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PROGRESS IN MODELLING AND SIMULATION OF ORGANIC SOLAR CELLS

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ABSTRACT

ORGAINC SOLAR CELLS (OSCs) is recently received a great urge as it is safe, secure and clean substitute for the current fossil fuel power plants and it can be synthesized by low temperature processes at low cost price with a good energy balance. During the preceding years, OSCs performance has enhanced remarkably but needs more improvements also. Simulations Or modelling are impressive tools for optimization of OSCs, disclose the new perception and predict the behavior, performance, limitations, stability, dependency of OSCs and maximum possible efficiency. In this paper we tells about the some various types of organic solar cells. In this research paper, we discuss about the chain of simulation models for modeling state of the art devices, their corresponding advancement in recent years on the basis of device physics and examine the photo absorption, working, principle, their quantum efficiency, short circuit current, open circuit voltage and fill-factor of the device to considered the photovoltaic needs.

KEYWORDS: *Organic Solar Cells, Small Molecules based Solar Cells, Drift Diffusion Model.*

Introduction

The largest hazards for the future of life on earth are energy disaster, global warming, exhalation of green house gases such as co2, water vapors, methane, nitrous oxide etc. Among all of the renewable resources, the many encouraging and defended fields which can be accepted as a safe, secure and clear imitative for their actual fossil fuel power plants is PV energy. On the basis of previous record, the renewable energy sources PV having the quick expanding rate. Solar energy is considered as an ideal green and renewable energy source due to which it attracts increasing awareness with developing the importance of energy sources and nature or habitat protection. OSCs is considered as a favorable solar energy source, the organic solar cells have been broadly studied because of its benefits of flexibility, light weight, lower price and comfort of its fabrication. An OSC, the firstly photo-generated state is an exciton (i.e. a strongly bound electron-hole pair) which is charge less or neutral and so travels by diffusion. The exciton wants to be beak into its constituent charges for photovoltaic action. After that the exciton can be isolated towards the material which has greater electron affinity and ionization potential. The electrons and hole are passed on by undertaking the photo generation has happened. During the photo generation process of OSCs, the way of charge generation and separation happens simultaneously at a material heterojunction. A problem in exciton separation is that excitons have a fix diffusion length, after that they will apparently recombine in place of releasing the free carriers. It set a limitation on the device thickness of organic cells. OSCs are a type of PV which uses organic electrons (i.e. branch of electronics that deals with conductive organic polymers or small organic molecules) for absorption of light and the charge transferred to producing the electricity from sunlight by using the PV effect. Those molecules which are used in OSCs are solution-processable.

Types of Organic Solar Cell

- **Small Molecules- based Solar Cells: In 1975,** the organic photovoltaic devices using small molecules is fabricated firstly. Nevertheless the efficiencies did not reach greater than 0.001% at that time. In 1986, Tang is generally cited as the groundbreaking analysis which provoked the recently interest in this field. By using the copper phthalocyanine as the electron donor and a

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perylene derivative, 3, 4, 9, 10-perylene tetracarboxylic bis-benzimidazole as the electron acceptor in a normal bilayer structure, power conversion efficiency of 1% was reported. The open circuit voltage come to 450 mV and the fill factor of 65% represents the excellent charge transport. C60 i.e. fullerene, does not show secure absorption properties in the visible region, its much larger exciton diffusion length compared to PTCB which is promising to attain larger efficiencies. Devices which are based on CuPc: C60 bulk heterojunctions reached power conversion efficiencies of up to 5%. The greatest efficiency for organic solar cell so far was reached by Xue et al. For a stacked solar cell comprising two CuPc: C60 bulk heterojunction cells separated via a layer of silver nanoclustors, which served as a charge recombination layer.

