Supporting Information

Effect of Composition Asymmetry on the Phase Separation and Crystallization in Double Crystalline Binary Polymer Blends: A Dynamic Monte Carlo Simulation Study

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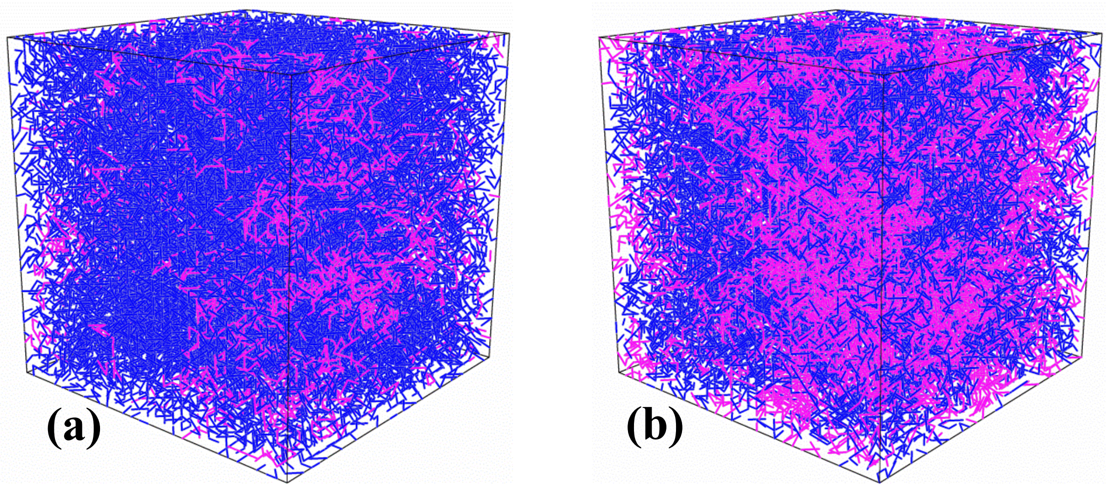
Figure S1. Snapshots at U_p = 0 for various compositions, x_B: (a) 0.125, (b) 0.375, (c) 0.5, (d) 0.625 and (e) 0.875. Blue and magenta colors represent bonds of A- and B-polymers, respectively.



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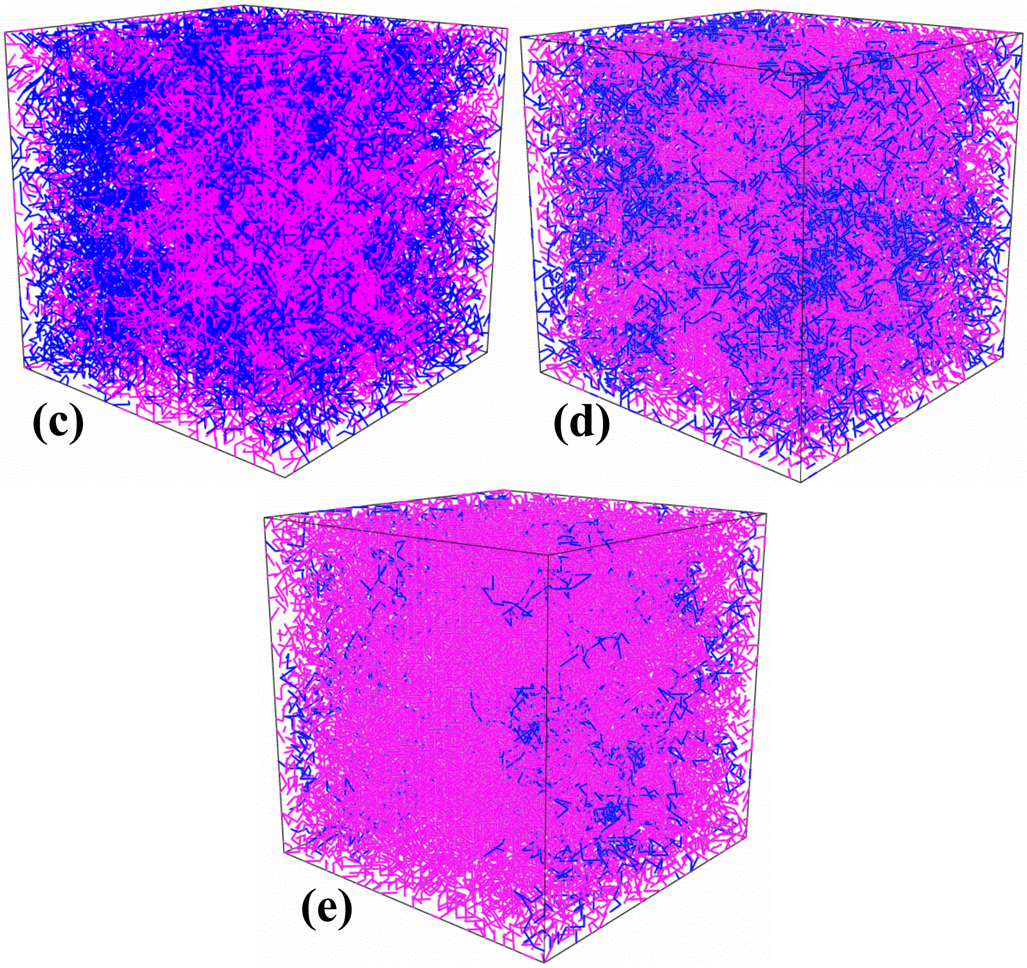

(c)
(d)
(e)

Figure S2. Change in mean square displacement of center of mass (d_{cm}^2) with U_p for A- and B-polymers: (a) $d_{cm\_A}^2$ vs. U_p at λ = 1, (b) $d_{cm\_A}^2$ vs. U_p at λ = 6, (c) $d_{cm\_B}^2$ vs. U_p at λ = 1, (d) $d_{cm\_B}^2$ vs. U_p at λ = 6.

