
Reliability and Physics Failure of Stretchable Organic Solar Cells

O. K. Oyewole, D. O. Oyewole, M. G. Zebaze Kana and W. O. Soboyejo

MRS Advances / *FirstView* Article / January 2016, pp 1 - 6
DOI: 10.1557/adv.2016.21, Published online: 13 January 2016

How to cite this article:
O. K. Oyewole, D. O. Oyewole, M. G. Zebaze Kana and W. O. Soboyejo Reliability and Physics Failure of Stretchable Organic Solar Cells. MRS Advances, Available on CJO 2016 doi:10.1557/adv.2016.21

MRS Advances © 2016 Materials Research Society
DOI: 10.1557/adv.2016.21

Reliability and Physics Failure of Stretchable Organic Solar Cells

O. K. Oyewole[1, 2], D. O. Oyewole[3], M. G. Zebaze Kana[1] and W. O. Soboyejo[4, 5, 6]
[1]Department of Materials Science and Engineering, Kwara State University, Malete, P.M.B 1530, Ilorin, Kwara State, Nigeria.
[2]Department of Theoretical and Applied Physics, African University of Science and Technology, Km 10, Airport Road, Galadimawa, Abuja, Federal Capital Territory, Nigeria.
[3]Physics Advanced Laboratory, Sheda Science and Technology Complex, Federal Capital Territory, Abuja, Nigeria.
[4]Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, USA.
[5]Princeton Institute of Science and Technology of Materials, Princeton University Princeton, USA.
[6]Department of Materials Science and Engineering, African University of Science and Technology, Km 10, Airport Road, Galadimawa, Abuja, Federal Capital Territory, Nigeria.

ABSTRACT

Organic solar (OPV) cells are cheap electronics that can replace the widely used high cost silicon-based electronics for electricity generation. They are cheap because of the easy techniques involved in their fabrication processes and they can be produced to cover a large surface area. However, the current low performance of organic electronics has been traced to failure due to interfacial adhesion problems, material processes, and service conditions. Therefore, transportation of charge carriers across the bulk heterojunction system of OPV cells becomes very difficult in the presence of these flaws. In this paper a combined experimental and computational technique is used to study the reliability and physics failure of stretchable OPV cells. Interfacial adhesion energies in the layered structures of OPV cells are measured and compared with theoretical estimated energies. The limit stresses/strains applied on layered OPV cells during service condition are estimated using critical values of the measured interfacial adhesion. The results obtained are, therefore, explained to improve the design of reliable OPV cells.

INTRODUCTION

Stretchable organic solar cells have emerged as interesting technologies where stretchability is considered important [1-11]. However, mechanical flexibility is a pre-requisite to achieve stretchable solar cells, where wrinkling and buckling deformations are used to create wavy, out of plane structures that can accommodate strain. This is done by pre-stretching the substrates [4, 7] before the deposition of the devices. The wrinkled and delamination-induced buckled structures of the devices are formed due to pre-stretch [4, 7] stress. The formation and deformation of wrinkling of thin films can then initiate failure that can overthrow the reliability of the devices.

Therefore, the basic understanding of deformation on the performance of stretchable solar cells becomes necessary. In this paper, a combined computational/analytical and experimental method is used to study the failure of stretchable organic solar cells. The results are then used to explain the reliability of the stretchable organic solar cells.

THEORY

Adhesion

The adhesion force between two materials can be measured by contact mode atomic force microscopy (AFM) [12, 13] The AFM measurements have been illustrated in Ref. 12. The adhesion force, F , is determined from Hooke's law to be:

$$F = -kx \tag{1}$$

where x is the tip displacement and k is the spring constant of the AFM tip, which can be measured using the thermal tune method [14]

The adhesion energy between the layers can be estimated using Derjaguin-Muller-Toporov (DMT) model. The DMT model is applicable to cases in which there are weak interactions between stiff materials with small radii [14-16]. The adhesion energy, γ, is related to the adhesion force, F, by the following expression:

$$\gamma_{DMT} = F_{adhesion} / 2\pi R \tag{2}$$

where R is the effective radius which is given by:

$$R = \left(1/R_{rms} + 1/R_{tip}\right)^{-1} \tag{3}$$

where R_{rms} and R_{tip} are the radii of the average roughness of the substrate and the coated AFM tip, respectively.

