

Supplemental Material

Dependence of Charge Carrier Transport on Molecular Relaxations in Glassy Poly(3-hexylthiophene-2,5-diyl) (P3HT)

Zhaojing Gao, Manuel Reali, Arthur Yelon* and Clara Santato*

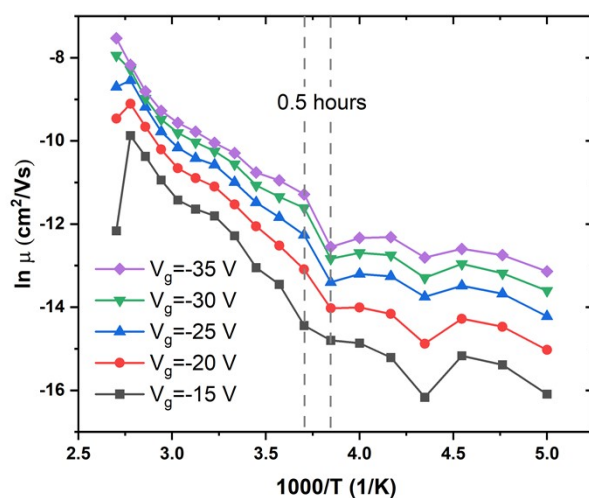


Figure S1. Dependence of μ on T under different V_g in medium MW RR P3HT. MW=30-50 kDa, $V_d=-15$ V, $T=200-370$ K. High T measurements were performed immediately after low T measurements.

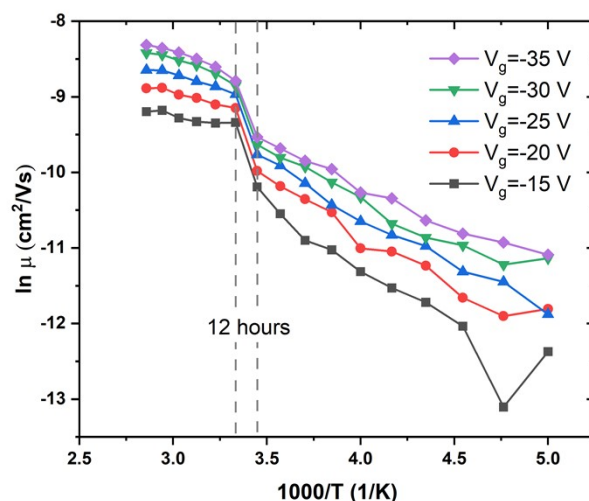


Figure S2. Dependence of μ on T under different V_g in medium MW RR P3HT. MW=30-50 kDa, $V_d=-15$ V, $T=200-350$ K. High T measurements were performed 12 hours later than low T measurements, during which the device was left at room temperature in a vacuum probe station.

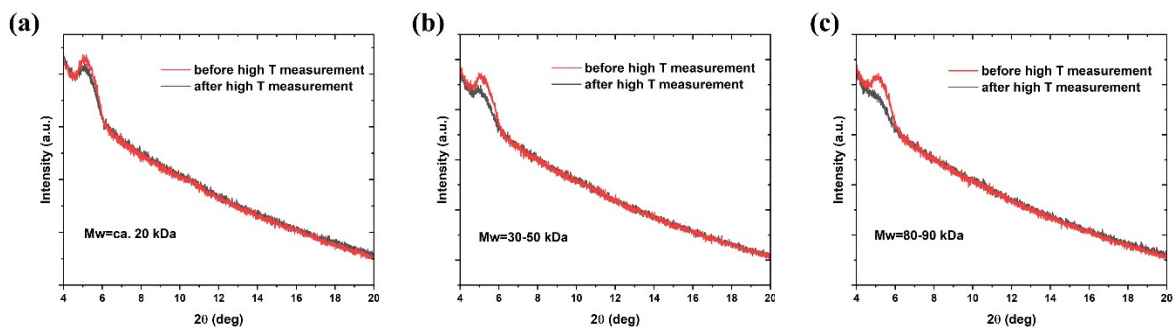


Figure S3. X-ray diffraction (XRD) patterns of three MW RR P3HT before and after the high T measurement.

Figure S3 shows the X-ray diffraction (XRD) spectra of the P3HT films (a) before and (b) after the high temperature measurement. We observe the same (100) diffraction peak at $2\theta=5.1^\circ$, which is the typical signal of the lamellar structure of P3HT.^{1, 2} The peaks of the P3HT film after the high temperature measurement are weaker, which signifies a more amorphous thin film after the glass transition.

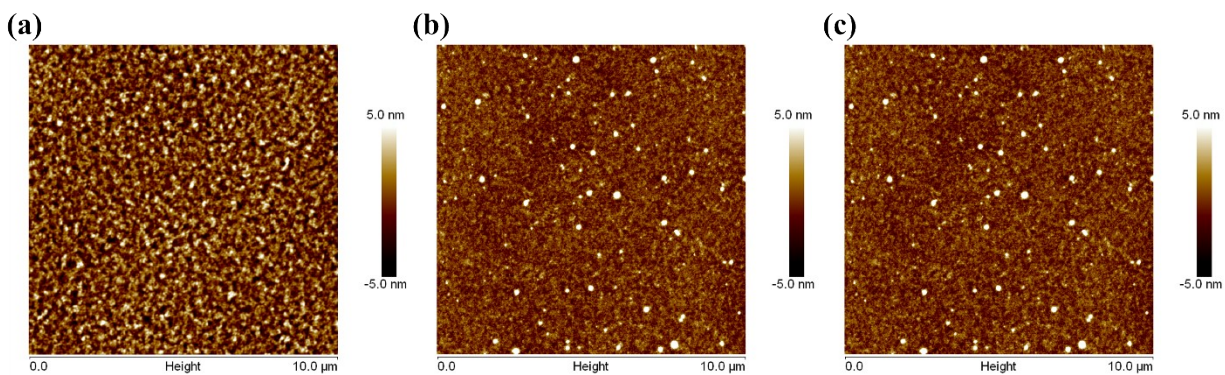


Figure S4. $10\ \mu\text{m}\times 10\ \mu\text{m}$ atomic force microscopy (AFM) images of (a) low, (b) medium, and (c) high MW P3HT.

Figure S4 shows the AFM images of (a) low MW P3HT, (b) medium MW P3HT, (c) high MW P3HT. The value of the root mean square roughness (rms) is $1.6\pm 0.1\ \text{nm}$ for low MW, $5.3\pm 0.6\ \text{nm}$ for medium MW and $13.8\pm 1.8\ \text{nm}$ for high MW. Lower MW polymers are expected to exhibit better solubility, resulting in films with a lower surface roughness.

References

1. Ballantyne, A. M.; Chen, L.; Dane, J.; Hammant, T.; Braun, F. M.; Heeney, M.; Duffy, W.; McCulloch, I.; Bradley, D. D.; Nelson, J., The effect of poly (3-hexylthiophene) molecular weight on charge transport and the performance of polymer: fullerene solar cells. *Advanced Functional Materials* **2008**, *18* (16), 2373-2380.
2. Sirringhaus, H.; Brown, P.; Friend, R.; Nielsen, M. M.; Bechgaard, K.; Langeveld-Voss, B.; Spiering, A.; Janssen, R. A.; Meijer, E.; Herwig, P., Two-dimensional charge transport in self-organized, high-mobility conjugated polymers. *Nature* **1999**, *401* (6754), 685-688.