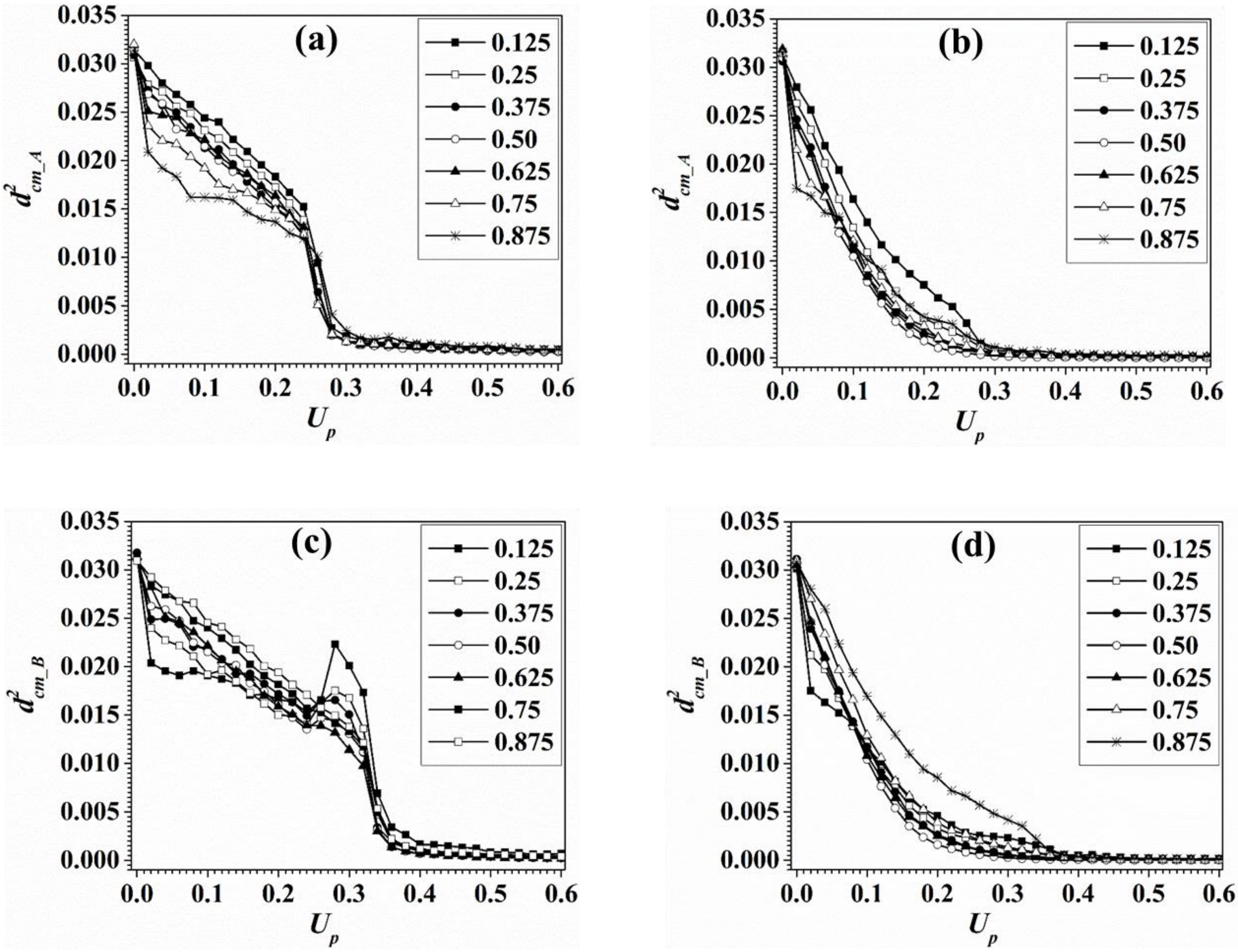
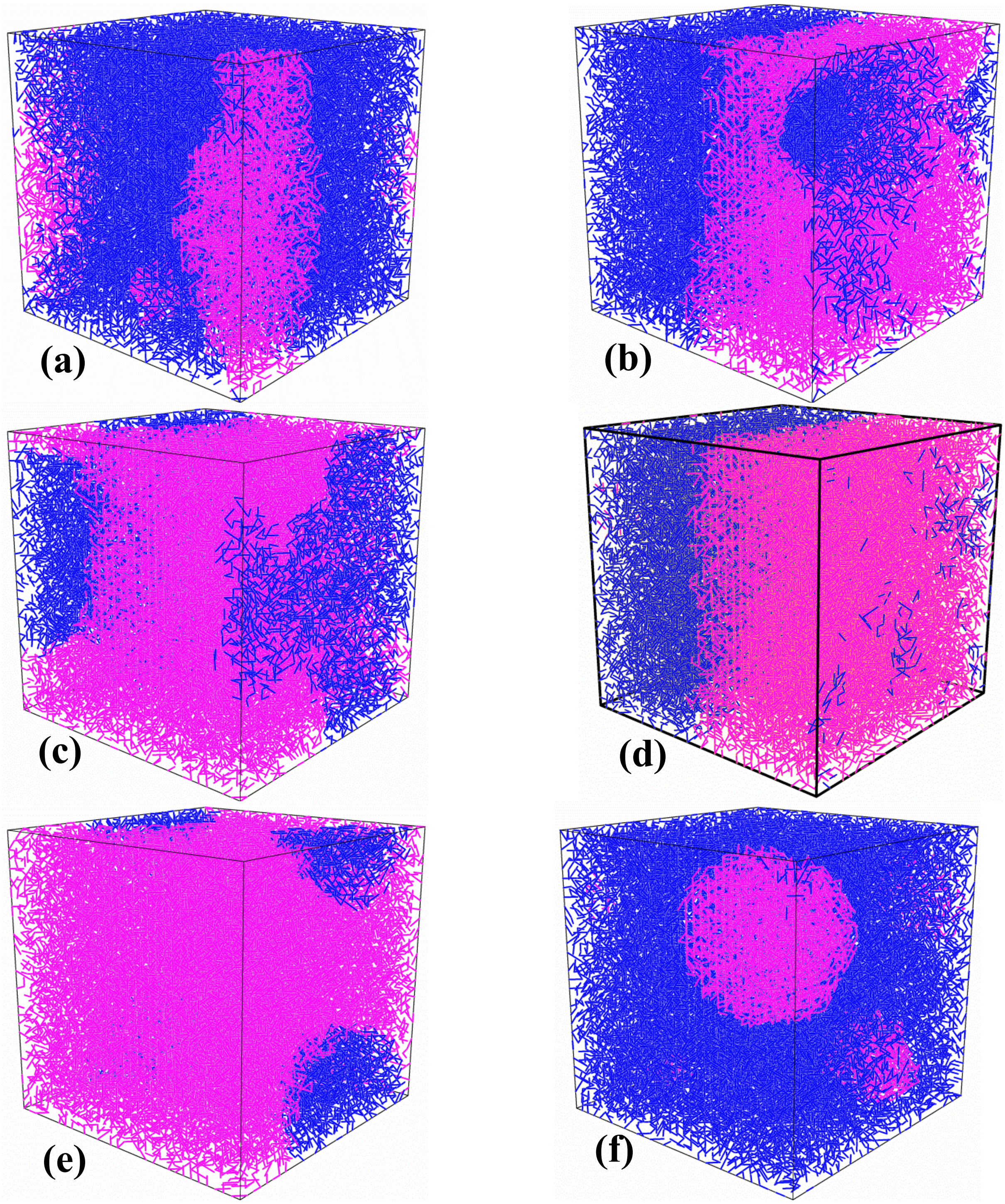


