Organic solar cells using imprinted P3HT nanostructures: The effects of geometry, crystallization and chain ordering

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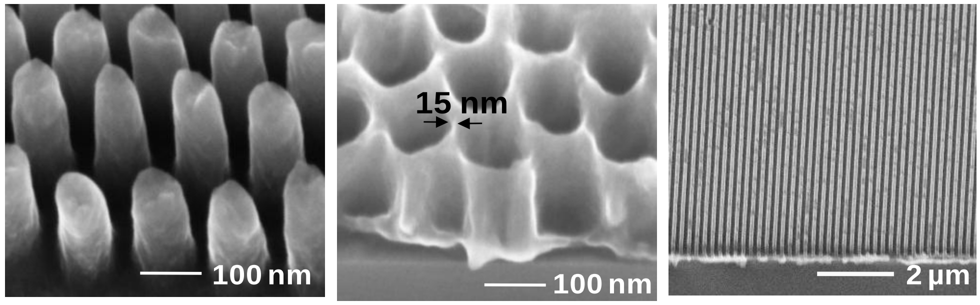
Significant progress in power conversion efficiency (PCE) of organic solar cells has been made with the introduction of donor-acceptor bulk heterojunction (BHJ) structures, e.g. polymer-fullerene blends. Control of nanoscale morphology of BHJ is the key to obtain high efficiency in charge dissociation and transport. However for popular polymer blend devices, the chemically defined morphology has fundamental limitations in achieving PCE higher than 5%. For example, the thermodynamically driven methods of spin-coating and phase segregation from a donor–acceptor mixture induced by thermal annealing lead to charge trapping at bottlenecks of distorted structures and cul-de-sacs in the conducting pathways to the electrodes. This architecture is also limited by low carrier mobility due to significant polymer chain disorder and poor light absorption due to the thin active layer (~100 nm) that results from such processing. Kim *et al* [1] and our previous work [2] have shown that nanoimprint lithography provides a unique method for precise control of the heterojunction morphology. By imprinting polymer nanostructures followed by deposition of electron transfer material on top, vertically interdigitized and bicontinuous heterojunction can be formed for efficient exciton dissociation and charge transport.

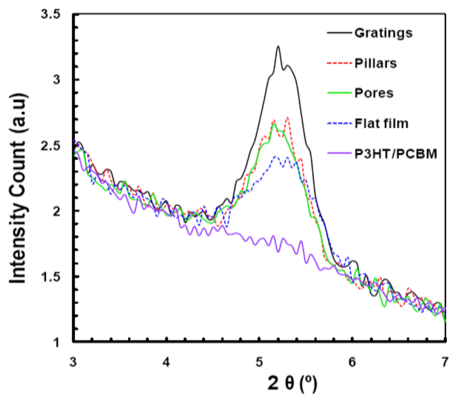
In this study, we further demonstrate that besides forming the interdigitized heterojunction morphology, the nanoimprint process also induces chain ordering and crystallization in polymer nanostructures, resulting in higher charge mobility and light absorption. By fabricating BHJ devices using imprinted poly(3-hexyl thiophene) (P3HT) nanostructures with various shapes, e.g. pillars, pores, gratings, as shown in Fig. 1, we investigate the effects of nanostructure geometry on chain ordering, crystallization, and device performance. Polymer chain ordering and crystallization originate from the polymer melt flow during pattern formation in thermal nanoimprint, which depend on the glass transition behavior of the P3HT (quite different from others), mold geometry and imprint conditions. The imprinted P3HT nanostructures were characterized with grazing incidence X-ray diffraction (GIXRD). Higher crystallinity and larger crystallite size are observed for imprinted P3HT nanostructures compared to non-imprinted films and P3HT and PCBM blend. In addition, the variation of nanoimprint-induced ordering and crystallinity and crystallite size is strongly correlated to the geometry of nanostructures as illustrated in Fig. 2. Organic solar cells were built using these nanoimprinted P3HT nanostructures as shown in Fig. 3. The preliminary I-V curves of BHJ devices indicate that the morphology geometry does affect device performance. We will present systematic study of the correlations among nanostructure geometry, polymer properties, imprint conditions, and device performance. We believe the fabrication technique and the fundamental studies are important for achieving high performance solar cells.

1. Kim, M.S. et al., *Appl. Phys. Lett.* 90, (2007).
2. Aryal, M et al., *J. Vac. Sci. Technol. B* 26(6), (2008).



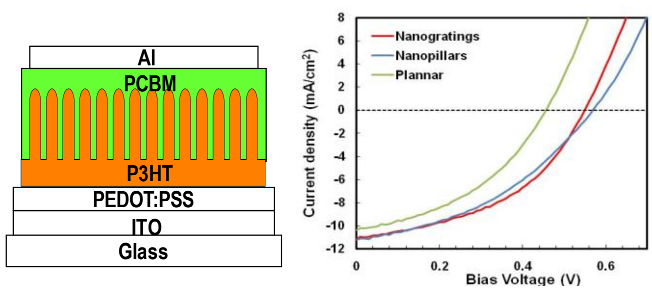
a) b) c)

Fig. 1: SEM of imprinted nanostructures in P3HT: a) 80 nm pillars; b) pores with 20 nm walls; and c) 100 nm line & space, 100 nm tall gratings.



Sample	HWFM(°) ($\Delta_{2\theta}$)	Crystallite size (nm)	Crystallinity (a.u)
Flat	0.532	14.9	6
Nanogratings	0.434	16.6	15
Nanopillars	0.447	17.8	10
Nanopores	0.487	16.3	9

Fig. 2: GIXRD results of imprinted polymer nanostructures. The table shows higher crystallinity and larger crystal size for imprinted structures as compared to blend or non-imprinted film. The crystallite size were calculated using $(L) = \frac{0.9\lambda}{\Delta_{2\theta}\cos\theta}$, where λ is the X-ray wavelength, $\Delta_{2\theta}$ is the half width full wave maximum (HWFM) and θ is the angle of incident.



Parameters	Planer	Nano-pillars	Nano-gratings
V_{oc} (V)	0.46	0.58	0.55
I_{sc} (mA/cm^2)	10.3	11.2	11.1
FF	0.40	0.39	0.45
Efficiency (η) %	1.96	2.55	2.75

a) b) c)

Fig. 3: a) Schematic of nanoimprinted organic solar cell, b) I-V characteristics of solar cells with nanopillars and nanogratings structures in comparison with planar heterojunction, and c) Summary of derived device parameters for nanoimprinted and planar devices.