

A Circuit Model for Polymer Solar Cells

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Abstract

In this simulation a polymer solar cell is modeled by resistors and diodes in a circuit. Voltage outputs and input are added to control voltage in the circuit. The effect of light is added to the circuit by modifying the IV characteristics of the diodes. The current as a function of voltage is calculated for several cases: a random resistor network, a resistor and diode network without light, and a resistor and diode network with a photocurrent.

Introduction

Solar Cells and Solar Energy

Solar cells are devices that convert the energy of sunlight directly into electricity by the photovoltaic effect. The photovoltaic effect involves the creation of a electrical current in a material upon exposure to electromagnetic radiation. Energy generated this way is an example of solar energy or power. Solar cells are desirable because they are a clean, environmentally safe, alternate source of energy. Many problems are related to energy in the world, and especially in the United States. Oil/fossil fuels are running out, we buy energy (oil) from other countries, and the greenhouse effect is causing global warming. Silicon solar cells are efficient but they are expensive as well; however, with improvements in technology we can use polymer solar cells instead at lower prices.

Figure 1 shows a P-N junction with a formed depletion zone. The purpose of this research is to create a model of a polymer solar cell with the long term goal of trying to improve their efficiency.

The most commonly known solar cell is configured as a large-area P-N junction. A P-N junction is formed by joining p-type and n-type semiconductors together in close contact. The junction refers to the boundary where the two regions of the semiconductors meet. P-N junctions are the elementary building blocks of almost all semiconductor electronic devices such as diodes and solar cells.

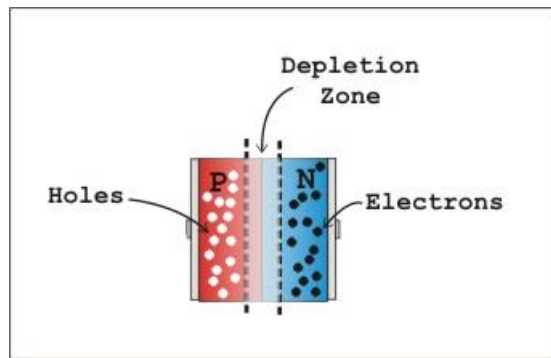


Figure 1: A basic P-N junction that creates a diode.

(<http://www.imagesco.com/articles/photovoltaic/photovoltaic-pg3.html>)

Definition of Polymers and Polymer Solar Cells

A polymer is a large molecule composed of repeating structural units (building blocks) typically connected by covalent chemical bonds. Polymer solar cells are a type of flexible solar cell that produces electricity from sunlight using polymers. Silicon solar cells are the most efficient solar cell made from a refined, highly purified silicon crystal which is costly. Compared to silicon-based devices, polymer solar cells are lightweight, potentially disposable, inexpensive to fabricate, flexible, customizable on the molecular level, and have lower potential for negative environmental impact. The disadvantages of polymers solar cells are serious: they offer 1/3 of the efficiency of hard materials, and they are relatively unstable toward photochemical degradation. Photochemical degradation is the reduction of strength, efficacy, or value of interactions between light and molecules or atoms. Because of these reasons, large arrays of solar cells rely on inorganic materials, but scientists are continuing advances in semiconducting polymers.

Properties of Organic Photovoltaics

Organic photovoltaics (OPVs) with polymers are solution processable and can be manufactured by using a technique called roll-to-roll printing [1]. I focused in on OPVs

fabricated from blends of either two conjugated polymers or a conjugated polymer and a fullerene derivative. Conjugated polymers are attractive solution-processable materials for optoelectronic applications because of the tunability of their optoelectronic properties afforded through control of their chemical structure. Examples of conjugated polymer chemical structures are shown in Figure 2.

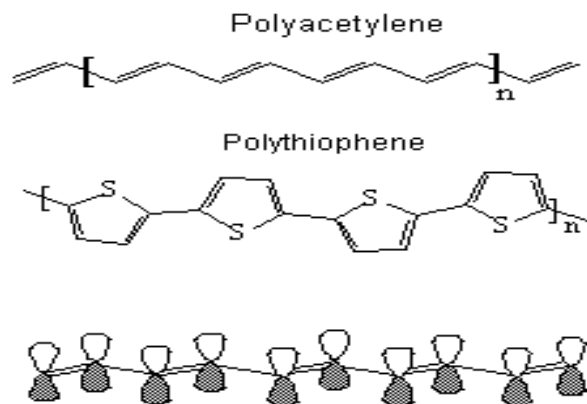


Figure 2: Conjugated polymers

(<http://www.dct.tudelft.nl/pcmt/html/grozema.html>)

Film morphology, or nanoscale texture, of the acceptor/donor blends is a critical variable which can dominate the performance of solar cells. The efficiency of organic solar cells has improved greatly in the last few years, but morphology optimization still occurs largely by trial and error.

