Electronic Supplementary Information

Utilizing 3-methyl-1-butene co-units to tailor phase transition behavior in butene-1 copolymers

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The below Figure S1 showed the ^{13}C NMR spectra of butene-1/3-methyl-1-butene random copolymers studied in this work. The quantitative concentration of co-units in copolymer was determined by the following equation:

$$\text{3M1B co - unit concentration} = \frac{\frac{1}{2}I_{18.30-18.92\text{ppm}}}{\frac{1}{3}(I_{39.53-40.20\text{ppm}} + I_{34.06-34.68\text{ppm}} + I_{26.58-}$$

in which $I_{39.53-40.20\text{ppm}}$, $I_{34.06-34.68\text{ppm}}$ and $I_{26.58-27.34\text{ppm}}$ are the integrated peaks of 1, 2 and 3 carbon of butene-1, respectively, and $I_{18.30-18.92\text{ppm}}$ is the integrated peaks of 5 carbon of 3M1B. [1]

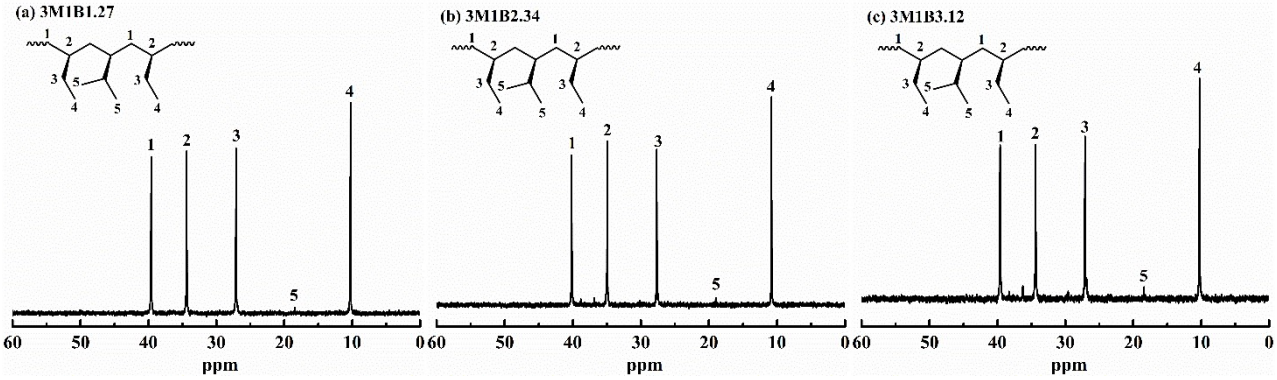

Figure S1. ^{13}C NMR spectra of butene-1/3-methyl-1-butene random copolymers with (a) 1.27 mol%, (b) 2.34 mol%, and (c) 3.12 mol% co-units

The below Figure S2 showed the FTIR data fitting to obtain the characteristic peaks located at 925 and 905 cm^{-1} for form I and II, respectively. During aging, the fraction of transformed form I in the total crystallites was estimated with the following equation [2]:

$$X_I = \frac{A_{925}}{A_{925} + A_{905}}$$

where A_{925} and A_{905} are the characteristic peak areas of form I and form II, respectively.

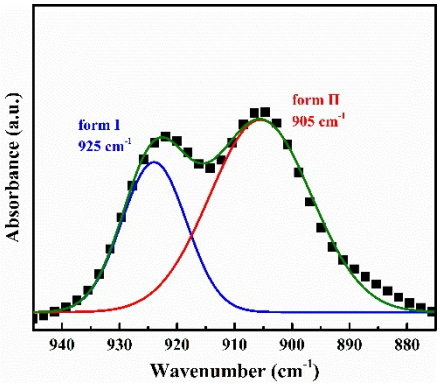

Figure S2. The peak fitting of FTIR spectrum during phase transition.

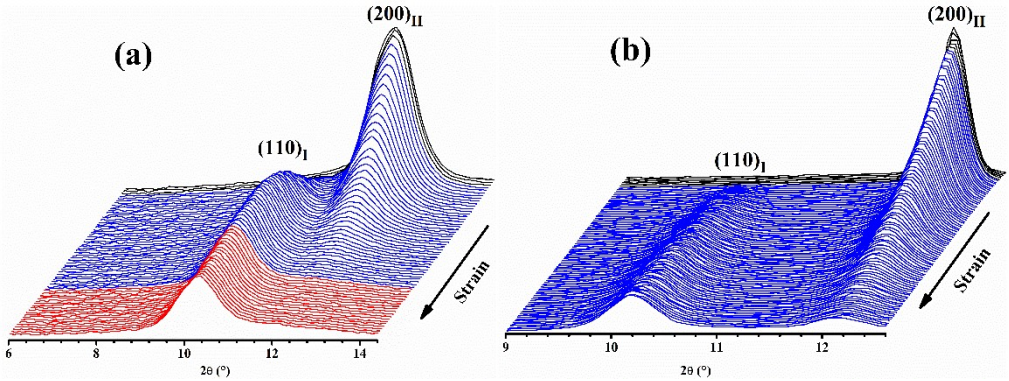

Figure S3. The integrated 1D diffraction intensity profiles of (a) PB and (b) 3M1B2.34. The blue lines represent the process of II-I phase transition and the red ones represent the stretching period after phase transition in PB. The stretching direction was horizontal.