- **Polymer -based Solar Cells:** An important portion of the cost of solar panels comes from the photoactive materials and worldly-wise, energy-intensive processing technologies. It proves that the inorganic components can be replaced by semiconducting polymers because these are proficient of accomplishing logically more power conversion efficiencies. As these polymers are cheap to manufacture and can be solution-processed in a roll-to-roll fashion with more production. Genetically, the poor polymer properties, such as low exciton, diffusion lengths and low versatility can be overcome by nanoscale morphology. The polymer-based solar cells reward specific attention to the design of device and potential increments. But conjugated polymers are good applicants for use in low-cost electronics and PV cells. This type of solar cells s having the good power conversion efficiencies of 5% in currently reports**.** Deposition of organics by screen printing, doctor blading, inkjet printing, and spray deposition is possible because these materials can be made soluble. There are various techniques such as doctor blading, inkjet printing, and deposition of organics by screen printing which are required for the high production roll-to-roll processing which will drive the cost of polymer-based PV down to that limit where it can compete with current grid electricity. These deposition techniques take place at a low temperature, which grants devices to be fabricated on plastic substrates for malleable devices. Malleable photovoltaic also come up with alcove markets such as portable power generation and aesthetic PV in building design**.** The fill factor and quantum efficiency wants to be doubled in order of 8-9% power conversion efficiency. Currently analysis indicates that their device performance is limited greatly by the low dissociation efficiency of the photo generated excitons into free charge carriers. The electrons tend to localize nearby the heterointerface in the electron accepting polymers due to their amorphous nature, even after dissociation.

Review of Literature

Firstly, the organic PV solar cells were based on single organic layers interceding between two metal electrodes of different work functions. Due to their rectifying behavior of a single layer devices was attenuated to the dissymmetry in the electron and hole injection. Their power conversion efficiencies reported were generally low, but attains the remarkable 0.7% for merocyanine dyes in the fresh days. The organic layer was sandwiched between a metal–metal oxide and a metal electrode in the case, thus increasing the Schottky-barrier effect. By introducing the bilayer heterojunction concept in which two organic layers with specific electron or hole transporting properties are interceding between the electrodes in the next progress was achieved. In 1986, Tang reported that approx 1% power conversion efficiency for two organic materials which are interceding between a transparent conducting oxide and a semitransparent metal electrode. This result having the excellent criterion for many years and only at the turn of the millennium it was overcome. A three layer p-i-n like structure with a co-deposited interlace between the p-type and n-type layers which are electron conducting is also developed. In the intervening time, conjugated polymers field grew mature, and the first single layer devices based on these newly developed materials were presented. The exciton were separates by organic-organic interface into its constituent charges. Actually, the resulting state is not a free electron and free hole in the acceptor and donor respectively after excition dissociation, instead a bound charge-transfer state known as a polaron pair, extending across the junction between the two materials. This probability in a process known as energy transfer, the exciton is transferred between the phases. Energy of the charge-transfer state which is lower as compared to an exciton on either material respectively. This is the reality for the occurrence of charge transfer. Due to their opposite spatial derivatives, the charges will diffuse in different directions.

Objectives

The essential energy supply in the EU is 85% which are dependents on fossil fuels. The energy system based on a low carbon model is recreating, so it becomes the one of the critical challenges of the

21st Century. Solar energy becomes the largest energy resources of all carbon-neutral energy sources. Most of the energy which is comes from sunlight is strikes with the Earth in 1 hour as compared to all the energy consumed on the planet in a year. Development of low-cost photovoltaic energy conversion technologies is more important.

Improvement for fabrication and doping processes to recognized the stable monolayer graphene p- and n-doped electrodes with sheet resistances less than 100 Ω/square and less than 10% change in sheet resistance over a time of fourteen days. The stability of the electrodes within the enclosed solar cells is enticipated to exceed one year.