Stresses

The controlled formation of wrinkles and buckles for applications in stretchable organic solar cells involves the deposition of thin films onto pre-stretched substrates [1-4, 17] using spin coating technique. The spin coating of films is usually done under ambient temperature. Hence the film is subjected to only the stress (σ_R) due to pre-stretch of the substrate. This is given by:

$$\sigma_R = E_f \varepsilon_{pre} \tag{4}$$

where ε_{pre} corresponds to the pre-strain and E_f is the film Young's modulus. The films start wrinkling or buckling when the induced stress reaches a critical value. The solutions of the critical stress, σ_c, for the onset of wrinkling or buckling of the thin films are given by [4, 18]:

$$\sigma_c = \left[E_f / \left(1-\nu_f^2\right)\right]^{1/3} \left[3E_s / 8\left(1-\nu_s^2\right)\right]^{2/3} \tag{5}$$

where E_f and E_s are the Young's moduli of the film and the substrate, ν_f and ν_s are the Poisson's ratios of the film and the substrate.

MATERIALS AND METHODS

Experimental methods

First, poly-di-methyl-siloxane (PDMS) was fabricated by mixing a Sylgard 184 silicone elastomer base with a Sylgard 184 silicone elastomer curing agent in a 10:1 weight ratio. The mixture was degassed in a vacuum oven of pressure 50 kPa for 60 minutes to remove the trapped bubbles. The degassed PDMS was cured in glass mold of dimensions of $25mm \times 50mm \times 1mm$ at $70^{o}C$ temperature for 2 hours. A 90 nm thick PEDOT:PSS was spin coated followed by spin coating of a 100 nm thick P3HT:PCBM using the protocol described in Ref. 19. Aluminum contact was thermally deposited onto P3HT:PCBM using vacuum thermal evaporator.

Adhesion force was measured using AFM. The tips of the etched silicon contact mode AFM tips (purchased from Bruker Instruments, Woodbury, NY) were dip-coated with P3HT:PCBM, while the PDMS substrates were spin coated with PEDOT:PSS. The AFM measurements were performed in air of a temperature range of 22-25 $^{\circ}C$ and a relative humidity range of 31-46%. The force-displacement measurements were obtained using a Digital Instruments Dimension 3000 AFM (Digital Instruments, Plainview, NY). The spring constant of each tip was measured using the thermal tune method [14]. The measurements were performed in a Digital Instruments Nanoscope IIIa atomic force microscope (Digital Instruments, Plainview, NY). The measurements of the tip deflections and the spring constants were then substituted into Equation (1) to determine the adhesion forces. Due to the high sensitivity of AFM measurements to surface roughness, the substrate roughnesses and the tip radii were measured. The surface roughnesses were obtained using tapping mode AFM. The AFM tips were examined before and after interaction under a Scanning Electron Microscope (SEM) (Philips FEI XL30 FEG-SEM, Hillsboro, OR).

Computational methods

In an effort to understand the failure and the conditions for reliable stretchable organic solar cells, computational methods were used to study the failure mechanisms and the delamination-induced buckling in the layered solar cell. First, the stress distributions in the wrinkled layers were simulated at different pre-strain levels using ABAQUS^{TM} software package (ABAQUS 6.12, Dassault Systèmes Incoporation, Rhoda Island). In the case of delamination-induced buckling, it was assumed that there were pre- existing interfacial cracks between the P3HT:PCBM and PEDOT:PSS-coated PDMS substrates. These cracks can be attributed to imperfections, such as voids, bubbles or impurities that are present at the interfaces. The energy release rates (G) at the tips of the cracks were computed in form of the path independent J-integral. Fine mesh was used to model the P3HT:PCBM/PEDOT:PSS interface. Four-node plane strain quadrilateral elements were used. All the materials properties that were used were assumed to exhibit isotropic behavior, while the active contact interface was maintained at zero rotation.