Figure S3. Snapshots of macrophase separated melt at U_p = 0.1 during non-isothermal crystallization, for various compositions and λ: (a) λ = 1, x_B = 0.125, (b) λ = 1, x_B = 0.375, (c) λ = 1, x_B = 0.5, (d) λ = 1, x_B = 0.625, (e) λ = 1, x_B = 0.875, (f) λ = 6, x_B = 0.125, (g) λ = 6, x_B = 0.375, (h) λ = 6, x_B = 0.5, (i) λ = 6, x_B = 0.625 and (j) λ = 6, x_B = 0.875. Blue and magenta colors represent bonds of A- and B-polymers, respectively.



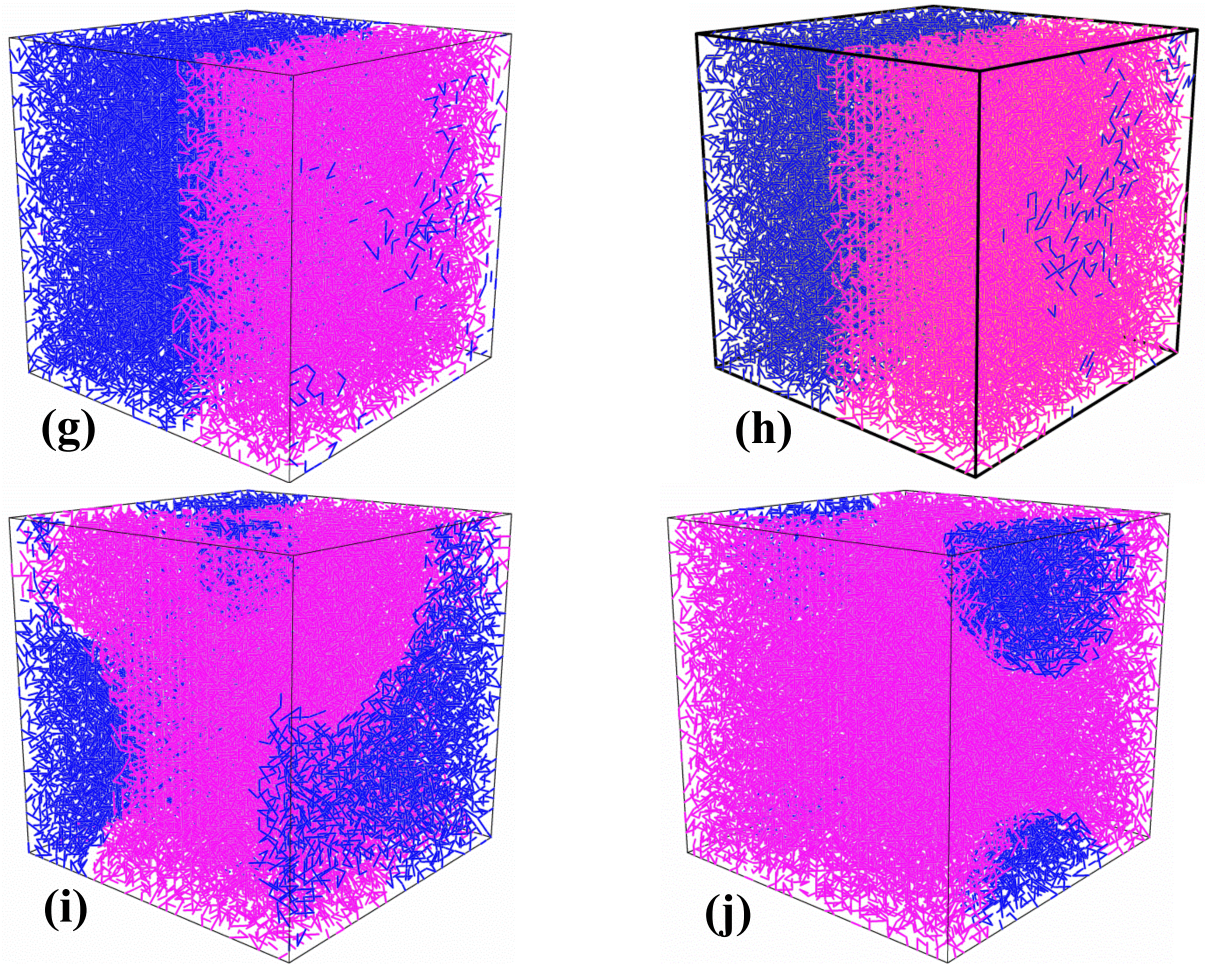
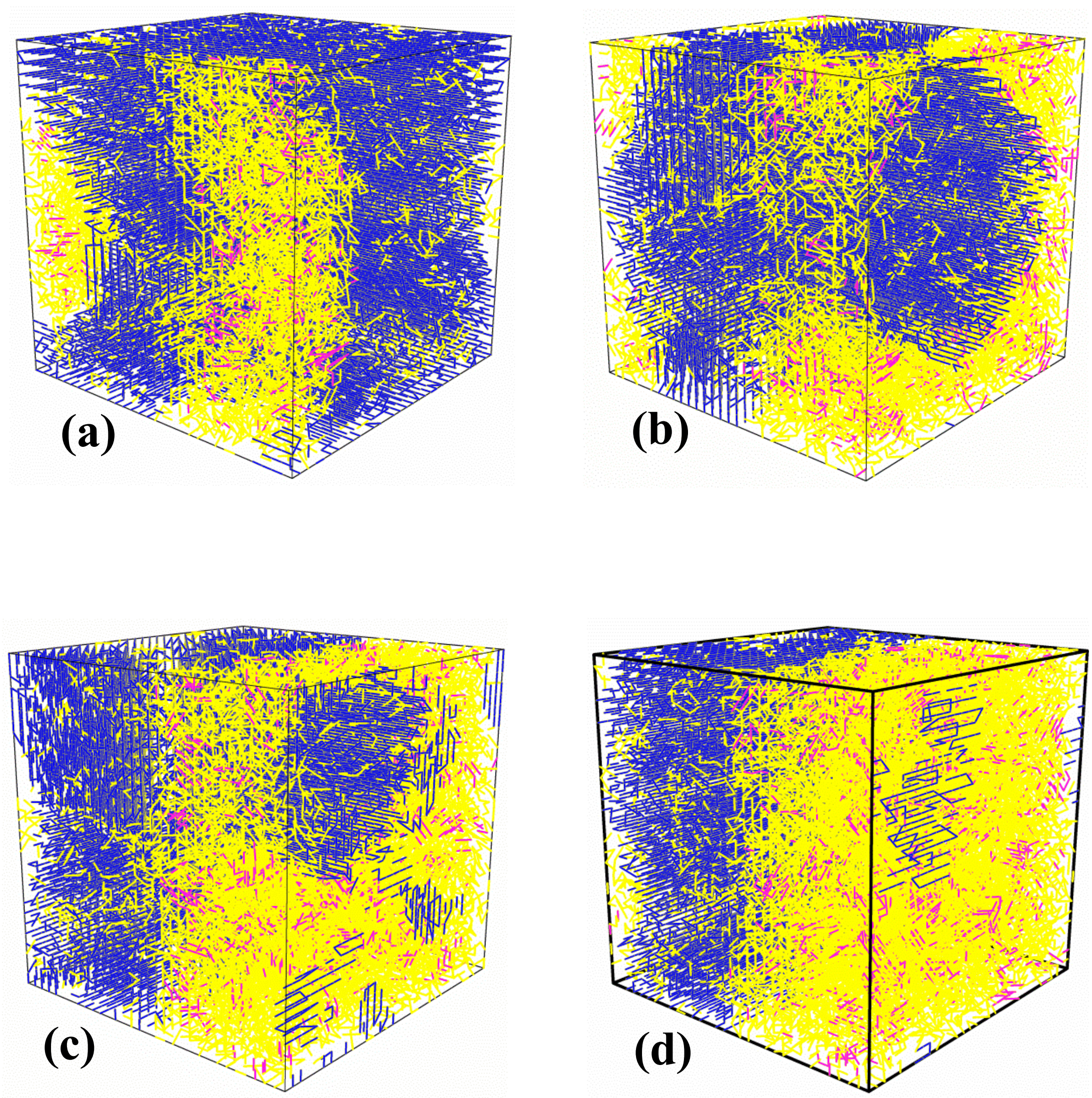
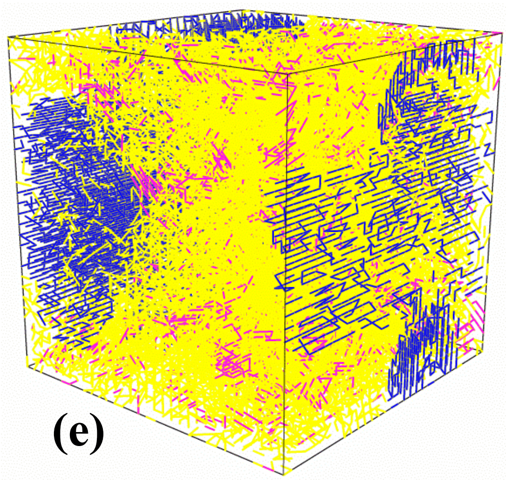
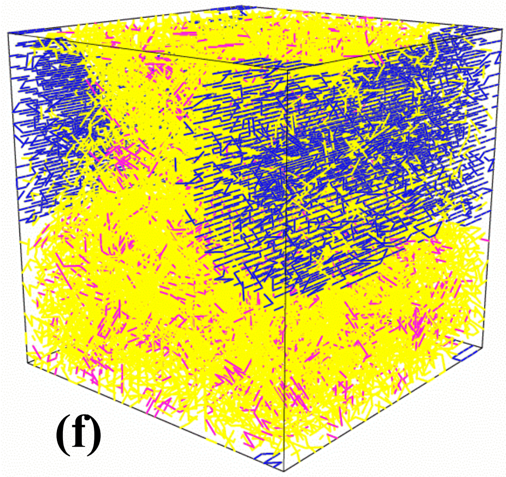

