

Deviation of Phase Transition Process in Surface-tethered Thermotropic Liquid Crystalline Polymer Nanocomposites with Graphene Oxide: A Spectroscopic Study

Ying Jing, Hui Tang* and Peiyi Wu*

1. TGA result of GO-PMPCS composite

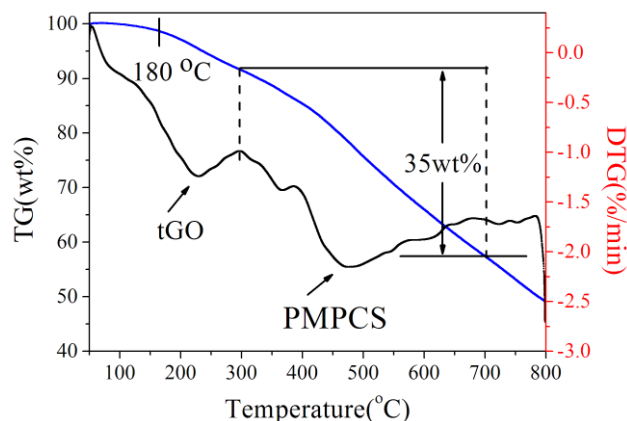


Fig. S1. TGA result of GO-PMPCS composite

2. 2D correlation analysis of PMPCS/GO-PMPCS system in 100~140 °C

Table S1. Symbols of the cross-peaks in synchronous and asynchronous spectra of the three representative spectral regions of PMPCS/GO-PMPCS system in 100~140 °C

| Cross-peak | Variation order | Cross-peak | Variation order |
|-----------------------------|-----------------|-----------------|-----------------|
| 2958/2910(+,-) ^a | 2910→2958 | 2910/2875 (+,+) | 2910→2875 |
| 3004/2910(+,+) | 3004→2910 | 2958/2875 (+,+) | 2958→2875 |
| 3032/2910(-,-) | 3032→2910 | 3080/2875 (+,+) | 3080→2875 |
| 3080/2910(+,+) | 3080→2910 | 2935/2875 (+,0) | 2935,2875 |
| 3004/2958(+,+) | 3004→2958 | 2935/2835 (+,-) | 2835→2935 |
| 3032/2958(-,-) | 3032→2958 | 2958/2935 (+,+) | 2958→2935 |
| 3080/2958(+,+) | 3080→2958 | 2935/2910 (+,-) | 2910→2935 |
| 3004/2875(+,+) | 3004→2875 | 3080/3032(-,+) | 3032→3080 |
| 3032/2875(-,-) | 3032→2875 | 3080/3004(+,0) | 3080,3004 |
| 2910/1508(+,-) | 1508→2910 | 2910/1498(-,+) | 1498→2910 |
| 2958/1508(+,-) | 1508→2958 | 3004/1498(-,+) | 1498→3004 |
| 3032/1508(-,+) | 1508→3032 | 3032/1498(+,+) | 3032→1498 |
| 1732/1508(+,-) | 1508→1732 | 2958/1732(+,-) | 1732→2958 |
| 1732/1498(-,+) | 1498→1732 | 2935/1732(+,-) | 1732→2935 |
| 2910/1732(+,-) | 1732→2910 | 3004/1732(+,+) | 3004→1732 |

^a The first symbol in the brackets represented symbol in synchronous spectrum, and the second symbol in the brackets represented symbol in asynchronous spectrum

^b “→” meant “prior to” and “,” meant “simultaneously”