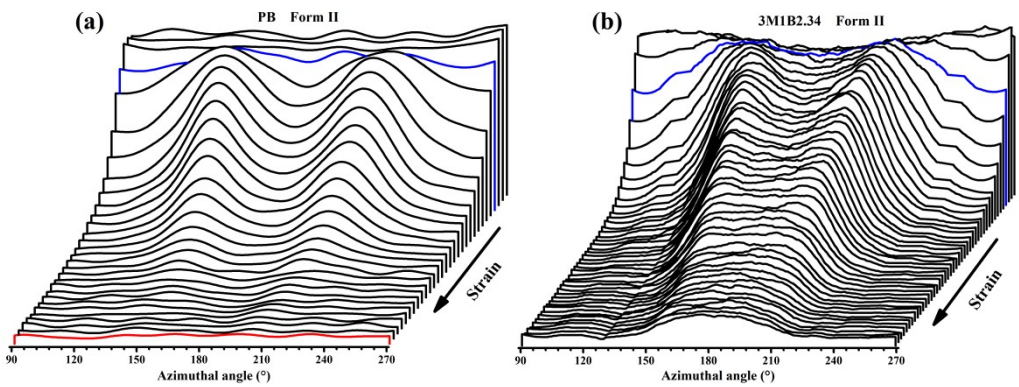

Figure S4. Evolution of intensity azimuthal scans of the form II $(200)_{II}$ plane of (a) PB and (b) 3M1B2.34. The blue and red lines represent the start and end of phase transition, respectively.

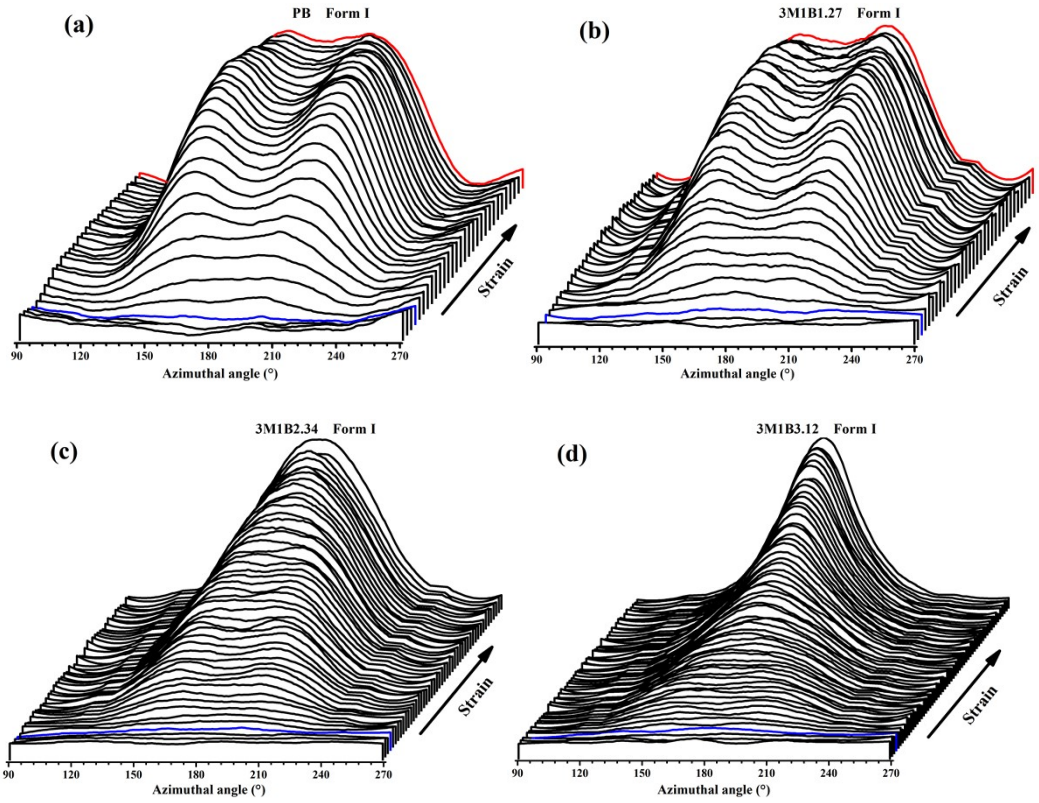

Figure S5. Evolution of intensity azimuthal scans of the form I $(110)_I$ plane of (a) PB, (b) 3M1B1.27, (c) 3M1B2.34 and (d) 3M1B3.12. The blue and red lines represent the start and end of phase transition, respectively.

References

[1] Stefanie D, Walter K. Copolymerization of Ethylene and Propylene with the Sterically Hindered Monomer 3-Methyl-1-butene by Homogeneous Catalysis[J]. Macromolecules, 2007, 40: 4130-4137.

[2] Zhong Z, Ge H, Su Z. Direct Formation of Form I' Crystals in Polybutene-1/Polypropylene Blend Enhanced by Cold Crystallization[J]. Polymer, 2018, 156: 30-38.