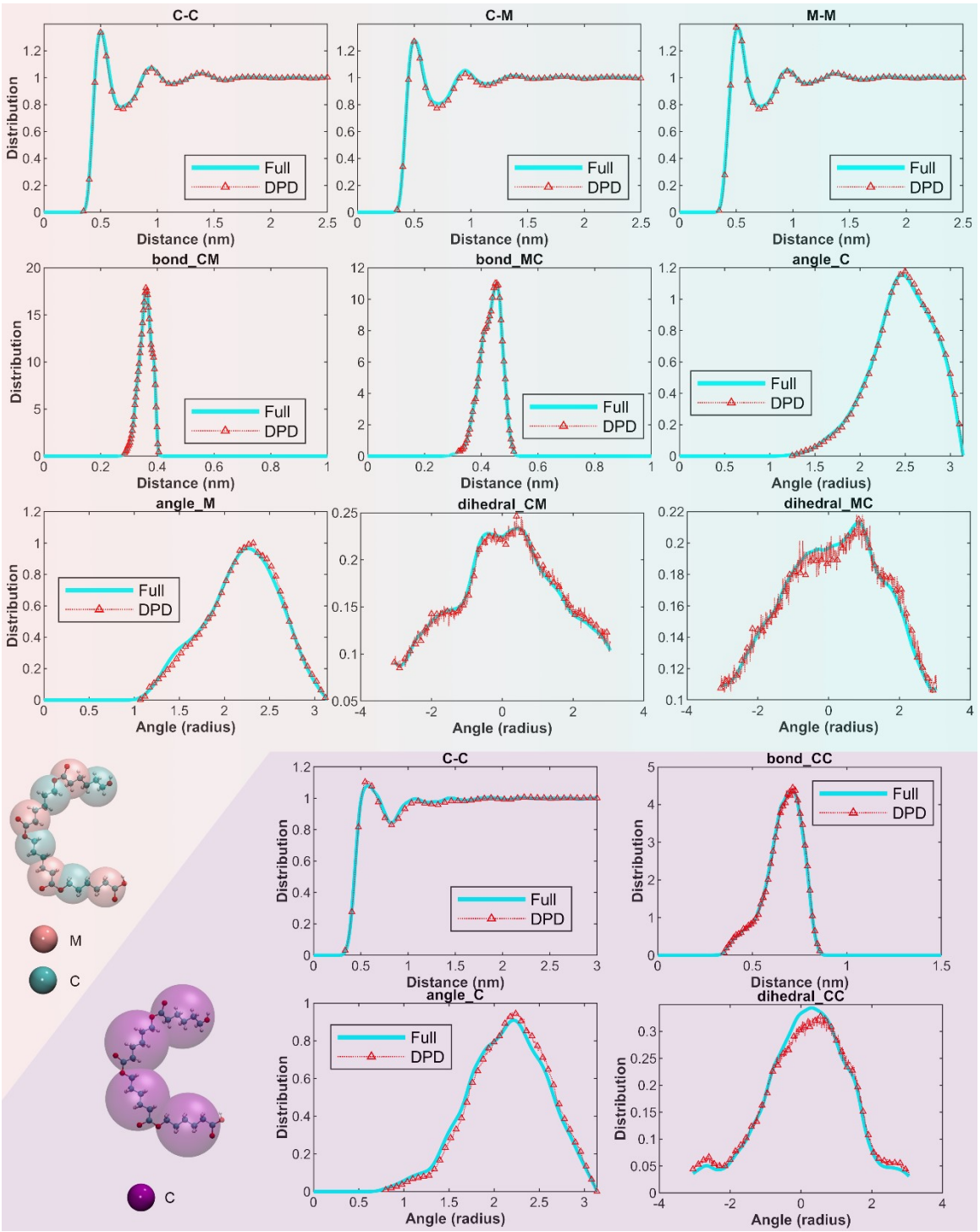


**Figure S4** The structural distribution functions in 2BD and 1BD model with IBI potential and DPD thermostat.

**S5 Mean squared displacement curves during the relaxation.**

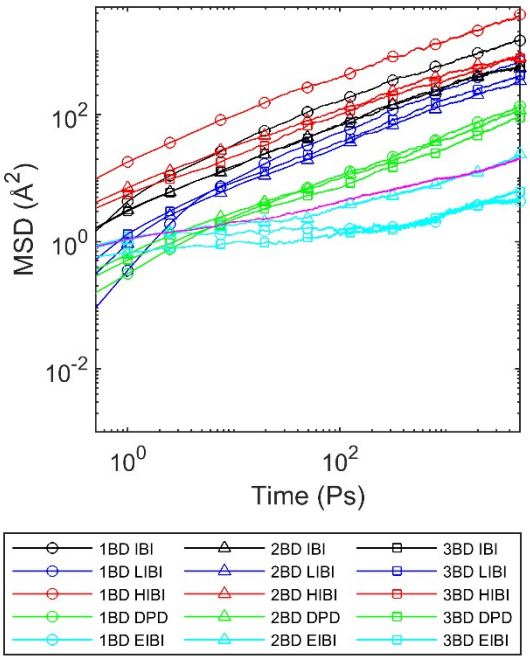


**Figure S5** The MSD curves of the atoms and CG beads for different models.

## S6 Enthalpy at different temperatures in different CG models

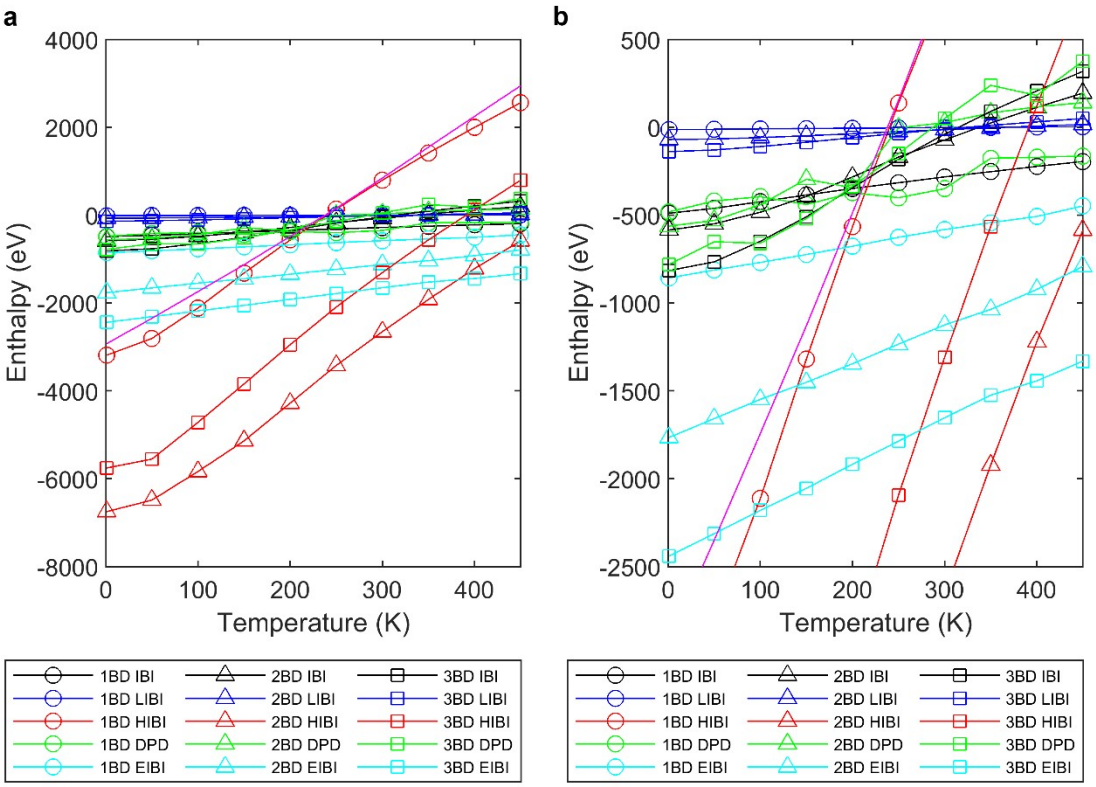


**Figure S6** For the DPD model, as the non-conservative force is added, the pressure has a larger