Supporting Information

Coarse-Grained Simulations on Polyethylene Crystal Network Formation and Microstructure Analysis

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Table S1. The density and box dimensions of the $10C_{1000}$ model at each stage of the MD simulations using PYS/R forcefield.

Conditions	**$10C_{1000}$**	
	ρ	Cell
Data file and NVT melting at 450K	*0.931*	a = 50.0
		b = 50.0
		c = 100.0
NPT Equilibration model at 450K	*0.769*	a = 53.282
		b = 53.282
		c = 106.564
Quenched model from 450K to 300K	*0.856*	a = 51.405
		b = 51.405
		c = 102.81
Isothermally cooled at 300K	*0.913*	a = 50.313
		b = 50.313
		c = 100.626

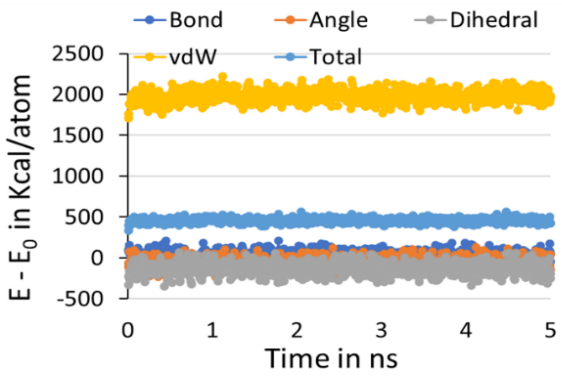

Figure S1. Potential energy decomposition of isotropically melting amorphous state at 450K and 1 atm pressure.

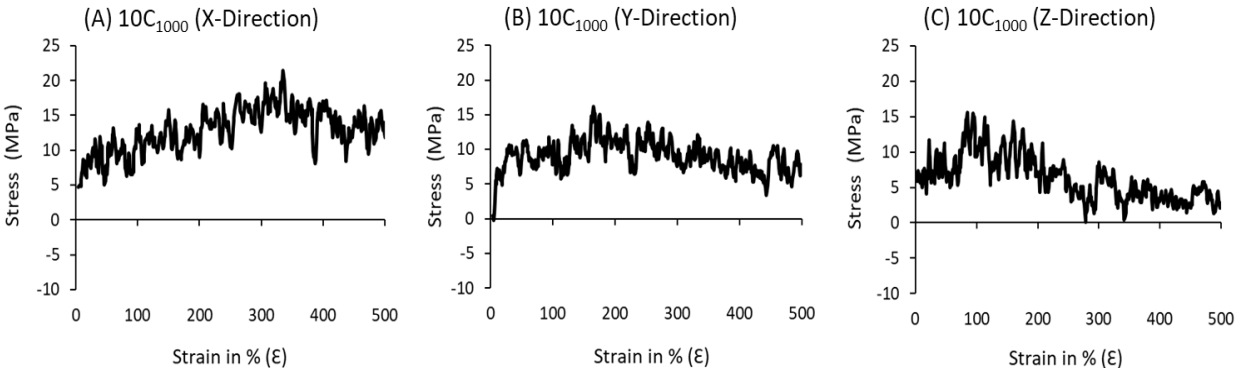

Figure S2. Amorphous state S-S curves for the $10C_{1000}$ model at 300K and zero pressure conditions using the NPT ensemble. Each model deformed to 500% of the initial box length of the simulation box's X, Y, and Z directions.