(g)
(h)
(i)
(j)

Figure S4. Snapshots of semicrystalline structure at U_p = 0.28 during non-isothermal crystallization for various compositions at $\lambda = 1$: (a) x_B = 0.125, (b) x_B = 0.25, (c) x_B = 0.375, (d) x_B = 0. 50, (e) x_B = 0.625, (f) x_B = 0.75, (g) x_B = 0.875. Blue and magenta colors represent crystalline bonds of A- and B-polymers, respectively. Yellow color represents non-crystalline bonds of both the polymers.




(e)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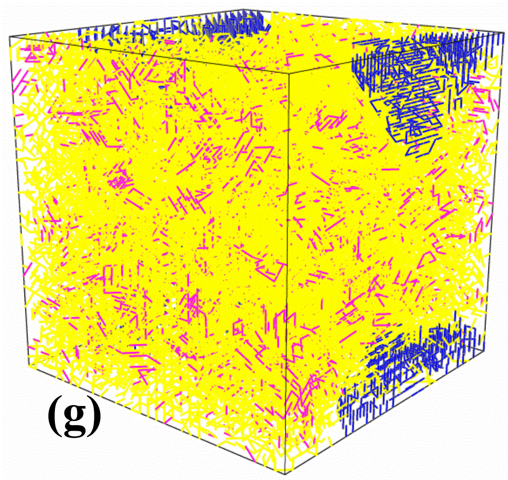

(g)

Figure S5. Change in crystallinity with U_p for A- and B-polymers: (a) X_A vs. U_p at λ = 1, (b) X_A vs. U_p at λ = 6, (c) X_B vs. U_p at λ = 1, (d) X_B vs. U_p at λ = 6.

