

Optimization of ZnO Nanorod Array Morphology and Chemistry for Polymer Hybrid Photovoltaic Devices

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Aligned ZnO nanorod arrays (NRAs) grown from aqueous precursors with subsequent infiltration of poly(3-hexylthiophene) (P3HT) represent a promising method to fabricate inexpensive, high surface area hybrid photovoltaic (PV) devices. Control of the ZnO NRA morphology and surface defects may improve exciton transport within the polymer, charge separation at the polymer-oxide interface, and carrier transport through both polymer and oxide, which in turn would enhance the efficiency of such nanostructured photovoltaic devices. Here, we systematically vary NRA alignment, nanorod diameter, and spacing between nanorods by controlling seeding and growth conditions. The resulting NRAs are characterized using scanning electron microscopy, x-ray diffraction, atomic force microscopy, surface area measurement, and UV-vis spectroscopy. After P3HT is infiltrated in the NRAs, the response and efficiency of ZnO-P3HT PV devices are correlated with the NRA characteristics. By increasing the thickness of a sol-gel seed layer, the degree of alignment of the resulting ZnO NRA changes from disordered to ordered, as demonstrated by XRD and SEM. The degree of NRA alignment affects both the infiltration and crystallinity of the P3HT, leading to competing effects on the performance of the PV devices. We adjust the inter-rod spacing in highly aligned NRA by changing the pH of the growth solution, and find a strong relationship between the amount of polymer infiltrated between rods and the performance of the PV device. Finally, we examine the effect of Mg doping on the conduction band position in the oxide and, consequently, the open circuit voltage of the PV device. By adding a magnesium precursor in the growth solution, highly aligned $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ arrays are synthesized. The amount of Mg doping is measured by UV-vis spectroscopy and x-ray diffraction, and the effect of Mg doping on NRA work function is determined by Kelvin probe measurement. Changes in the PV device performance as a function of Mg doping will be presented. Possible strategy for further improvements in the PV device efficiency will also be discussed.