Solar cells made from conjugated polymers function differently than devices made from inorganic semiconductors. One of the most important differences is the absorption of photons in an organic semiconductor does not directly produce free charges. Absorption of a photon in an OPV leads to the formation of a neutral excited

state called an exciton. An exciton consists of a tightly bound electron-hole pair that must be dissociated to yield the charge carriers needed for a photocurrent.

Efficient bulk heterojunction photovoltaic cells

As stated by G. Yu, in polymer photovoltaic cells, the exciton diffusion bottleneck has been removed through the introduction of bulk heterojunction [2]. A heterojunction is the interface between two materials having different band gaps, such as a p-type semiconductor and an *n*-type semiconductor. In organic photovoltaic devices, the term "bulk heterojunction" has been used to describe a heterojunction composed of two different band gap materials such as electron acceptor fullerenes and electron donor polymer, mixed together in a bulk and thus containing several discrete interfaces. The donor-acceptor interface, in a bulk heterojunction, is highly folded such that photogenerated excitons find an interface within a distance of their generation site. Currently, state-of-the-art bulk heterojunction polymer photovoltaic cells have power conversion efficiencies of up to 3.5%. The bulk heterojunction is fabricated by spin-coating a mixture of the donor and acceptor materials.

My Circuit Model Project

In this project I model the charge transport in a bulk heterojunction solar cell with a circuit consisting of resistors and diodes. The diodes represent the P-N junction. Each stage of my project added complexity to the previous ones until the final stage was a model of a bulk heterojunction solar cell.

Resistors Only Warm-Up Program

Dr. Hershfield created a warm-up program with only resistors and no diodes that I later ran and modified. This program used a system with M rows and N columns

between two electrodes at V_{plus} (top) and V_{minus} (bottom). For testing purposes I started with a 3 by 4; I called the horizontal resistors G_{horiz} and the vertical resistors G_{vert} . Each pack of resistors had their own matrix of values; in the beginning, I let the resistors be random numbers. Figure 3 shows my circuit model for a matrix of resistors.

