Characterization of the microstructure of spin-coated and blade coated all-polymer solar cells

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Abstracts

All-polymer solar cells have active layers based on blends of two semiconducting polymers.[1] With a view to commercialisation, all-polymer solar cells have a number of potential advantages over other organic PV technologies including improved morphological stability.[2] The fact that two polymers are blended together means that an all-polymer blend, as distinct to a blend based on a semiconducting donor polymer and small molecule acceptor, has a lower tendency to phase segregate due to the entanglement of polymer chains rendering them with a low physical mobility.[3,4] The blending of two polymers can be challenging to produce an optimum nanoscale morphology as required for the efficient operation of a bulk heterojunction solar cell.[4] As tightly bound excitons – which are the primary product of photoexcitation in organic semiconductors – can only diffuse around 10 nm or less before they recombine,[5] donor and acceptor materials must be intermixed such that there are donor/acceptor heterojunctions within 10 nm of exciton generation to ensure that excitons are dissociated into electron-hole pairs at the donor/acceptor interface before they recombine.[4] The long chains of semiconducting polymers means that there can be a tendency for all-polymer blends to phase separate into mesoscale domains (with domain size much larger than the exciton diffusion length) due to the reduced entropy of mixing of two polymers compared to a polymer and small molecule.[4] Furthermore, the extended nature of polymer chains means that polymer chains begin to interact earlier in the solution coating process potentially initiating phase separation earlier in the film drying process.

While active layer films in the laboratory are generally prepared via spin-coating, the commercial production of polymer solar cells will rely on in-line or roll-to-roll coating processes.[6] Due to the different kinetics of drying in a small spin-coating vs. a large area coating process, the morphologies produced via spin-coating may not be reproduced when device production is scaled up.[7] As a lab-based alternative to spin-coating, blade coating can enable the fabrication of test-size devices minimising material wastage for device optimisation, with drying kinetics comparable to roll-to-roll coating enabling.[8] Thus the efficiencies and morphologies realised in small area blade-coated cells can be more directly transferred to large area cells produced via commercially relevant processes. In this report the efficiency and morphology of all-polymer solar cells produced via spin-coating and via blade coating are directly compared. As shown in Table one, Six different all-polymer systems are compared, including 3 not previously reported (as shown in Figure 1). Microstructure is characterised using a combination of atomic force microscopy (AFM), transmission electron microscopy (TEM) and synchrotron-based grazing-incidence wide-angle X-ray scattering (GIWAXS). These three techniques provide a comprehensive overview of surface roughness and topography (AFM), bulk phase separation and morphology (TEM) and thin film crystallinity (GIWAXS).

Table 1 *Summary of film preparation conditions and surface roughness values for the six systems studied.*

