Cohesion and Adhesion in Thin-Film Organic Nanostructured Materials for Photovoltaic Applications

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Abstract:

The main focus of this project was to study the nano-mechanical properties, cohesion, and reliability of advanced thin-film architectures used in polymer organic photovoltaics. Photovoltaics are devices that convert incident light into usable energy. The cohesion of the photoactive layer, which consists of the semiconducting polymer poly(3-hexylthiophene-2, 5diyl) (P3HT) and small molecule Phenyl-C60-butyric acid methyl ester, or $PC_{60}BM$, are characterized using micromechanical analysis. The goal of the work was to develop an understanding of how the films adhesive/cohesive and thermo-mechanical properties are related to their nanostructure and processing conditions. In addition, we used a cross-linking agent (BABP) to minimize molecular diffusion, improving thermal stability. In particular, we were interested in how the films were affected under operating conditions; including exposure to air, solar UV irradiation, and temperature. By correlating the results to the efficiencies for our organic photovoltaics and analyzing the trends, we intend to design processing methods that will improve the mechanical reliability of these devices while maximizing thermal stability.

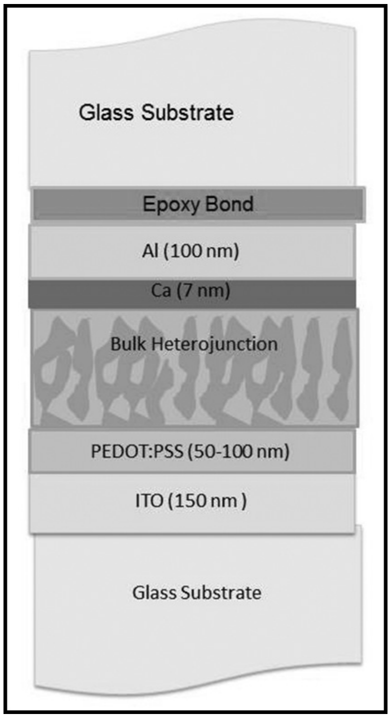

Figure 1: Organic solar cell thin film layer profile.

Introduction:

Having a finite amount of fossil fuels is one of the main reasons the development of alternative sources of energy is necessary. Additionally, the burning of said fossil fuels in such large quantities causes severe environmental alterations such as global warming. The project at hand aimed to offer a reliable alternative for fossil fuels with the use of photovoltaics.

Organic cells can be printed into very thin sheets making them weigh significantly less than inorganic based solar cells and allow for flexibility. However, organics tend to be more sensitive to air and moisture, meaning that environmental effects can severely degrade their performance. Our research also indicates that the polymers with small molecules used are relatively fragile from a mechanical perspective. This is important to note since barrier delamination of the solar cell may lead to catastrophic failure within the device. Our main concern for this project was the need for the cells to operate under severe environmental conditions.

The operational principle of an organic cell begins when light is incident upon the device, which is then followed by the absorption of the photon. This process then results in electrons being excited from the highest occupied molecular orbital to the lowest unoccupied molecular orbital. Charge splitting then occurs allowing for the collection of electrons and holes.

Experimental Procedure and Results:

The organic solar cells at hand consisted of eight layers as shown in Figure 1. The core of the cell was the bulk heterojunction (BHJ) layer, which consisted of a 1:1 weight ratio of P3HT and $PC_{60}BM$ and a particular amount of BABP ranging from 0%-10%.

First, a thin layer of BHJ solution was spin-coated onto a glass substrate and observed under a microscope after various thermal annealing times. As shown in Figure 2, BABP prevented the crystallization of $PC_{60}BM$ with annealing time. This is important to note since it is consistent with past literature and supports the argument that BABP allows for thermal stability of the BHJ layer via preventing the diffusion of $PC_{60}BM$ molecules.

Next, one of the most important techniques used to test the mechanical properties of the solar cell devices was the four-point bend test (4PB). The 4PB test applies an equivalent amount of force on four parallel directions on the device, two forces acting on top of the device and two on the bottom of the device, in order to propagate a crack within the cell. This technique provided a method for analyzing the cohesion values of the devices. These values are significant because if the cohesion is low failure is more likely to occur. As shown in Figure 3, the cohesion values of the devices decreased significantly when BABP was included in the BHJ layer. These results helped us understand that although BABP increased the thermal stability of the cell, it decreased the mechanical reliability by about 50%. Though the cohesion values decreased significantly, they still remained around 5 J/m^2, which is the optimal value desired for the devices.

Finally, after analyzing the cohesive strength of the device, it was important to investigate where exactly the failure occurred. In order to do so, an x-ray photoelectron spectrometer (XPS) was used.

