Supplementary Information

Molecular dynamics simulation and non-isothermal crystallization kinetics of polyamide 4 and different bio-based polyamide blends

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Methods

The simulations were conducted using LJ units, and all quantities are unitless. The units of mass, length, time, and energy are defined by m, r_c, τ, and k_BT, respectively. The time unit τ can be formulated by[S1]

$$\tau = \sqrt{mr_c^2 / k_BT} \quad \text{(S1)}$$

where T and k_B are the absolute temperature and Boltzmann constant, respectively. k_BT and m are equal to 1.0 in our simulations. This simulation only considers the nonbonding potential energy (U_{nb}), bond potential energy (U_b), bond-angle-bending potential energy (U_A), and hydrogen-bond interaction potential energy (U_{hb}). The parameters of the beads, nonbonding potential energy, bonds, and angles are shown in Table S1-S4.

Table S1 Parameters for beads.

Bead type	Description	m	ε	σ
A	N atom in the amide group	1.0	1.0	1.0
B	Carbonyl group in the amide group	1.0	1.0	1.0
C	Methylene group in the molecular chain of PA4	1.0	1.0	1.0
D	Methylene group in the molecular chain of PAX	1.0	1.0	1.0
H	H atoms attached to the N atoms	1.0	1.0	1.0

Table S2 Parameters for nonbonding potential energy.

Bead 1	Bead 2	Δ	ε	σ	r_{nb}
A	A	0	1.0	1.0	4.5 r_c
A	B	0	1.0	1.0	4.5 r_c
A	C	0	1.0	1.0	4.5 r_c
A	D	0	1.0	1.0	4.5 r_c
A	H	-0.8	1.0	1.0	4.5 r_c
B	B	0	1.0	1.0	4.5 r_c
B	C	0	1.0	1.0	4.5 r_c
B	D	0	1.0	1.0	4.5 r_c
B	H	-0.8	1.0	1.0	4.5 r_c
C	C	0	1.0	1.0	4.5 r_c
C	D	0	1.0	1.0	4.5 r_c
C	H	-0.8	1.0	1.0	4.5 r_c
D	D	0	1.0	1.0	4.5 r_c
D	H	-0.8	1.0	1.0	4.5 r_c
H	H	-1.6	1.0	1.0	4.5 r_c

Table S3 Parameters for bonds.

Bead 1	Bead 2	K_b	R_b
A	B	$30\varepsilon/\sigma^2$	1.5σ
A	H	$30\varepsilon/\sigma^2$	1.5σ
B	C	$30\varepsilon/\sigma^2$	1.5σ
B	D	$30\varepsilon/\sigma^2$	1.5σ

Table S4 Parameters for angles.

Bead 1	Bead 2	Bead 3	θ_0	K_A
A	B	C	180	10.0
A	B	D	180	10.0
B	C	C	180	10.0
B	D	D	180	10.0
C	A	B	180	10.0
D	A	B	180	10.0

S1 Y. S. Lv, L. Q. Wang, F. Liu, W. S. Feng, J. Wei and S. L. Lin, *Polym. Chem*, 2020, **11**, 4798-4806.