3. 2D correlation analysis of pure PMPCS system in 100~140 °C

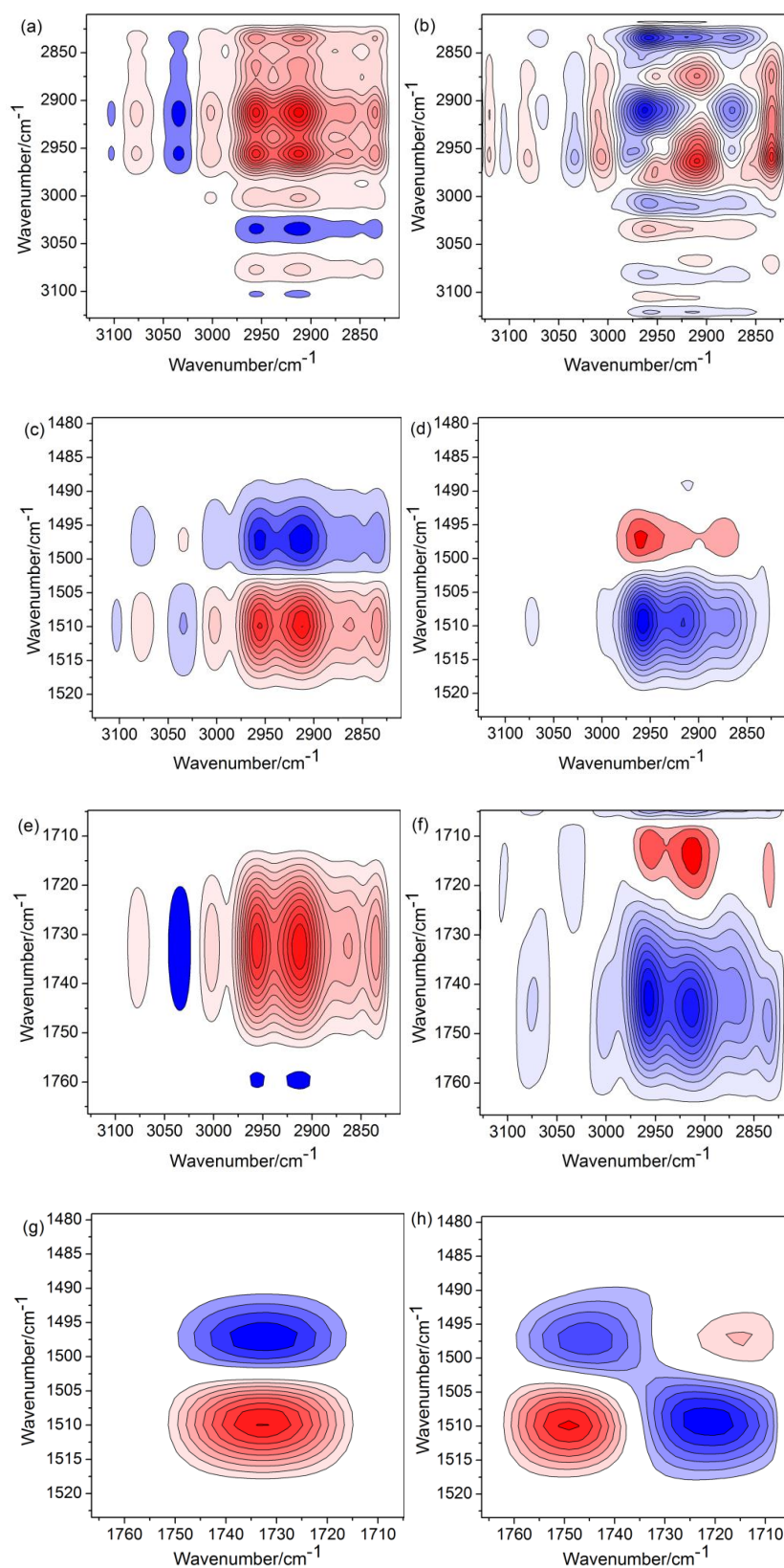


Fig. S2. 2D synchronous spectra of (a) C-H stretching vibration region 3127-2811 cm⁻¹; (c) C-H stretching vibration region 3127-2811 cm⁻¹ with skeleton vibration of aromatic ring II 1540-1474 cm⁻¹; (e) C-H stretching vibration region 3127-2811 cm⁻¹ and carbonyl stretching vibration of

1766-1706 cm^{-1} ; (g) carbonyl stretching vibration of 1766-1706 cm^{-1} and skeleton vibration of aromatic ring II 1540-1474 cm^{-1} and 2D asynchronous spectra of (b) C-H stretching vibration region 3127-2811 cm^{-1} ; (d) C-H stretching vibration region 3127-2811 cm^{-1} with skeleton vibration of aromatic ring II 1540-1474 cm^{-1} ; (f) C-H stretching vibration region 3127-2811 cm^{-1} and carbonyl stretching vibration of 1766-1706 cm^{-1} ; (h) carbonyl stretching vibration of 1766-1706 cm^{-1} and skeleton vibration of aromatic ring II 1540-1474 cm^{-1} .