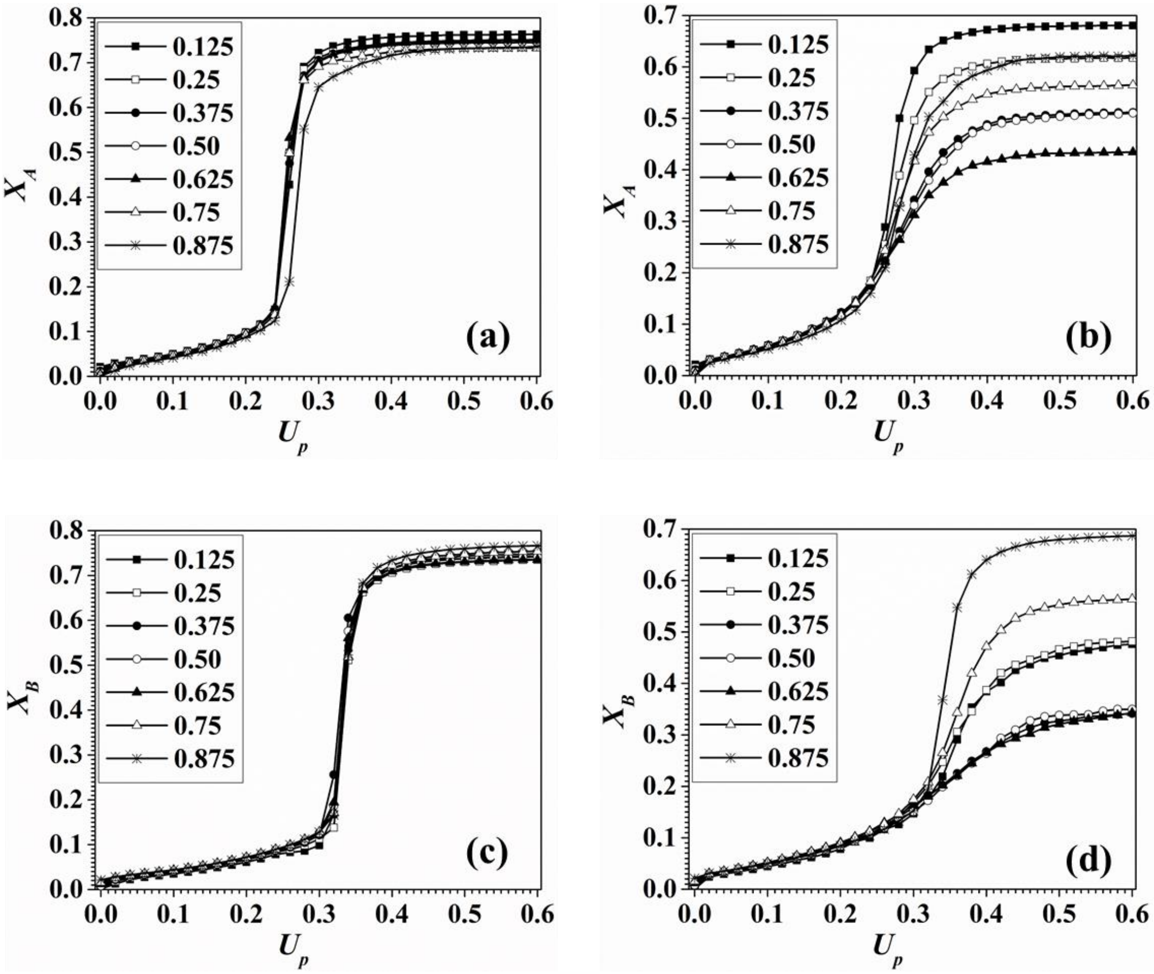
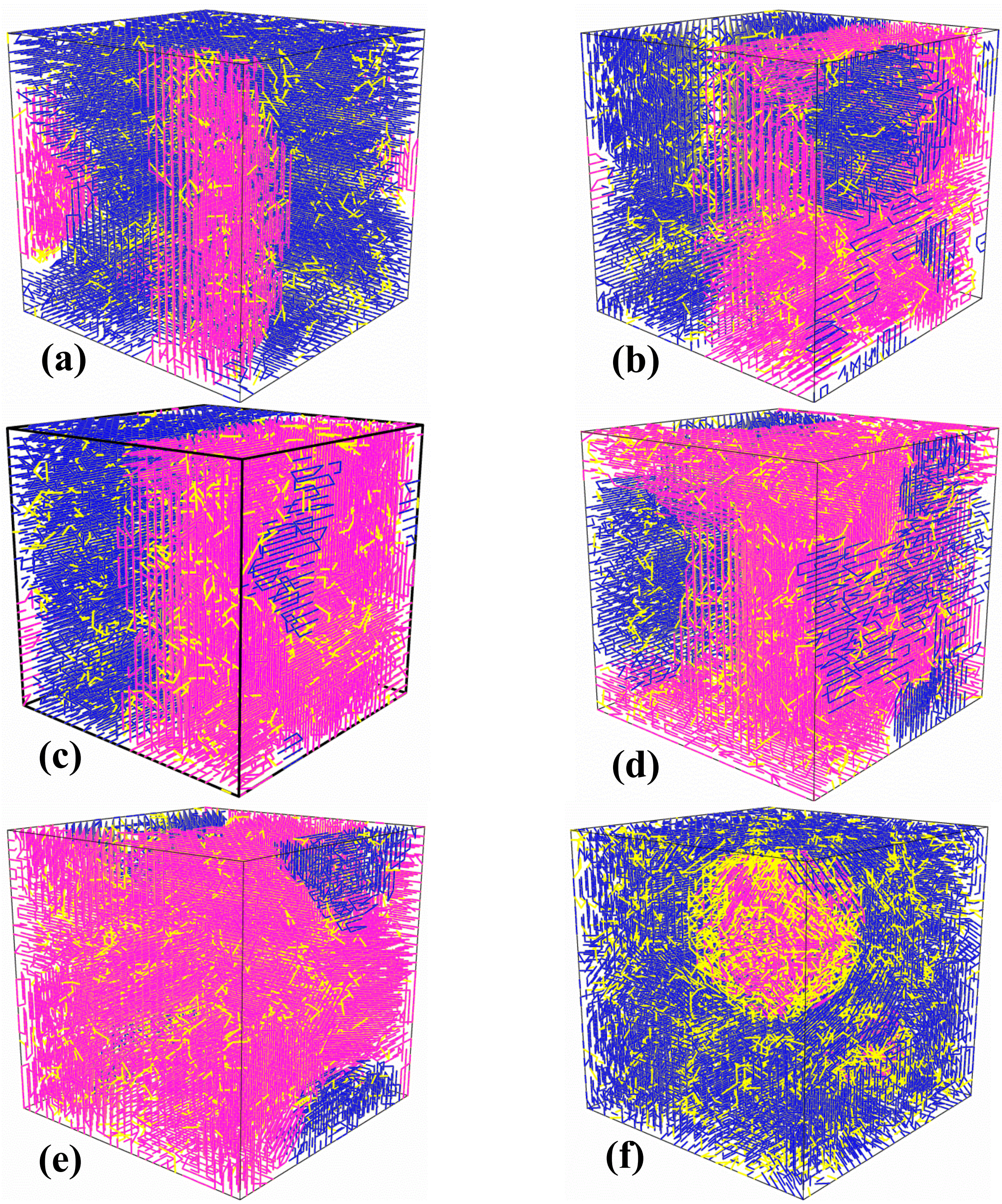


