Hole Mobility Enhancement by Chain Alignment in Imprinted P3HT Nanogratings for Organic Solar Cells

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Organic solar cells have received considerable attention mainly due to their low production cost. However, efficiency of organic solar cells is relatively lower than their inorganic counterparts, partially due to the poor charge carrier mobility in organic materials[1]. For instance, bulk hetero-junction (BHJ) solar cells typically have hole mobility on the order of 10^{-4} due to random chain configuration. Studies have shown improved charge carrier mobility can improve short circuit current by several folds [2]. Recently, we have shown nanoimprint lithography can improve chain ordering of the polymer (P3HT) in nanoscale confinement. A nano-grating mold of 65 nm in width, 200nm in pitch, and 200 nm in depth is used to define the polymer structures by imprinting at 50 bars and 170ºC for 10 minutes, and the SEM image for nano-gratings are shown in figure 1(a). Then, XRD is used to measure the chain orientation in the nanoimprinted structures. The XRD data proves these nano-gratings have an ordered three dimensional morphology with π-π stacking along grating direction (hopping distance (d_h) is 3.8Å), backbone alignment perpendicular to the grating direction (d_h = 16.8 Å) and polymer chains in the vertical direction (d_h = 3.8Å) [3].

We believe this ordered morphology (especially vertical d_h of 3.8Å) will give enhanced hole carrier mobility in solar cells. To measure this mobility, field effect transistors (FET) using the imprinted P3HT nano-gratings are fabricated with top contact and bottom gate configuration as shown in figure 1(b). Electrical characterizations were performed using a cascade probing station at room temperature (298K) and ambient condition (atmospheric pressure). I_d-V_d curves are shown in figure 2. The mobility values are extracted according to equation: $\frac{\partial I_d}{\partial V_g} = \mu_{FE} W c_i V_d / L$, where W, L and C_i are the channel width, channel length and gate capacitance respectively [4]. The calculated mobility values are shown in table 1. These nano-grating P3HT FETs exhibit highly anisotropic conductance behaviors. Hole carrier mobility parallel to the nano-grating direction is over 150 times as much as the perpendicular direction. The mobility of thin film P3HT FETs (5×10^{-4} cm^2/Vs) is higher than the perpendicular direction (5×10^{-5} cm^2/Vs) but much lower than the parallel direction (3×10^{-2} cm^2/Vs) of the nano-grating FETs. A higher mobility value along the grating direction can be achieved through optimizing nanoimprint quality, minimizing oxygen and water exposure, and annealing treatment. These results clearly demonstrated that nanoimprint lithography is an effective method to increase the hole carrier mobility in P3HT, showing high potential in enhancing power conversion efficiency of organic solar cells.

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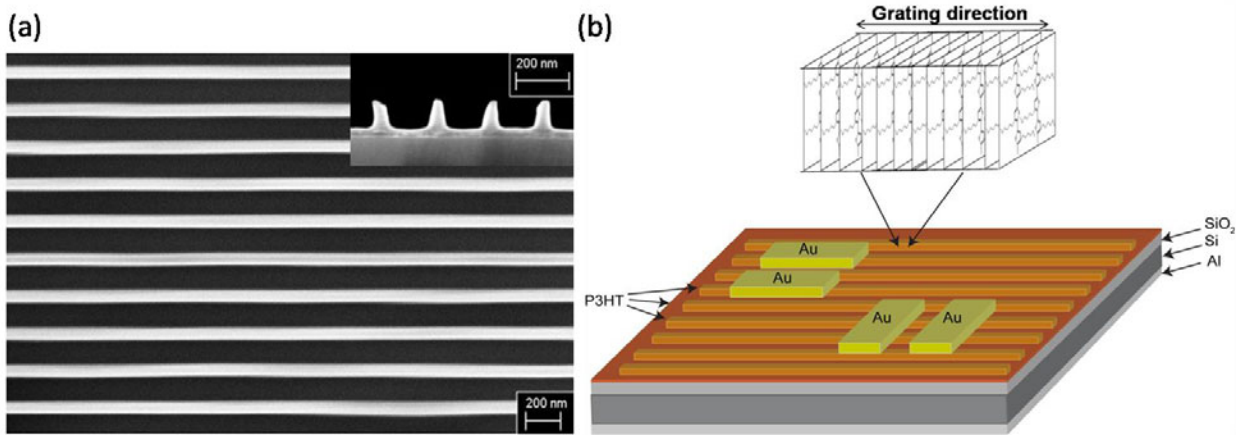

Figure 1: (a) SEM image of P3HT nano-gratings made by nanoimprint lithography. The grating has 20 nm residual layer and 150-170 nm grating height. (b) Schematic of the nano-grating field effect transistor with source and drain along perpendicular and parallel to the nano-gratings.

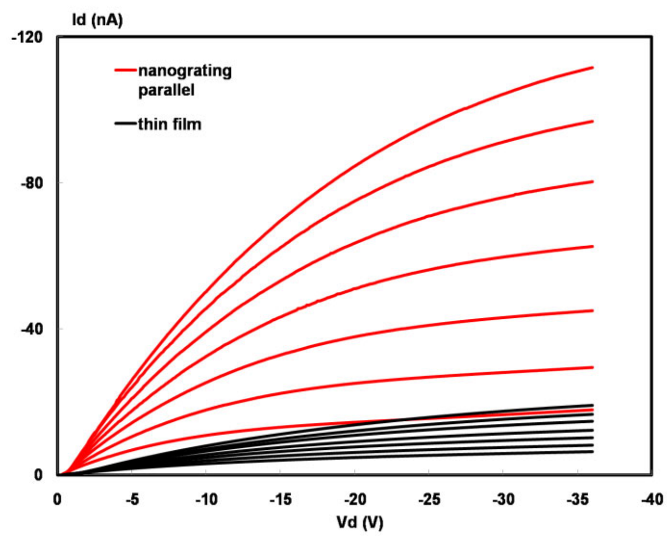

Figure 2: I_{DS} vs V_{DS} characteristics of nano-grating FETs (in red) and thin film FET (in black) with effective channel length of 30 μm, showing the accumulation mode operation when different negative gate bias applied.

(100μm)	Parallel	Perpendicular	Thin Film
Mobility (cm^2/Vs)	3.04×10^{-2} +/- 3×10^{-3}	5.48×10^{-5} +/- 5×10^{-6}	5.62×10^{-4} +/- 5×10^{-5}

Table1: Hole mobility data for nano-grating parallel, perpendicular and thin film transistors