Table S2. Symbols of the cross-peaks in synchronous and asynchronous spectra of the three representative spectral regions of pure PMPCS system in 100~140 °C

| Cross-peak | Variation order | Cross-peak | Variation order |
|------------------------------|------------------------|-----------------|-----------------|
| 2910/1508 (+,-) ^a | 1508→2910 ^b | 2910/1732(+,-) | 1732→2910 |
| 3004/1508(+,-) | 1508→3004 | 3004/1732(+,-) | 1732→3004 |
| 3080/1508 (+,-) | 1508→3080 | 3080/1732(+,-) | 1732→3080 |
| 1732/1508(+,-) | 1508→1732 | 3032/2910 (-,-) | 3032→2910 |
| 3004/2910(+,+) | 3004→2910 | 3080/2910 (+,+) | 3080→2910 |
| 3080/3004(+,0) | 3004,3080 | 3032/3004(-,-) | 3032→3004 |
| 3032/1508 (-,+) | 1508→3032 | 3032/1732(-,+) | 1732→3032 |

^a The first symbol in the brackets represented symbol in synchronous spectrum, and the second symbol in the brackets represented symbol in asynchronous spectrum

^b “→” meant “prior to” and “,” meant “simultaneously”

4. 2D correlation analysis of PMPCS/GO-PMPCS system in 140~180 °C

Table S3. Symbols of the cross-peaks in synchronous and asynchronous spectra of the three representative spectral regions of PMPCS/GO-PMPCS system in 140~180 °C

| Cross-peak | Variation order | Cross-peak | Variation order |
|----------------|-----------------|----------------|-----------------|
| 3004/2958(+,-) | 2958→3004 | 3080/2875(+,-) | 2875→3080 |
| 3004/2910(+,-) | 2910→3004 | 2910/2875(+,-) | 2875→2910 |
| 3004/2875(+,-) | 2875→3004 | 2958/2875(+,-) | 2875→2958 |
| 3080/2958(+,-) | 2958→3080 | 3080/3004(+,0) | 3080,3004 |
| 3080/2910(+,-) | 2910→3080 | 2910/1508(+,+) | 2910→1508 |
| 2958/2910(+,+) | 2958→2910 | 2958/1508(+,+) | 2958→1508 |
| 3004/1508(+,+) | 3004→1508 | 3080/1508(+,+) | 3080→1508 |
| 2910/1732(+,+) | 2910→1732 | 2958/1732(+,+) | 2958→1732 |
| 3004/1732(+,+) | 3004→1732 | 3080/1732(+,+) | 3080→1732 |

^a The first symbol in the brackets represented symbol in synchronous spectrum, and the second symbol in the brackets represented symbol in asynchronous spectrum

^b “→” meant “prior to” and “,” meant “simultaneously”