Figure S6. Snapshots of crystalline structure at U_p = 0.6 during non-isothermal crystallization, for various compositions and λ: (a) λ = 1, x_B = 0.125, (b) λ = 1, x_B = 0.375, (c) λ = 1, x_B = 0.5, (d) λ = 1, x_B = 0.625, (e) λ = 1, x_B = 0.875, (f) λ = 6, x_B = 0.125, (g) λ = 6, x_B = 0.375, (h) λ = 6, x_B = 0.5, (i) λ = 6, x_B = 0.625 and (j) λ = 6, x_B = 0.875. Blue and magenta colors represent crystalline bonds of A- and B-polymers, respectively. Yellow color represents non-crystalline bonds of both the polymers.



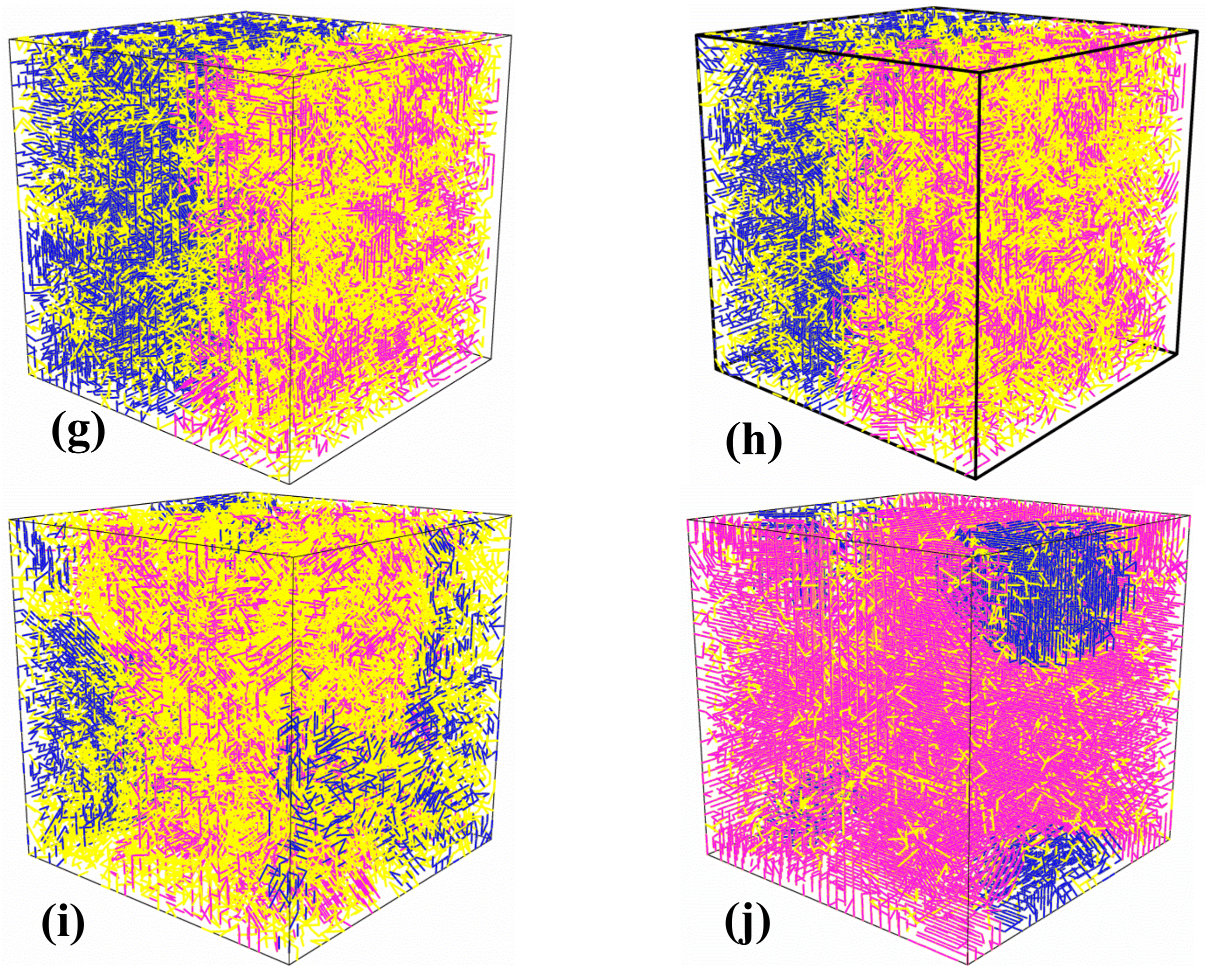

(g)
(h)
(i)
(j)

Figure S7. Change in average crystallite size with U_p for A- and B-polymers: (a) $\langle S_A \rangle$ vs. U_p at λ = 1, (b) $\langle S_A \rangle$ vs. U_p at λ = 6, (c) $\langle S_B \rangle$ vs. U_p at λ = 1, (d) $\langle S_B \rangle$ vs. U_p at λ = 6.

