Supplementary Materials

Analysis of the Structure and the Thermal Conductivity of Semi-Crystalline Polyetheretherketone/Boron Nitride Sheet Composites Using All-Atom Molecular Dynamics Simulation

Yuna Oh [1,2], Kwak Jin Bae [1], Yonjig Kim [2] and Jaesang Yu [1,*]

List of abbreviations

PEEK	Polyetheretherketone
BN	Boron nitride
MD	Molecular dynamics
h-BN	Hexagonal boron nitride
DSC	Differential scanning calorimeter
N-DFF	Newly proposed dreiding force field
DFT	Density functional theory
DFF	Dreiding force field
LLSF	Linear least square fitting
NPT	Isothermal-isobaric ensemble
RNEMD	Reverse non-equilibrium molecular dynamics
NVE	Microcanonical ensemble
PDOS	Phonon density of states
VACF	Velocity autocorrelation function
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
RMSE	Root mean squared error

List of symbols

R_g	Radius of gyration (Å)
R_{bulk}	Radius of gyration on the bulk polymer (Å)
M	Total mass of the polymer chain (g/mol)
m_i	Mass of the atom (g/mol)
r_i	Coordinate of the atom
r_{cm}	Coordinate of the center of mass on a polymer chain
$R_{a,g}$	Average value of radius of gyration of the amorphous polymer chains (Å)
R_{bulk}	Radius of gyration on the bulk polymer (Å)
M_b	Total mass of the amorphous polymer chains (g/mol)
$r_{cm,bulk}$	Coordinate of the center of mass on the bulk amorphous polymer
ns	Nanosecond
fs	Femtosecond
K	Thermal conductivity (W/mK)
J	Total heat flux (W/m^2)
t	Heat transfer time (s)
A	Cross-sectional area (m^2)
m_h	Atomic masses of the heat source (g/mol)
m_c	Atomic masses of the heat sink (g/mol)
v	Velocity of atom (m/s)
T	Temperature (K)
ω	Frequency (THz)
τ	Total integration time (s)
$v(t)$	Velocity of atoms at time t (Å/ps)
K_B	Force constants
l	Bond length (Å)

Calculation of parameters for the bond stretching term

The force constants of the B-H and N-H bonds were obtained by linear least square fitting (LLSF) using the density functional theory (DFT) potential energy, which was calculated according to the bond length between boron atom and nitrogen atom in the unit cell. The bond potential energy of the newly proposed Dreiding force field (N-DFF) is expressed as

$$E_B = \sum_{Bonds} \frac{K_B}{2}(l - l_0)^2 \tag{S1}$$

where K_B is the force constants on the bond stretching and l is the bond length between two atoms. Figure S1 shows the bond potential energy obtained by the DFT and the molecular dynamics (MD) simulation using N-DFF. The root mean squared error (RMSE) values of the B-H and N-H bond terms calculated by the residuals between the DFT and MD potential energy were 0.004 and 0.015, respectively. These results mean that the force constants were accurately calculated with low error. Table S1 shows the force constants and the parameters of N-DFF. The sigma and epsilon of the B-H and N-H bonds on the Lennard-Jones function were calculated using the parameter values on the boron and nitrogen atoms of N-DFF, and the parameter values of the hydrogen atoms of the original Dreiding force field.

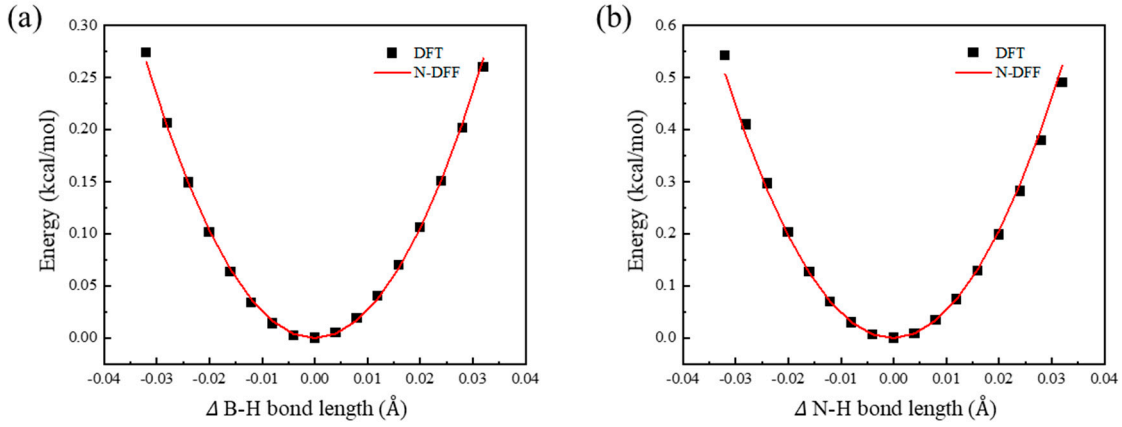

Figure S1. Energy of the bond stretching term using DFT and the N-DFF: (**a**) B-H bond and (**b**) N-H bond.

Table S1. Parameters of the N-DFF used in the MD simulations.

Bonding term	**Value**	**Force constant (kcal/mol)**
B-H (l_0)	1.202 Å	521.102
N-H (l_0)	1.014 Å	1006.20
Lennard-Jones	**Sigma (Å)**	**Epsilon (kcal/mol)**
B-H	3.2035	0.03309
N-H	2.9526	0.02480