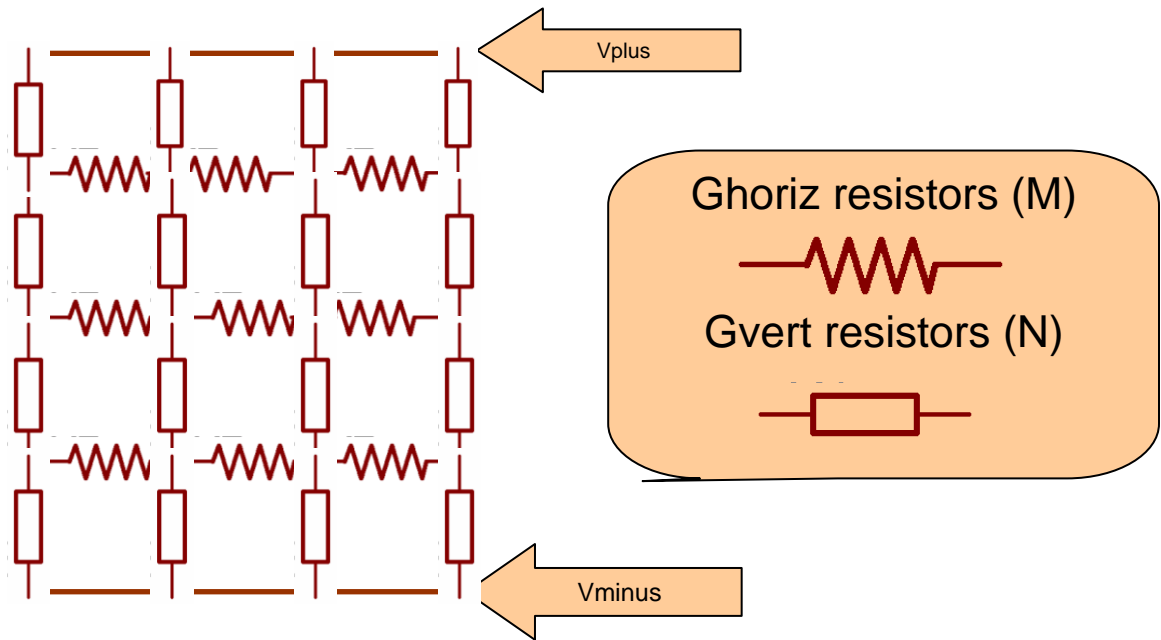


Figure 3: A matrix of resistors (vertical & horizontal)

This circuit model shows two matrices of resistors overlapping each other. The top line of this diagram is the V_{plus} or the voltage at the top going into the circuit. The V_{minus} at the bottom is the voltage leaving this circuit. I used both V_{plus} and V_{minus} to maintain the voltage across the circuit. The arrow on the right side label what each line is. The legend shows what each resistor in the diagram is

After creating my matrix of resistors diagram, I measured the voltage points across the diagram. The total number of voltage points in the diagram depends on N and M because the total number of voltage points is equal to $N \cdot M$. To have information to

compare to, I solved for the voltage points manually by using Kirchhoff's current law. For this case of random resistors the computer program and solving for the voltages by hand gave the same result, which was an important check.

Program Details

By setting values for my resistors, I was able to look for the voltage. Dr. Hershfield did some programming and then we set some boundary restrictions. The boundary restrictions were put on the resistor to the left, right, top, and bottom. To find the voltage, I created a Gmatrix that responded to each point on the resistor network and also created a constant to keep in place. After creating the Gmatrix and constant, I found a matrix of voltages for my voltage points. To place my findings in a more organized order, I placed my voltages on top of where there were voltage points as I reshaped my voltages to create a Vmatrix to get my values. This program was written in MATLAB Editor; I then ran it in MATLAB to get some values for Vmatrix.

Setting Size Limitations

By adding an extra set of resistors horizontally, I tested the program with periodic boundary conditions. This models an infinite system. The two new boundary restrictions include a left side added resistor and right side added resistor, which are the same. I found that for the computer, I am using a matrix of 49 by 50 is the highest I can go without MATLAB having problems with finding the voltage points. I found that the program needs about 10 seconds to calculate all the voltage points when it previously needed about 2 or 3 seconds.

Solving for Current

After those test cases, I began to solve for the current through the matrix along with the voltage. I found that creating loops in my program to solve the voltage points and current resulted in fewer errors in the values. After taking some data, I made all the Gverts standardized at 100 and the Ghorizs standardized at 50 to test my results. The program proved it was working correctly because I found the current the same going down each column. Also I found that no current was going across the horizontal resistors. I found the voltages at each point were showing values that made sense.

Adding Diodes

By adding a row of diodes, I was able to evaluate if the program matched a measured current and voltage across a diode. With this program working, my circuit model became closer to a polymer model. I found I had to set a loop to evaluate V_{plus} from negative 3 to positive 3, and V_{minus} equal to 0 because I needed to first test the IV curve over a small voltage. I have all the Ghoriz resistors as 50 and the Gvert resistors at 100. Setting all six of my boundary restrictions on, I was able to use a more general code for current. Because these results converged, they led me to my final project of a realistic PN Junction model without light as shown in Figure 5.