RESULTS AND DISCUSSION

Stress analysis

The critical stresses obtained from equation (5) for different moduli of the substrate are presented in Figure 1(a). The critical stresses increased with increasing Young's modulus of the substrate. This can be used to predict the limiting critical stress of the layered films of stretchable organic solar cells. The von Mises stress distributions in the layered structure of stretchable organic solar cell are presented in Figure 1(b). These show the dependence of substrate elastic modulus on stress distributions and profile amplitude. The increasing elastic modulus of the substrate increases the concentration of stress in the wrinkled structure. This shows that the processing of stiffer PDMS substrate will increase the overall Mises stresses. Furthermore, the wrinkling profile became well defined with increasing substrate Young's modulus. However, there is a high possibility that failure would be introduced by higher Von Mises stresses. Hence, a balanced approach is, therefore, needed to obtain well defined profiles without inducing failure.

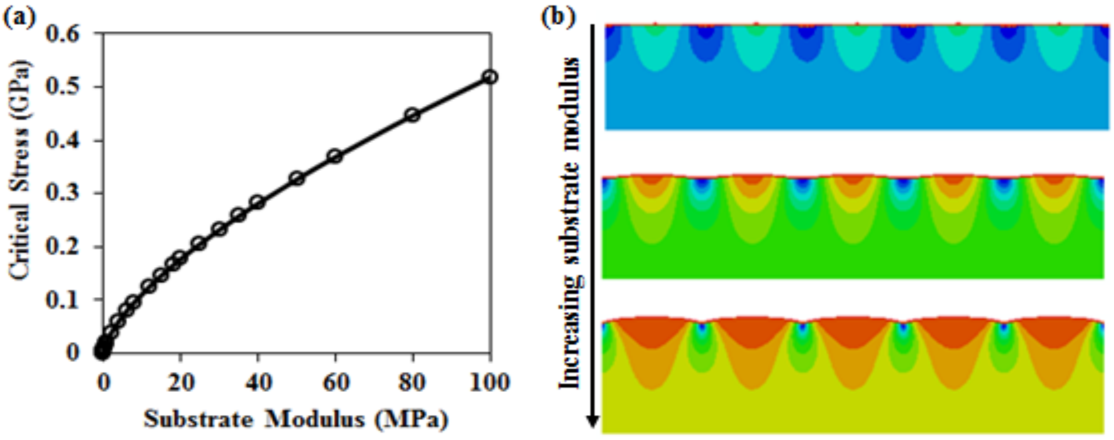

Figure 1: (a) Dependence of substrate on modulus critical stress (b) Von Mises showing the dependence of elastic modulus of the substrate on stress distribution and wrinkled profile

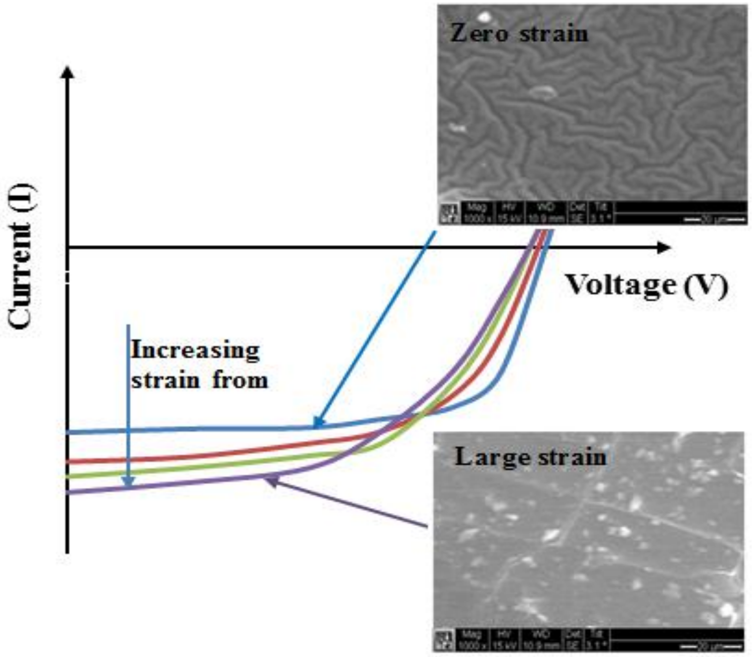

Figure 2: I-V curves of stretchable organic solar cell showing the microstructures of layered films