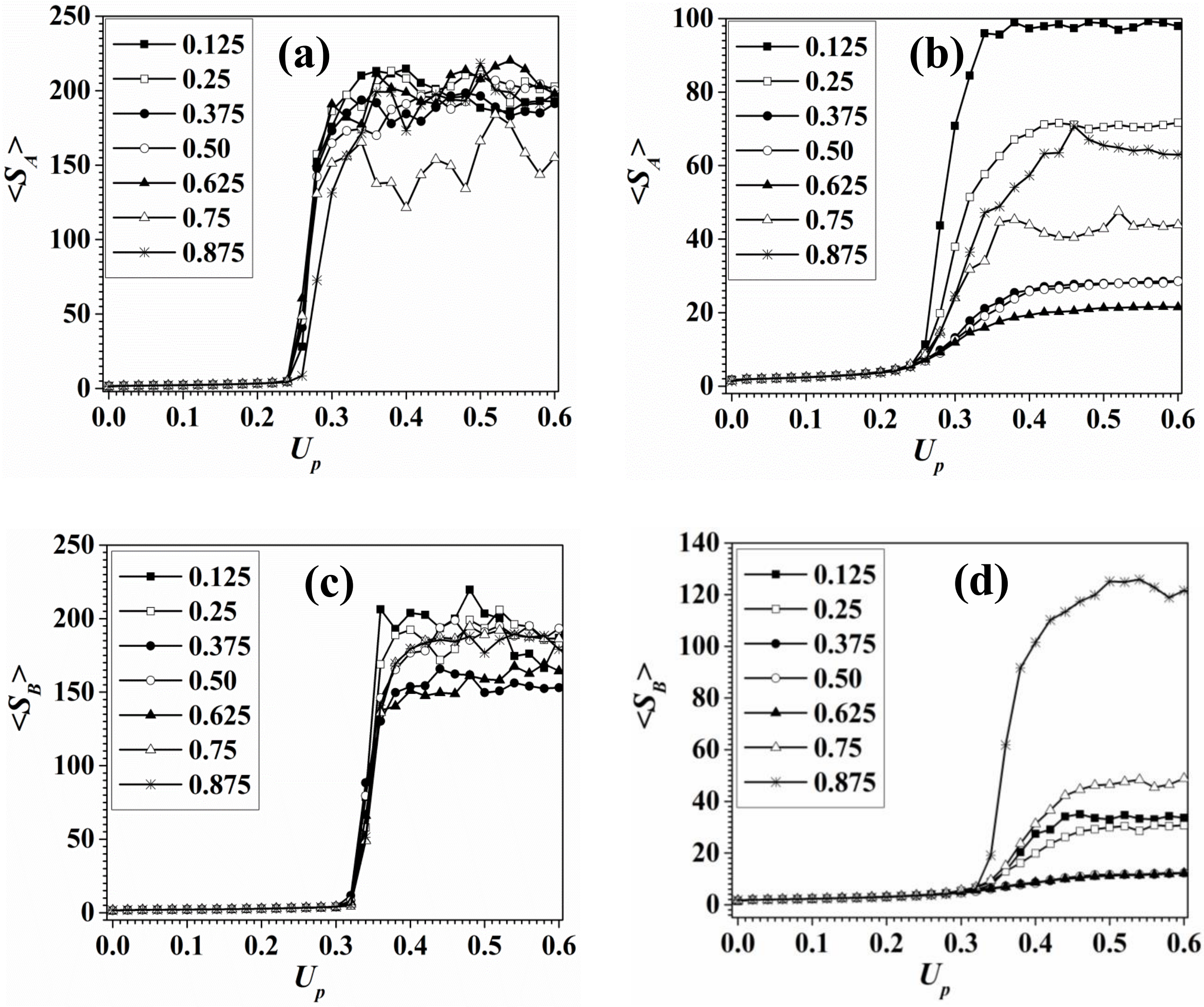


Figure S8. Change in average lamellar thickness with U_p for A- and B-polymers: (a) $\langle l_A \rangle$ vs. U_p at λ = 1, (b) $\langle l_A \rangle$ vs. U_p at λ = 6, (c) $\langle l_B \rangle$ vs. U_p at λ = 1, (d) $\langle l_B \rangle$ vs. U_p at λ = 6.