Improvement of organic PV solar cells with single or both electrodes fabricated from doped graphene. Improvement of all those processes which are fabricated of nano structured graphene-based photonic crystal electrodes addressing the improved light trapping in the organic PV cells in the visible or near-infrared spectral ranges. Improvement and comprehension of graphene-based high-efficiency tandem solar cells. Improvement of experimentally approved models for the simulation of solar cells with graphene contacts and Distribution of the simulation tools implemented under BSD open-source license

Parameters of Organic Solar Cells

Now we considered the device physics which is relevant to the study of solar cells. Out of the particular relevance there are the four parameters which are given as:

- Short circuit current
- Open circuit voltage
- Power conversion efficiency at maximum power point
- Fill factor
  - Jsc – it represents the short circuit current density which is defined as the current density under illumination at zero applied bias and according to these conditions the potential difference between the electrodes is called the built-in bias, i.e. Vbi.
  - Voc – it indicates that the open circuit voltage which is applied bias at which the photogenerated, extracted current equals the injected current and so the total current is zero.
  - ηmpp – it indicates that the efficiency at maximum power point which is the power density that delivered to the external circuit divided by the incident illumination power density, P0.
  - FF – it represents that tha fill factor whic is a measure of the 'squareness' of the current-voltage characteristic.

The performance of OSCs is a function of several variables, like as the thickness of the layer, energy band-gap, absorption coefficient, carrier mobility, contact barrier, recombination coefficient and device architecture. All these factors conveys a important affect on the performance of BHJ OSCs. Wide understanding of the physics related to the device is necessary for device optimization and further progress. For exploring the physics of the device modeling and numerical simulation are favorable tool which provides key insights into the internal mechanisms of OSCs.

Models of OSCs

A normal OSC is involves the incident light that passes through a transparent substrate and its successive layers. Then the excitons are produced and undergoes to dissociation into free electrons and holes in the BHJ layer after the light absorption. The charge carriers are compelled by an internal electric field and the they collected by the electrodes before the recombination and at the metal electrode the light reflects back. That generation, recombination, drift, diffusion, and collection process of the electron and hole of the photovoltaic structure is considered by the electrical model and to calculate the numbers of the absorbed photon in the structure is done by applying the optical model.

Electrical Model

This model fall into three main categories:

Equivalent circuits, Microscopic models and Continuum models.

Equivalent circuits –this model is based on the equivalent lumped circuits few models,for e.g. the single diode model (SDM), the double diode model (DDM) as shown in fig 1.

The SDM-based approach by the Lambert W-function

The DDM also known as Mazhari's model which are often used to characterise the electrical characteristics which are mature to directness and flexibility; nevertheless, their features do not fully take into account the physical phenomena of organic cells.

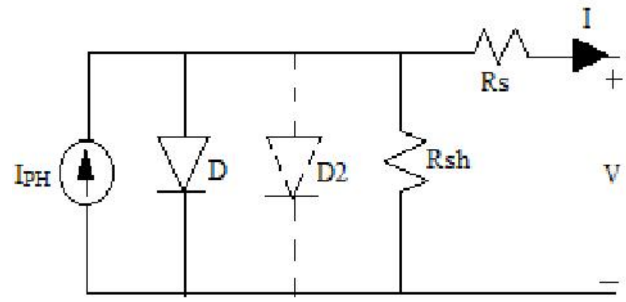

fig. 1: single diode and double diode model

- **Microscopic Models:** This model based on kinetic Monte Carlo (kMC) simulations. Their main advantage is the possibility to correctly include the effect of the real morphology. The kMC represents an priceless tool to analysis these processes in time domain and gives the suggestion for optimization strategies for the device fabrication. But there are some drawback of kMC which is given as, the extremely high computational cost, particularly if the entire active layer has to be included in a 3-D structure. Due to this reason, only a portion of the entire device has been effectively simulated.
- **Continuum Models:** Mostly this model is consider the blend as a homogeneous medium. Good concurrence has been achieved with calculated current–voltage characteristics in OSCs for these types of models. Nevertheless, computationally efficient at the same time such models are unable to describe carrier interactions in sufficient detail.
- **The Effective Medium Model:** The BHJ layer is a combination of donors and acceptors demonstrate a complex morphology. In this model, the BHJ layer is considered as a homogeneous semiconductor. The energy difference between the LUMO of the acceptor and the HOMO of the donor functions is considered the effective energy band gap of the semiconductor. The electrons-holes transportation in the semiconductor under operation condition is a shown in Figure 2.