XPS emits an x-ray beam onto the surface of the device and utilizes the photoelectron effect to eject core shell electrons from the elements on the surface. The XPS then records peaks at specific binding energies that correspond to each element on the periodic table.

In this case, the two peaks that occurred around 200 eV corresponded to sulfur and the large peak around 300eV corresponded to carbon. XPS analysis showed that failure occurred in the (organic) BHJ layer. This was due to the prominent peaks for sulfur and carbon within the analyzed spectra (see Figure 4).

The presence of sulfur and carbon indicated failure at the BHJ since those were the two common elements of P3HT and $PC_{60}BM$. Also, the failure occurring at the BHJ did not change with BABP concentration and/or anneal time, which reinforced the conclusions made.

Conclusions:

Although organic solar cell devices have many improvements to be made, this project was able to yield a few key conclusions. First, BABP increases the thermal stability yet decreases the cohesion values of the solar cells. Next, failure occurs at the BHJ layer no matter the concentration of BABP in the device, or the anneal time it undergoes. This allows for further analysis to be done on the BHJ in order to maximize its mechanical strength. Finally, devices are able to withstand 5-11.9 J/m^2, which are optimal values for these kinds of organic devices.

Acknowledgements:

Thank you to Professor Dauskardt, Christopher Bruner, and the 2014 Stanford NNIN REU group and staff. Also to the NNIN REU Program and National Science Foundation (NSF) for funding.

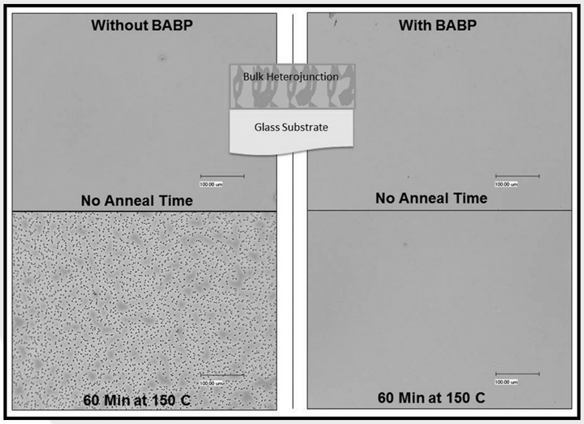

Figure 2: Microscopic images of BHJ layer on glass.

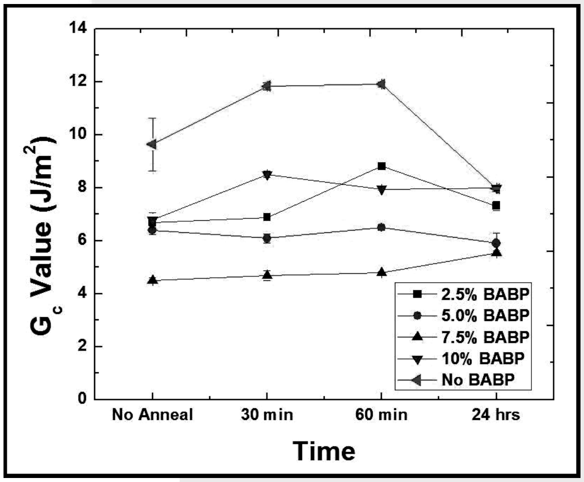

Figure 3: Cohesion values for devices with various BABP concentrations.

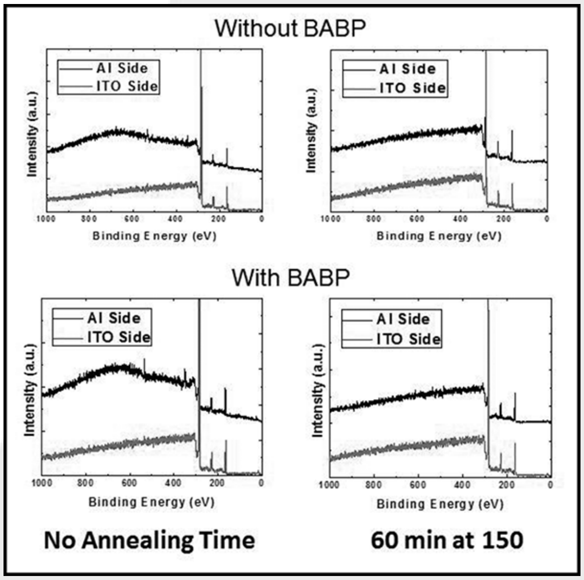

Figure 4: XPS results showed peaks at the sulfur and carbon binding energies.