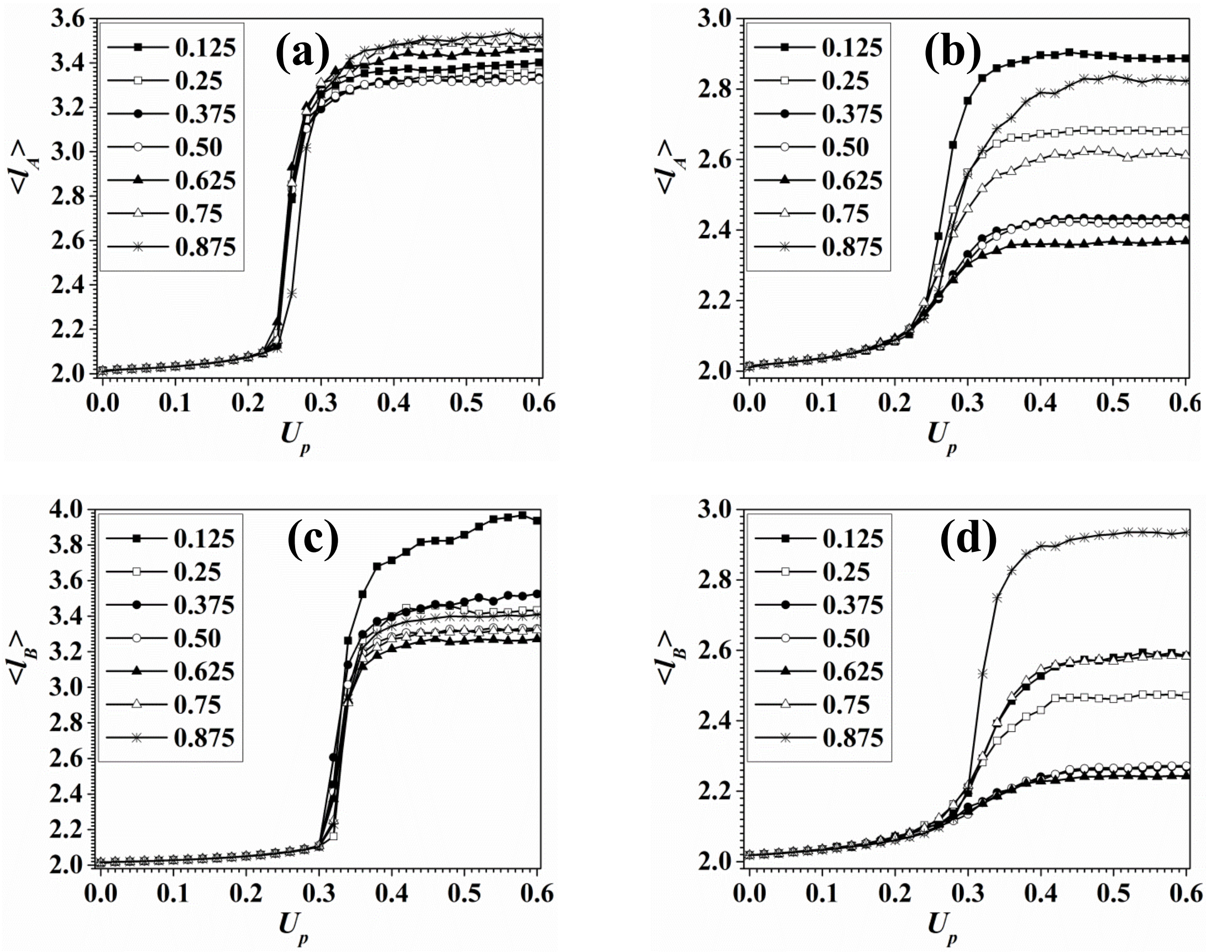


Figure S9. Change in isothermal overall crystallinity with number of Monte Carlo steps (*MCS*) at (a) λ = 1 and (b) λ = 6.

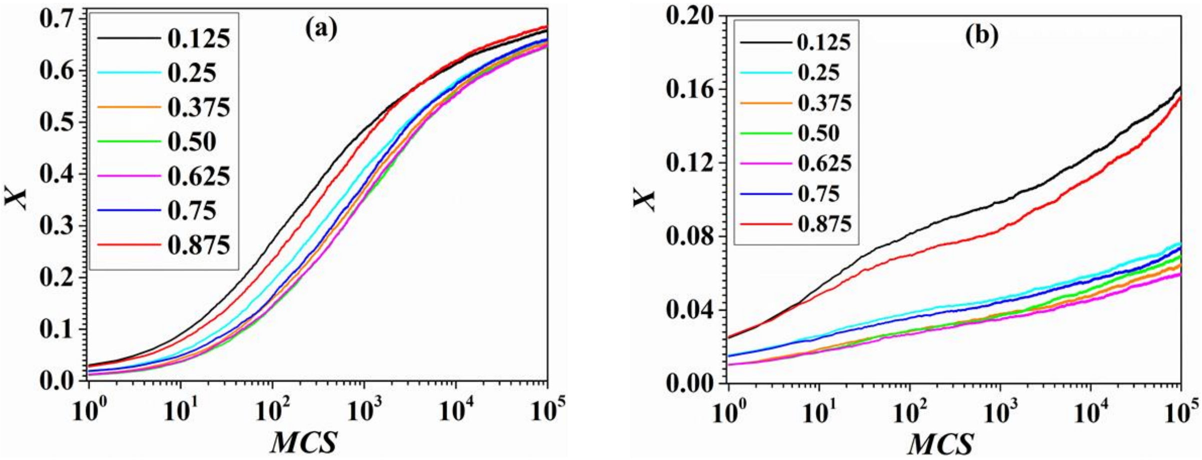


Table S1. Comparison in saturated crystallinity of A-polymer, X_A, B-polymer, X_B, with composition, x_B, during one-step isothermal crystallization, at λ = 1 and 6.

	Weak segregation, λ = 1		**Strong segregation, λ = 6**	
Composition (x_B)	X_A	X_B	X_A	X_B
0.125	**0.683**	**0.632**	**0.175**	**0.053**
0.25	**0.664**	**0.639**	**0.085**	**0.048**
0.375	**0.660**	**0.639**	**0.070**	**0.054**
0.5	**0.653**	**0.641**	**0.072**	**0.066**
0.625	**0.645**	**0.648**	**0.051**	**0.064**
0.75	**0.645**	**0.663**	**0.051**	**0.080**
0.875	**0.641**	**0.690**	**0.067**	**0.167**

Table S2. Comparison in average lamellar thickness of A-polymer, $\langle l_A \rangle$, with composition, x_B, during one- and two-step isothermal crystallization, at λ = 1.

	Two-step cooling		One-step cooling
Composition (x_B)	U_p **= 0.28**	U_p **= 0.6**	U_p **= 0.6**
0.125	**3.47**	**3.51**	**2.7**
0.25	**3.46**	**3.46**	**2.67**
0.375	**3.39**	**3.44**	**2.68**
0.5	**3.43**	**3.47**	**2.74**
0.625	**3.45**	**3.47**	**2.73**
0.75	**3.53**	**3.63**	**2.81**
0.875	**3.61**	**3.72**	**2.95**

Table S3. Comparison in average lamellar thickness of B-polymer, $\langle l_B \rangle$, with composition, x_B, during one- and two-step isothermal crystallization, at λ = 1.

	Two-step cooling	One-step cooling
Composition (x_B)	U_p **= 0.6**	U_p **= 0.6**
0.125	**3.00**	**3.01**
0.25	**2.83**	**2.85**
0.375	**2.79**	**2.79**
0.5	**2.78**	**2.74**
0.625	**2.77**	**2.74**
0.75	**2.78**	**2.75**
0.875	**2.86**	**2.80**

Table S4. Comparison in saturated crystallinity of A-polymer, X_A, with composition, x_B, during one- and two-step isothermal crystallization, at λ = 6.

	Two-step cooling		One-step cooling
Composition (x_B)	U_p **= 0.28**	U_p **= 0.6**	U_p **= 0.6**
0.125	**0.623**	**0.668**	**0.175**
0.25	**0.397**	**0.473**	**0.085**
0.375	**0.294**	**0.335**	**0.070**
0.5	**0.384**	**0.426**	**0.072**
0.625	**0.358**	**0.422**	**0.051**
0.75	**0.276**	**0.329**	**0.051**
0.875	**0.429**	**0.523**	**0.067**

Table S5. Comparison in saturated crystallinity of B-polymer, X_B, with composition, x_B, during one- and two-step isothermal crystallization, at λ = 6.

	Two-step cooling		One-step cooling
Composition (x_B)	U_p **= 0.28**	U_p **= 0.6**	U_p **= 0.6**
0.125	**0.126**	**0.342**	**0.053**
0.25	**0.144**	**0.243**	**0.048**
0.375	**0.145**	**0.180**	**0.054**
0.5	**0.151**	**0.250**	**0.066**
0.625	**0.143**	**0.259**	**0.064**
0.75	**0.150**	**0.246**	**0.051**
0.875	**0.137**	**0.523**	**0.167**