fluctuation than the IBI with the Nose-Hoover thermostat, which results in a larger fluctuation in enthalpy, but the value is close to IBI results on average. As for the EIBI method, the enthalpy is lower than that of the IBI results.

**S7 Young's modulus at different strain rates in different CG models**

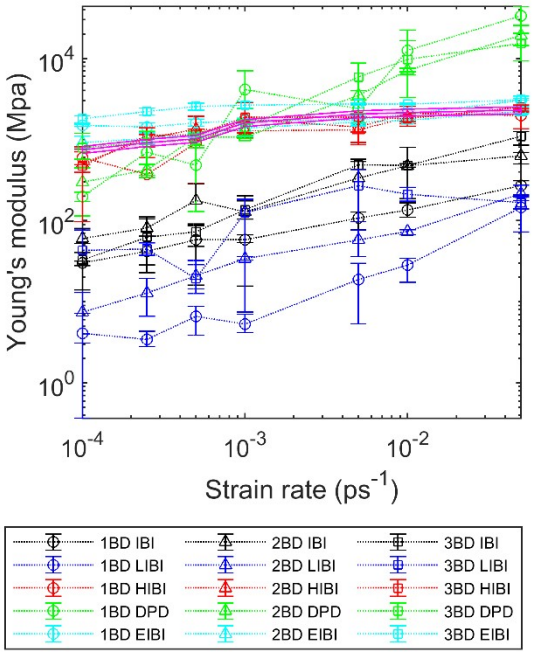


**Figure S7** The Young's modulus in different CG models with different strain rates. The error bar shows the variance from the tensile tests in the three orthogonal directions for each model.