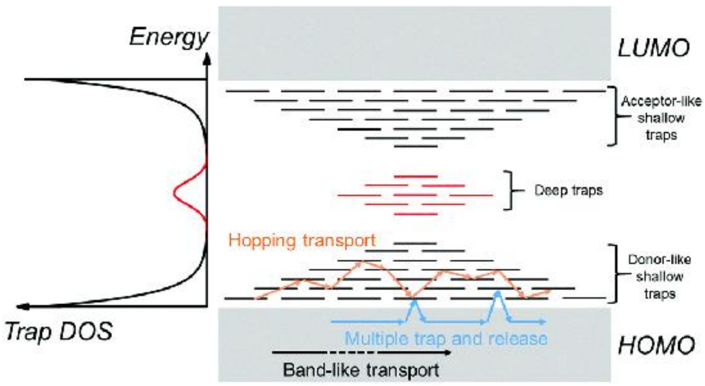

Fig. 2: This is the electrical model that showing energy level of materials with Be and Bh representing the energy barrier for the electron and hole respectively.

Inside the BHJ layer the 1-D equations that characterized the behavior of electrons and holes are similar to those which are used in inorganic semiconductor devices. The electrostatic attraction between the charge carriers in organic semiconductors is not able to screened as of their low dielectric constant. Thus, the charge carriers feels stronger attraction. The absorption of a photon primarily leads to the formation of a strongly bound exciton in organic semiconductors. For obtaining the free charge carriers, the exciton must be breaked that can be accomplished by blending two organic semiconductors with different energy levels so that an electron can easily undergo a charge-transfer process from the bound exciton state to transform into a less tightly bound charge-transfer exciton leading to efficient generation of free electrons and holes. This one is the solution for a steady-state diffusion equation which characterized the dissociation and recombination kinetics of ion pairs in an applied electric field. Ions in solutions having the long range order lives.

Optical Model

To illuminate the optical strength of OSCs, that having a clear explanation of the illumination direction and active layer thickness effects on their performanace and transparency of the device, optical simulations are necessary. The introductory step requires the calculation of the respective number of photons absorbed in the active layer (Nph) under AM. But their optical interference effect should not be ignored in multilayer structure, especially when highly reflective metal electrode is used because the layer thicknesses in OSCs are comparable with the wavelength of sunlight. The optical transfer-matrix theory is given by Heavens which was applied to organic heterojunction solar cells by Pettersson et al and others than deliberated the interference effects for light wave propagating in thin films to OSCs. According to the optical transfer-matrix theory has been widely applied to simulate optical absorption and light intensity distribution within organic thin film solar cells. This theory is based on the Fresnel relations, that mean the light wave undergoes Fresnel reflection and transmission, and apply matrix formulae to calculate the optical intensity in various thin layers. There are some assumptions for applying this theory which are given as:

- Layers of OSCs are homogeneous and isotropic
- Parallel and flat interfaces,
- The incident light is a plane wave normal to the substrate interface.
- Based on these assumptions the 1-D model is accurate to calculate the optical electric field.

Annotations on Simulation/ Modeling

To optimization of OSCs, to disclose the new insights, anticipate the behaviour, performance, limitations, stability, dependency of OSCs and maximum attainable efficiency, simulations/modeling are powerful tools. Their modeling is characterized into two parts:

- Electrical modeling and
- Optical modeling,

Generally we used jointly to simulate the performances of a device. Electrical modelling is used to supply key insights into the internal mechanism, that derives the manipulation of factors limiting the electrical transport processes which are based on the drift-diffusion model that included of the Poison's equation and continuity equations.