5. 2D correlation analysis of pure PMPCS system in 140~180 °C

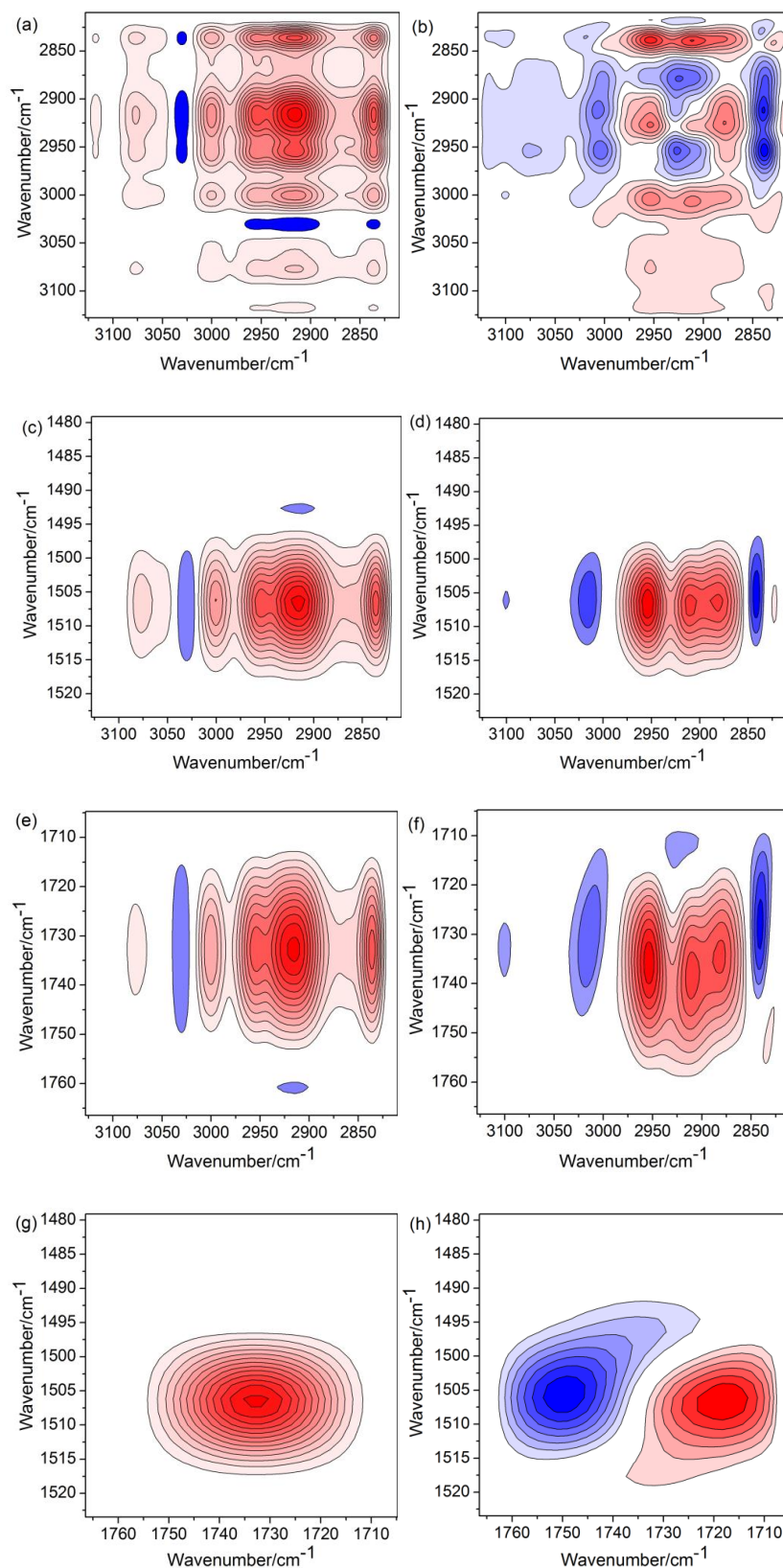


Fig. S3. 2D synchronous spectra of (a) C-H stretching vibration region 3127-2811 cm⁻¹; (c) C-H stretching vibration region 3127-2811 cm⁻¹ with skeleton vibration of aromatic ring II 1540-1474 cm⁻¹; (e) C-H stretching vibration region 3127-2811 cm⁻¹ and carbonyl stretching vibration of 1766-1706 cm⁻¹; (g) carbonyl stretching vibration of 1766-1706 cm⁻¹ and skeleton vibration of

aromatic ring II 1540-1474 cm^{-1} and asynchronous spectra of (b) C-H stretching vibration region 3127-2811 cm^{-1} ; (d) C-H stretching vibration region 3127-2811 cm^{-1} with skeleton vibration of aromatic ring II 1540-1474 cm^{-1} ; (f) C-H stretching vibration region 3127-2811 cm^{-1} and carbonyl stretching vibration of 1766-1706 cm^{-1} ; (h) carbonyl stretching vibration of 1766-1706 cm^{-1} and skeleton vibration of aromatic ring II 1540-1474 cm^{-1} .

Table S4. Symbols of the cross-peaks in synchronous and asynchronous spectra of the three representative spectral regions of pure PMPCS system in 140~180 °C

| Cross-peak | Variation order | Cross-peak | Variation order |
|----------------|-----------------|-----------------|-----------------|
| 2910/2835(+,+) | 2910→2835 | 3080/2835 (+,0) | 3080,2835 |
| 3004/2910(+,-) | 2910→3004 | 2925/2835 (+,+) | 2925→2835 |
| 3080/2910(+,-) | 2910→3080 | 2925/2910 (+,-) | 2910→2925 |
| 3080/3004(+,0) | 3080,3004 | 3080/2925 (+,-) | 2925→3080 |
| 2835/1508(+,-) | 1508→2835 | 3004/2925 (+,-) | 2925→3004 |
| 2910/1508(+,+) | 2910→1508 | 2835/1732 (+,-) | 1732→2835 |
| 3004/1508(+,-) | 1508→3004 | 2910/1732 (+,+) | 2910→1732 |
| 3080/1508(+,-) | 1508→3004 | 3004/1732 (+,-) | 1732→3004 |
| 2925/1508(+,+) | 2925→1508 | 3080/1732 (+,-) | 1732→3080 |
| 2925/1732(+,+) | 2925→1732 | 1732/1508 (+,+) | 1732→1508 |

^a The first symbol in the brackets represented symbol in synchronous spectrum, and the second symbol in the brackets represented symbol in asynchronous spectrum

^b “→” meant “prior to” and “,” meant “simultaneously”