Failure of stretchable organic solar cells

The current-voltage (I-V) curves of a typical stretchable solar cell are presented in Figure 2 with the microstructures of the failure of layered structures. The curves tend to change from a "knee" curve to a "blunt" curve with increasing strain. This trend can be attributed to interfacial failure due to delamination and cracking of the films as the applied strain increases. At a large strain above the pre-strain, the intrinsically non-stretchable films begin to delaminate and crack. It is, therefore, necessary to bear in mind the threshold of the applied strain when applying strain on stretchable solar cells.

Interfacial energies and failure prediction

The measured interfacial energies in the layered stretchable solar cells are presented in Figure 3(a). The energy between PDMS and PEDOT:PSS layers was 1.14 J/m^2, while the energy in PEDOT:PSS/P3HT:PCBM was 2.6 J/m^2. The energy between P3HT and PCBM was also 1.3 J/m^2. The computed interfacial energy release rate is presented as a function of pre-strain in Figure 3(b) for PDMS/PEDOT:PSS and PEDOT:PSS/P3HT:PCBM interfaces. The energy increases with increasing pre-strain.

Failure due to interfacial delamination can be predicted using the critical measured energies as shown in Figure 3(b). For example, from Figure 3(b), the critical pre-strain on PEDOT:PSS/P3HT:PCBM interface is ~18% at the critical measured interfacial energy of 2.6 J/m^2. For reliability of the layered stretchable organic solar cells, the applied strain on structures of the stretchable organic solar cells should be controlled below the range of predicted values.

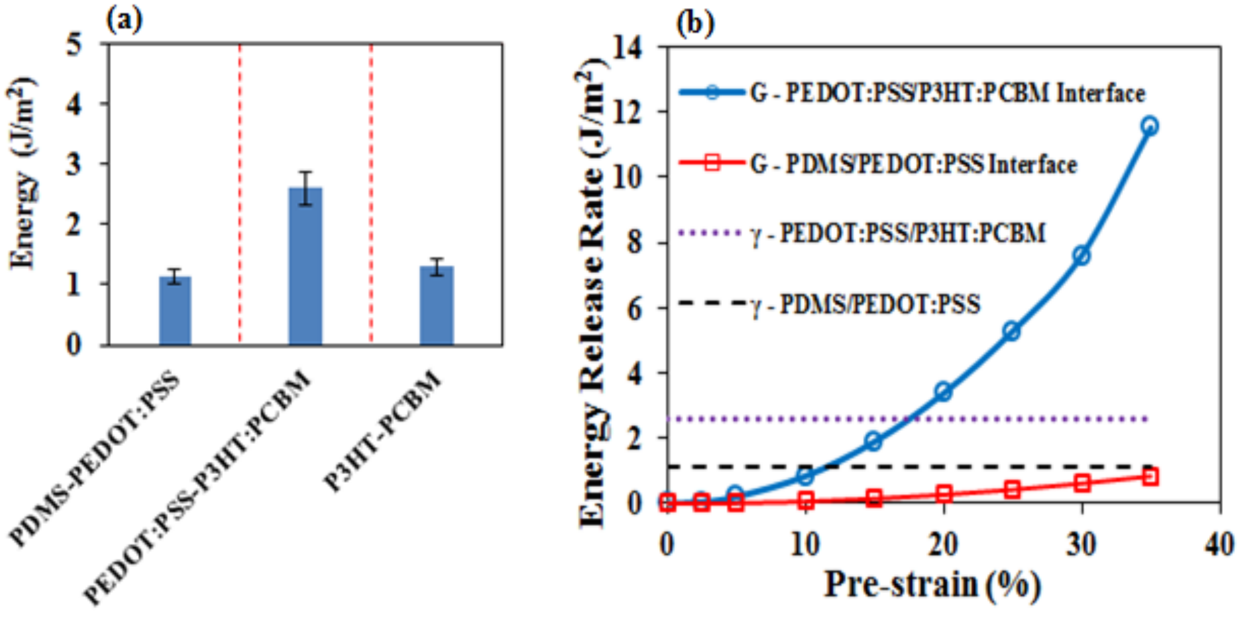

Figure 3: (a) Measured interfacial adhesion energies (b) Interfacial energy release rate (G) versus pre-strain