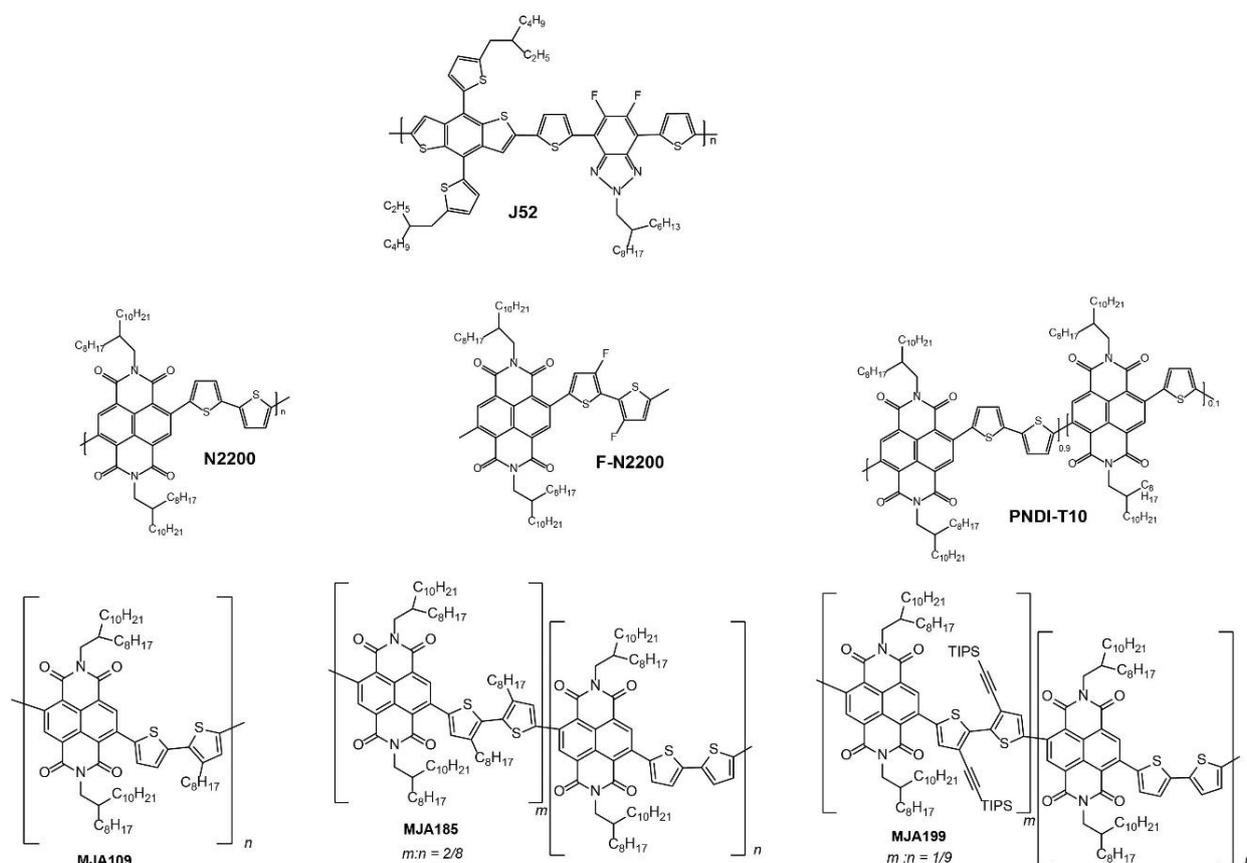| System	Weight ratio	Solvent	Spin-coated Rq (nm)	Blade-coated Rq (nm)
J52:N2200	1:1	Chlorobenzene	1.38	0.83
J52:F-N2200	1:1	Chlorobenzene	0.91	1.38
J52:PNDIT10	1:1	Chlorobenzene	2.29	1.11
J52:MJA109	1:1	Chlorobenzene	2.01	1.19
J52:MJA185	1:1	Chlorobenzene	4.04	1.40
J52:MJA199	1:1	Chlorobenzene	2.36	1.63

Figure 1 *Chemical structures of polymers studied.*

References

1.   McNeill, C. R.; Greenham, N. C., Conjugated-Polymer Blends for Optoelectronics. *Adv. Mater.* **2009,** 21, 3840 - 3850.

2.   Wang, G.; Melkonyan, F. S.; Facchetti, A.; Marks, T. J., All-Polymer Solar Cells: Recent Progress, Challenges, and Prospects. *Angewandte Chemie International Edition* **2019,** 58, 4129-4142.

3.   Kim, T.; Choi, J.; Kim, H. J.; Lee, W.; Kim, B. J., Comparative Study of Thermal Stability, Morphology, and Performance of All-Polymer, Fullerene–Polymer, and Ternary Blend Solar Cells Based on the Same Polymer Donor. *Macromolecules* **2017**, DOI: 10.1021/acs.macromol.7b00834.

4.   McNeill, C. R., Morphology of all-polymer solar cells. *Energy & Environ. Sci.* **2012,** 5, 5653-5567.

5.   Blom, P. W. M.; Mihailetchi, V. D.; Koster, L. J. A.; Markov, D. E., Device Physics of Polymer:Fullerene Bulk Heterojunction Solar Cells. *Adv. Mater.* **2007,** 19, 1551-1566.

6.   Krebs, F. C.; Tromholt, T.; Jørgensen, M., Upscaling of polymer solar cell fabrication using full roll-to-roll processing. *Nanoscale* **2010,** 2, 873-886.

7.   Ro, H. W.; Downing, J. M.; Engmann, S.; Herzing, A. A.; DeLongchamp, D. M.; Richter, L. J.; Mukherjee, S.; Ade, H.; Abdelsamie, M.; Jagadamma, L. K.; Amassian, A.; Liu, Y.; Yan, H., Morphology changes upon scaling a high-efficiency, solution-processed solar cell. *Energy & Environ. Sci.* **2016,** 9, 2835-2846.

8.   Krebs, F. C., Fabrication and processing of polymer solar cells: A review of printing and coating techniques. *Solar Energy Materials and Solar Cells* ***2009***, 93, 394-412.