MONTE CARLO SIMULATION OF POLYMER SOLAR CELLS

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ABSTRACT

Monte Carlo method was successfully employed to study the mechanism inside a three dimensional bulk hetero-junction polymer solar cell using a model based on a novel architecture of adjustable structural parameters. The amorphous properties of the conjugated polymers were modelled to determine the operating conditions and structural properties and dimensions that maximize current generation efficiency. The dimensions of the best morphology of a polymer solar cell in terms of the charge carrier collection efficiency by the electrodes were found. The effect of applied external voltage, internal structural design and the simulated performance of polymer solar cell fabrication materials, MDMO-PPV:PCBM, M3EH-PPV:PCBM and P3HT:PCBM on efficiency were obtained. For polymer solar cells with practical dimensions, the charge carrier collection efficiency was almost governed by the strength of the applied electric field. For strong electric field, charge carrier efficiency in the range of 10%-20% was achieved. Reduction of the interfacial height from 30*nm* to 10*nm* resulted in a drop of almost 13% in the charge carrier generation efficiencies. The impact of the valance and conduction band energies of the three hole transporting materials on the charge carrier collection efficiencies was significant.

KEY WORDS: Monte Carlo simulation, polymer solar cell, excitons, morphology, charge carrier collection efficiency, applied external voltage, fabrication materials.