CONCLUSIONS

In this paper, the reliability and failure of stretchable organic solar cells have been presented using a combined experimental, analytical and computational approach. The critical stress of the layered stretchable solar cells increases with increasing elastic modulus of the PDMS substrate. The failure of the stretchable solar cells was attributed to the delamination and cracking of the films. The measured interfacial adhesion energies were then used to predict the limiting pre-strain for reliable stretchable organic solar cells.

ACKNOWLEDGMENTS

The research was supported by the National Science Foundation (DMR 0231418), the Nigerian Tertiary Education Trust Fund (TETFUND), the Princeton University Grand Challenges Program, the African Development Bank, the World Bank STEP B Program, the World Bank African Centers of Excellence Program and the Nelson Mandela Institution.

REFERENCES

1. S. P. Lacour, J. Jones, S. Wagner, T. Li and Z. Suo, Proceedings of the IEEE **93**, 1459 (2005).
2. T. Li, Z. G. Suo, S. P. Lacour and S. Wagner, J. Mater. Res. **20**, 3274 (2005).
3. S. P. Lacour, J. Jones, Z. Suo and S. Wagner, IEEE Electron Device Lett. **25**, 179 (2004).
4. D-H. Kim, J. Xiao, J. Song, Y. Huang and John A. Rogers, Adv. Mater. **22**, 2108 (2010).
5. C. Yu, K. O'Brien, Y-H. Zhang, H. Yu and H. Jiang, Appl. Phys. Lett. **96**, 041111 (2010).
6. N. Bowden, W. T. S. Huck, K. E. Paul and G. M. Whitesides, Appl. Phys. Lett. **75**, 2557 (1999).
7. C. M. Stafford, B. D. Vogt, C. Harrison, D. Julthongpiput and R. Huang, Macromolecules **39**, 5095 (2006).
8. M. Watanabe, H. Shirai and T. Hirai, Journal of Applied Physics **92**, 4631 (2002).
9. D. J. Lipomi, B. C. Tee, M. Vosgueritchian and Z. Bao, Adv. Mater. **23**, 1771 (2011).
10. M. Pretzl, A. Schweikart, C. Hanske, A. Chiche, U. Zettl, A. Horn, A. Boker and A. Fery, Langmuir **24**, 12748 (2008).
11. M. T. Lam, W. C. Clem and S. Takayama, Biomaterials **29**, 1705 (2008).
12. T. Tong, B. Babatope, S. Admassie, J. Meng, O. Akwogu, W. Akande and W. O. Soboyejo, Journal of Applied Physics, **106**, 083708 (2009).
13. O. Akogwu, D. Kwabi, A. Munhutu, T. Tong and W. O. Soboyejo, Journal of Applied Physics **108**, 123509 (2010).
14. Veeco Instruments Inc.: Improving the Accuracy of AFM Measurements, the Thermal Tune Solution, Bruker Corporation, Billerica, MA (2005).
15. B.V. Derjaguin, V.M. Muller and Y.P. Toporov, Progress in Surface Science **45**, 131 (1994).
16. N. Rahbar, K. Wolf, A. Orana, R. Fennimore, Z. Zong, J. Meng, G. Papandreou, C. Maryanoff and W. Soboyejo, Journal of Applied Physics **104**, 103533 (2008).
17. O. K. Oyewole, D. Yu, J. Du, J. Asare, D. O. Oyewole, V. C. Anye, A. Fashina, M. G. Zebaze Kana and W. O. Soboyejo, Journal of Applied Physics 117, 235501 (2015).
18. M. Watanabe, Soft Matter **8**, 1563 (2012).
19. Yu, O. K. Oyewole, D. Kwabi, T. Tong, V. C. Anye, J. Asare, E. Rwenyagila, A. Fashina, O. Akogwu, J. Du and W. O. Soboyejo, Journal of Applied Physics **116**, 074506 (2014).