Optimization and Characterization of Organic Solar Cells based on regio-P3HT and C_{60}-PCBM Blends

By

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APPROVAL

This dissertation of Mr. Given Kalonga is approved as fulfilling part of the requirements for the award of the degree of Master of Science in Physics by the University of Zambia.

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I, Given Kalonga, declare that no portion of this work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institution of learning.

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ABSTRACT

Bulk Hetero-Junction - (BHJ) - Organic photovoltaic (OPV) cells based on the conjugated polymer poly (3-hexylthiophene-2, 5- diyl) (region-P3HT) also referred to as P3HT and a fullerene derivative [6, 6] Phenyl-C61-butyric acid methyl ester (C60-PCBM) also referred to as PCBM. The optimization, realization and characterization of these cells were done on both glass and aluminium substrates. The aluminium provided a flexible substrate for the cells whilst the glass provided a rigid substrate and acted as a control. The thin films for the solar cells were deposited by means of the spin coating method.

The integrity of the starting materials were evaluated using Fourier Transform infra-red (FTIR) and x-ray diffraction (XRD) spectroscopy whilst the particle size and distribution, were examined using XRD spectroscopy and transmission electron microscopy (TEM). The electrical characterization was done using a 4-point probe and gas sensing methods. The morphology and roughness of the local composition of TiO_2 thin films before and after annealing were evaluation by means of atomic force microscopy (AFM).

The study eventually evaluated the effects of blend ratio and annealing temperature on photo-absorption of the blends. Blend ratios examined in the study fell within the range of 1:0.8 to 1:1 by weight of P3HT to PCBM. The range was divided into 11 intervals with a step increment of 0.02 for PCBM while P3HT was kept constant. The optimum blend ratio was determined and found to be 1:0.96 at 130 ^{o}C annealing temperature and duration of 30 minutes. The annealing temperature dependence of each blend ratio with respect to photon-absorbance was found not to be symmetric but random. Each blend ratio was found to have own optimum annealing temperature.

The efficiency of the cells was enhanced by the use of TiO_2 thin film as a back reflector and optical spacer on aluminium substrate. The study compared the performance of cells on glass substrate to those on aluminium substrate. The

cells built on aluminium substrate showed a power conversion efficiency of 2.8 % whilst those on glass substrate showed 1.9 % efficiency.

The main objective of the study was to determine the optimum blend ratio, the optimum annealing temperature, and to eventually build solar cells from the optimized parameters.

DEDICATION

To my dad Robinson Kalonga

To my lovely wife Lucy Nalwimba Kalonga

And

To my lovely Daughter Luyando Naluse Kalonga

GK

Given Kalonga

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LIST OF SYMBOLS

A	electron acceptor
AM	air mass
AFM	Atomic Force Microscopy
CB	conduction band
D	donor
EA	electron affinity
ECD	equivalent circuit diagram
EQE	external quantum efficiency
FF	fillfactor
HOMO	highest occupied molecular orbital
IP	ionisation potential
IQE	internal quantum efficiency
ITO	indium tin oxide
LED	light emitting device
LUMO	lowest unoccupied molecular orbital
PCBM	[6,6]-phenyl C61 butyric acid methyl ester
PEDOT	poly(ethylene dioxythiophene)
P3HT	poly (3-hexylthiophene)
SR	spectral response
TOF	time of flight
VB	valence band
A/D	acceptor/donor interface
HOMO/LUMO gap	band gap
Irradiance	light intensity
n-type	negative charge transporter
W	Watt
V_{max}	maximum voltage
J	current density
s	shadow length
Φ_B	barrier potential
E_{EM}	electromagnetic field

E_{vacuum}	vacuum energy level
h	vertical structure height
K	Kelvin temperature
q	positive elementary charge
kB	Boltzmann constant
$\alpha(\lambda)$	absorption coefficient at wavelength, λ
T	temperature in degrees Celsius
eV	electron volts
QTH	quartz tungsten halogen-lamp
BHJ	bulk hetero-junction
E_f	Fermi-level
N_C	density of states in conduction band
N_V	density of states in valence band
N_D	concentration of donor charge carriers
N_A	concentration of acceptor charge carriers
$P_{AM1:5d}$	power at air mass 1.5
E_{FN}	the quasi-Fermi level of electrons
E_{FP}	the quasi-Fermi level of holes
V	the potential applied at the barrier contact
V_d	the potential drop across the dipole layer
V_{sc}	short circuit voltage
PANI	polyaniline
E_g	band gap
IPV	inorganic photovoltaic
OPV	organic photovoltaic
μ	charge mobility
μ_0	zero-field mobility
F	field strength,
Y	field activation parameter
W_{ij}	phonon-assisted hopping from i_{th} to j_{th} state
ε_j	energy at j_{th} state
υ_0	the attempt-to-jump frequency
R_{ij}	the distance between the states i and j

γ	the inverse localization length
Σ	positional disorder
a	intersite spacing and
Γ	positional disorder of transport sites
E_r	intramolecular reorganization energy
ITO	indium tin oxide
□$_M$	metal work function
MIM	metal-insulator-metal
ECD	equivalent circuit diagrams
I_L	light current
I_0	zero current
I_{sh}	shunt resistance.
V_d	diode voltage
I_d	diode current.
R_s	series resistances
R_L	load resistances
R_{sh}	shunt resistance
V_{oc}	open circuit voltage
η	power conversion efficiency
Φ	work function
SR	solar radiation
XRD	x-ray diffraction
FTIR	Fourier Transform Infra-red
β_{hkl}	width of peak at half maximum intensity
L_{hkl}	particle size or crystallite length
c	speed of light in air
V	speed of light in the non-air medium.
χ	energy of the LUMO above vacuum
n	electron density
p	hole density
J_n	electron flux in the organic layer

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