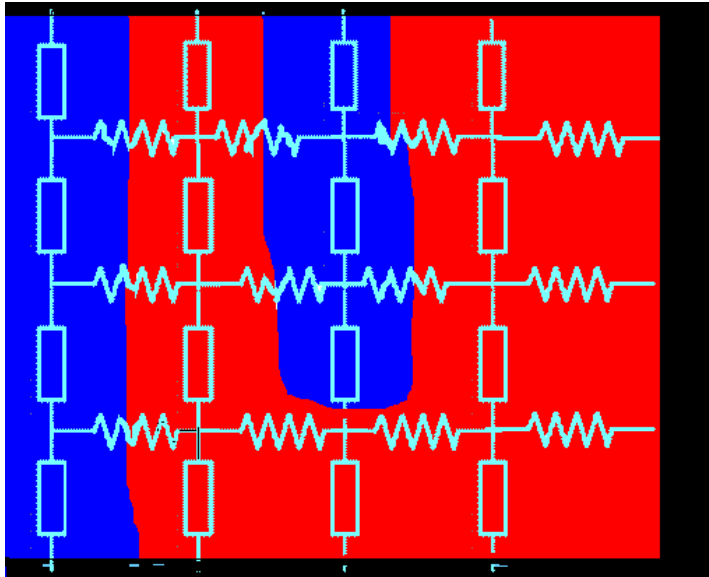


Figure 5: A circuit model for a PN Junction (Polymer Solar Cell Circuit).

Model for a Polymer Solar Cell

In this final part of my simulation, I labeled the red and blue, or N-type and P-type, resistors as such. The parts of this figure where red (N-type) touches blue (P-type) coloring are where diodes form. The figure above has 8 diodes, 6 blue resistors, and 14 red resistors. I then measured for the IV curve at a point through my circuit using the current at that point. I increased the voltage through the circuit to get a much smoother graph. My final results are shown in Figure 6.

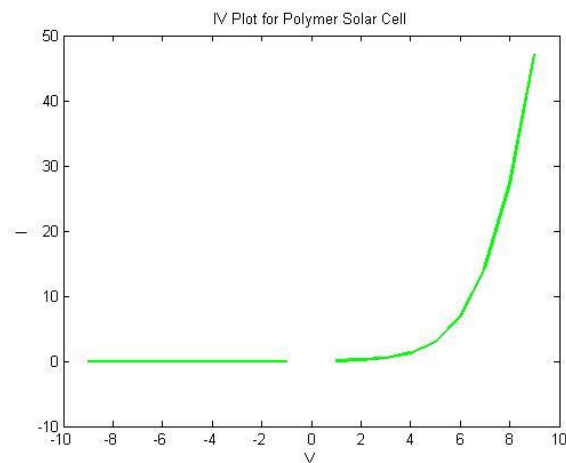


Figure 6: IV curve of my polymer solar cell without light (I_0).

My polymer circuit findings were the desired IV curve of a diode. Adding light to my device caused current to change. In the presence of light the current coming out of the junctions takes the form of $I = 0.1 * (\exp(b * V) - 1) - I_0$, where I_0 increases with the amount of light. To test how much photocurrent could add to the circuit, I slowly increased the I_0 to see the effect of the light. To test the changes in the IV curve, I increased the I_0 , and the plot slowly moved down. Figure 7 shows a polymer solar cell with $I_0=10$.

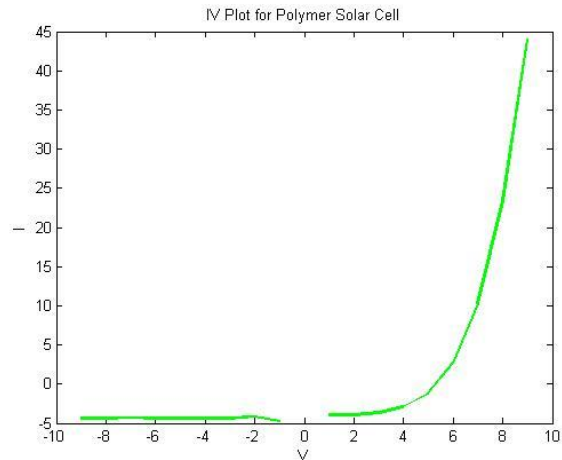


Figure 7: IV curve of my polymer solar cell with light (I_0).

After getting these results, I found that for the discussion of efficiency of the polymer it was best to use the total current for my program. So to get these results, I first used the program without light to show the IV curve of the entire polymer solar cell without light. The IV plot of the total current without light is shown in Figure 8, and the IV plot of the polymer with light is shown in Figure 9.