On the other hand Optical modelling is used to determine the characterization of absorbed light energy inside the device and for obtaining the optimum thickness of film layers used in the device. Even though the large active layer thickness can be increased the short-circuit current density and external quantum efficiency, while devices needed the higher mobility to assure the separated charges to reach their respective electrodes. Electrical modeling with a constant 327 exciton generation rate will be accurate for BHJ OSCs with an active layer thinner than 250 nm, but the optical interference effects should be considered for devices with a thicker active layer. Those materials which are used in active layer of OSCs with small energy gap is improve the device efficiency but lowering which will decreased the open-circuit voltage. In tis manner, the optimized efficiencies of OSCs are acquired at balanced level tuning and the band gap. Because of the temperature dependency of a carrier mobility and bimolecular recombination, the short-circuit current is dependent on temperature. The local electric field affects the charge dissociation and the transformation to the appropriate electrodes. The activity of OSCs is also based on the collection of charges at the electrodes. Higher anode work function develops in higher energy conversion efficiency. But for further improvement the performance of OSCs must be necessarily improved.

Methodology

Polymer solar cells are widely used during the past few decades because of their low manufacturing cost and discrepancy for flexible substrates. For solution-processed organic solar cells, the optimal thickness, annealing temperature, and morphology are main components for achieving a high efficiency. For this work we generally used the response surface methodology (RSM) to find optimal fabrication conditions for polymer solar cells. To optimize cell efficiency, the central composite design (CCD) with three seperate variables polymer concentration, polymer-fullerene ratio, and active layer spinning speed was used. The device performance was achieved by using the 10.25 mg/ml polymer concentration, 0.42 polymer-fullerene ratio, and 1624 rpm of active layer spinning speed.

Response Surface Methodology

RSM is a combination of mathematical and statistical processes which are used to fitting an empirical model to the experimental data formed in relation to an experimental design. So, with the help of these methods, we discovered and improved with applications in different scientific areas. In a experiment, the choice of design region depends on the required properties expected in the experiment. The classical design properties measured in developing an RSM involves the orthogonality, rotatability, and uniform precision.

RSM is a very good technique having the important applications in the design of an experiment, the improvement and design of a new product. Also in the optimization of existing products and process designs. In reality, the word "response surface" comes from a graphical perspective created which using a mathematical model. Generally, RSM is used in chemometrics, food science, and biochemistry since that time. Most of the applications of RSM for optimization is involve of the following various stages:

A screening factor is rush to decrease the number of factors of independent variables to a relative few, therefore the process will be more effectivet and wants the less number of experiments. Decovery of current levels of the major effect factors which resulting in a value for the response that is close to the optimum region. If current levels of the factors not having the ragularly with optimum performance, then the experimente must allocate the process variables that will lead the process toward the optimum level.

Researchers are chosen experimentalal design according to the selected experimental matrix. And mathematical or statistical models of these models data are developed by fitting linear or quadratic polynomial functions. For the fitness of the models, needs to be evaluated. Finally the optimum values are obtained for the variables.

Conclusion

We concluding that the linearly decreasing of the excitons generation function is associated to the loss of free charge carriers at the electrodes or organic interface that causing the raising of the interrnal dissociation rate and a diffusivity of the electron-hole pair at an interface and observed that the rate of total exciton generation does not regularly increase with the increase of the active layer thickness, but it behaves like a wave which produces the corresponding variation of Jsc. The lifetime of carrier also influence the Jsc on large scale. If lifetimes of both electrons and holes are long enough then the dissociation probability act an important role in thick active layer. The excitons dissociation probability decreases exponentially and the internal quantum efficiency charge generation constantly increases when the electron-hole pair separation distance increases.

Optimization of OSCs is one of the largest challenges in OPV technology. Various complex mathematical tools are introduced to simplify and understand the solar cell performance. The aim l was to find the optimum polymer solar cell performance through a statistical model which was found that the RSM is very useful in optimizing solar device performance. Best model found that the 97% of the data was explained, which might help in impending the optimum device performance efficiently. Their performance is also dependent on the collection of charges at these electrodes. Higher anode work function gives the higher energy conversion efficiency. The performance of OSCs has significantly improved but needs further improvement.

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