**S8 The stress- strain curves for each model under different tensile rates.**

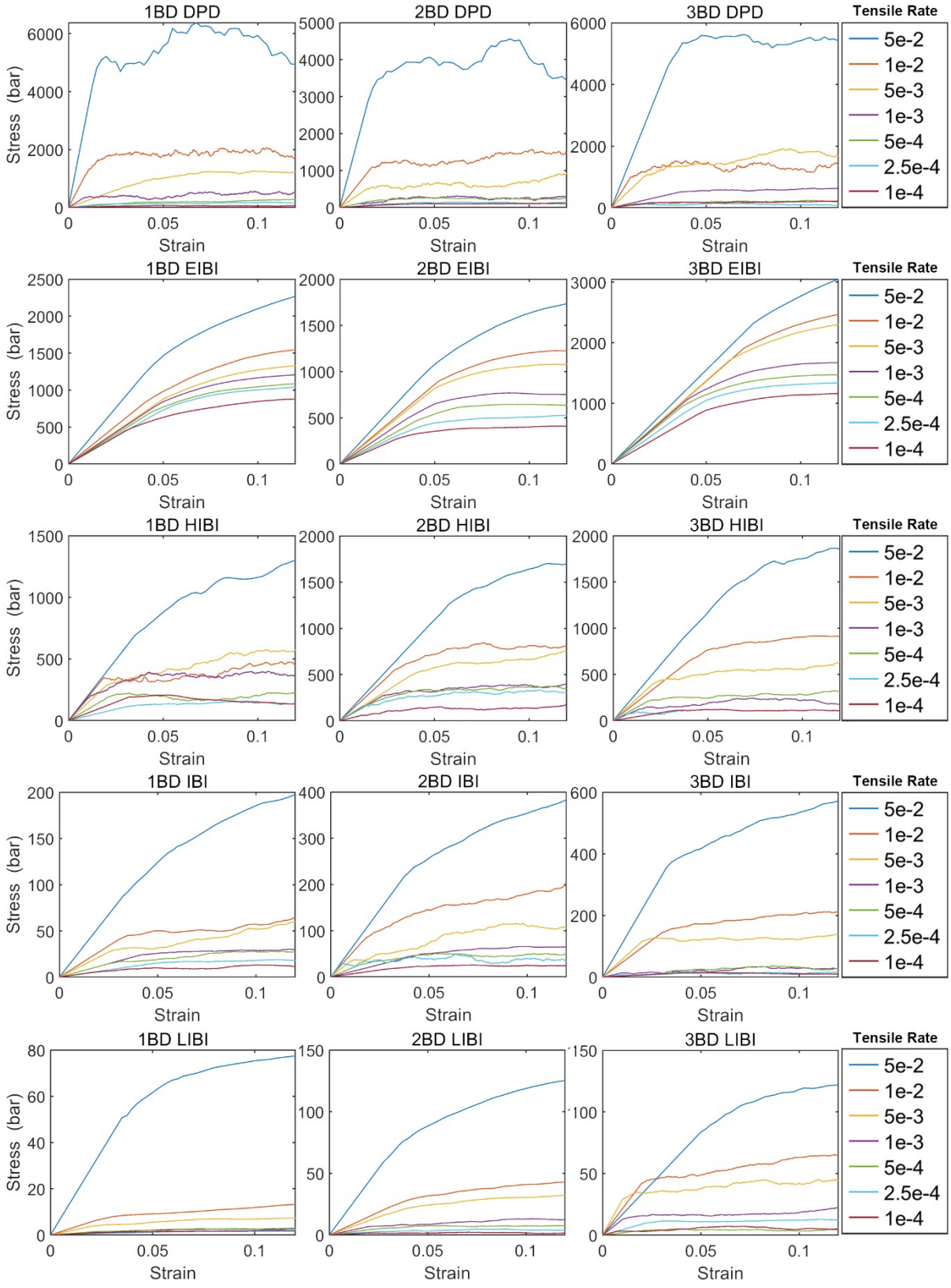


**Figure S8** The stress-strain curve for each model under different tensile rates. The stress-strain curve is the averaged result from the tensile test in three directions.