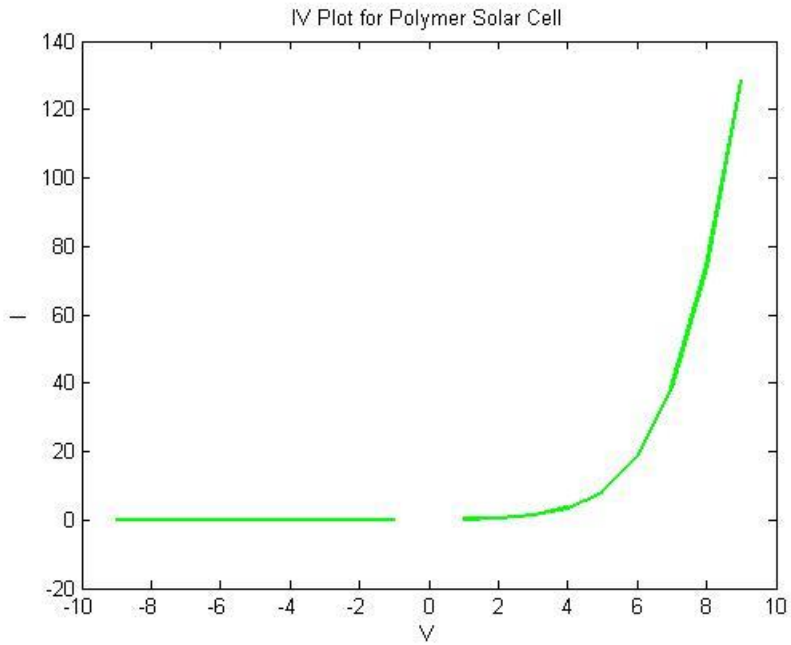


Figure 8: IV curve of the entire polymer solar cell.

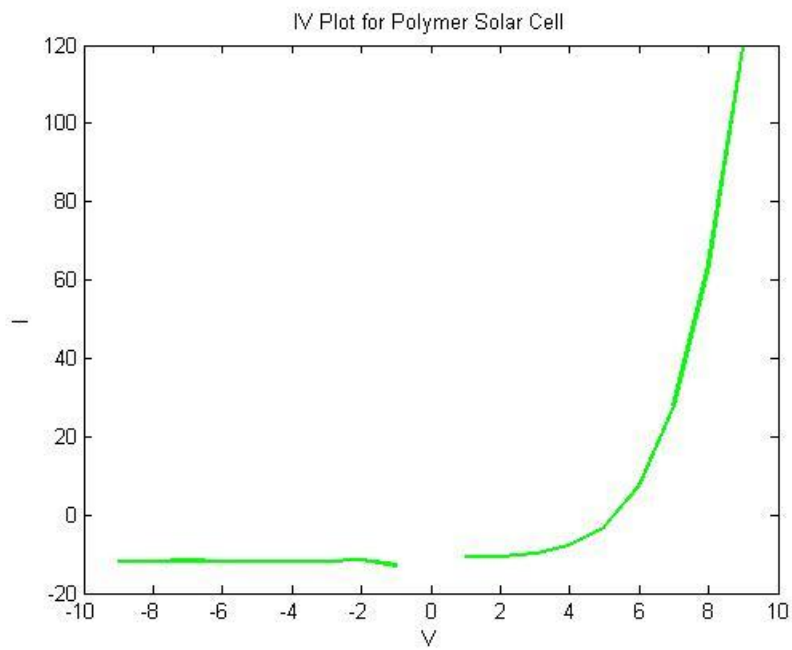


Figure 9: IV curve of the entire polymer solar cell while illuminated.

Conclusion

In this project the current voltage characteristic was calculated for a circuit model of a bulk heterojunction organic solar cell. The computer code was tested on several cases such as a random resistor case before proceeding to the case of a solar cell. We did find that a photocurrent is created by the light, but further research is needed to determine the optimum arrangement of the P and N materials for an organic photovoltaic cell.

Acknowledgments

I'd like to acknowledge Dr. Selman Hershfield for all of his help and guidance in this project. Also I like to thank him for all his help with MATLAB and programming methods. Also I like to thank the Physics REU program at University of Florida for the monetary support. I also like to thank Mark Hannel for his help with MATLAB. Last, I'd like to thank all the professors for their talks on physics and the English professors for their help with the final reports and presentations.

Documentation

[1] C. Groves, O. G. Reid, and D. S. Ginger, "Heterogeneity in Polymer Solar Cells", *Acc. Chem. Res.*, **43**, 612 (2009).

[2] P. Peumans, S. Uchida, and S. R. Forrest, "Efficient bulk heterojunction photovoltaic cells using molecular-weight organic thin films", *Nature*, **425**, 158 (2003).