Monochromated Electron Energy-Loss Spectroscopy Spectrum Imaging of Organic Photovoltaic Devices

Frank J. Scheltens¹, Michael F. Durstock², Christopher E. Tabor², Benjamin J. Leever², Lawrence F. Drummy², Michael D. Clark^{2,3}, Dennis P. Butcher^{2,3}, Jessica A. Alexander¹, and David W. McComb¹. Department of Materials Science and Engineering, The Ohio State University, College Road, Columbus OH 43210, United States

Bulk heterojunction (BHJ) organic photovoltaic (OPV) based solar cells hold the promise of achieving the highly desirable objective of low cost, clean renewable electrical power via solar energy collection in a flexible device architecture. A very active OPV research and development effort is being driven by the potential to produce large active areas on flexible substrates at low cost and high throughput [1, 2]. Recent developments in polymeric OPV device technology have increased power conversion efficiencies (PCE) into the 10% range [3], pushing OPV devices closer to being viable low-cost, environmentally friendly alternative to contemporary inorganic based solar cells. Extending OPV performance significantly beyond the 10% PCE barrier is a critical challenge. The active layer of the BHJ OPV device studied here consists of a bi-continuous network of electron donor and electron acceptor constituents, in this case poly(3hexylthiophene) (P3HT) and [6,6]phenyl C61butyric acid methylester (PCBM), respectively. Only photo-generated excitons that diffuse to the interface between these electron donor and acceptor materials can dissociate into holes and electrons. Factors such as the amount of light absorption, efficiency of photo-generation of electrons and holes, and their collection efficiency at the respective electrodes must be optimized in order to improve the device PCE.

The development of light trapping strategies such as the utilization of surface plasmon polaritons (SPPs) in metal nanostructures can be an effective method of improving the amount of light absorption inside the active layer of a thin-film solar cell [4]. While incorporation of plasmonic nanostructures into thin-film PV cells is an attractive solution for enhancement of the optical absorption and current density in an OPV, little is known about the detailed structure, chemistry and bonding between the active layer and the plasmonic structure. In this presentation we will explore the application of monochromated scanning transmission electron microscopy (STEM) and high resolution electron energy loss spectroscopy spectrum imaging (EELS SI) to the illumination of these topics (Figure 1).

High resolution EELS can be used to probe the interfaces in the blended film active layer containing plasmonic nanostructures. In particular, monochromated STEM valence loss spectra can probe the complex dielectric function of a material with high spatial resolution [5] yielding information about the effect of the interface between the organic phase and metal nano-particle on the observed resonances. Knowledge about the changes in the chemical bonding at this interface can be gained from studying the single electron transitions and collective excitations in the organic phase resulting from Kramers-Kronig analysis of these spectra. This analysis would then result in a signal that is related to the interactions between the acceptor/donor and gold nanoparticle interfaces, which could be studied and analyzed to try and understand why the insertion of gold nanoparticle in the P3HT/PCBM films improves the efficiency of these OPV devices.

² Materials and Manufacturing Directorate, Air Force Research Laboratory, WPAFB, Ohio 45433, United States

³.UES, Inc., Dayton, Ohio 45432, United States

A successful Kramers-Kronig analysis requires as input the energy-loss function (ELF). The extraction of the ELF from the collected valence loss data is not a trivial process. Substantial issues related to the removal of the monochromated zero-loss peak (ZLP) from the low loss EELS spectra (Figure ld-lg) will be discussed in the presentation [6].

References:

- [1] C.J. Brabec, N.S. Sariciftci, et al, Advanced Functional Materials 11 (2001), 15.
- [2] N.S. Lewis, Science 315 (2007), 798.
- [3] R.F. Service, Science 332 (2011), 293.
- [4] H. A. Atwater, A. Polman, Nature Materials 9 (2010), 205.
- [5] Koh, A. L., Fernández-Domínguez, A. I., McComb, D. W., et al, (2011). Nano Letters 11 (2011), 1323.
- [6] The authors acknowledge the Air Force Office of Scientific Research and the Air Force Research Laboratory Materials and Manufacturing Directorate for funding as well as The Ohio State University Center for Electron Microscopy and Analysis for technical support.

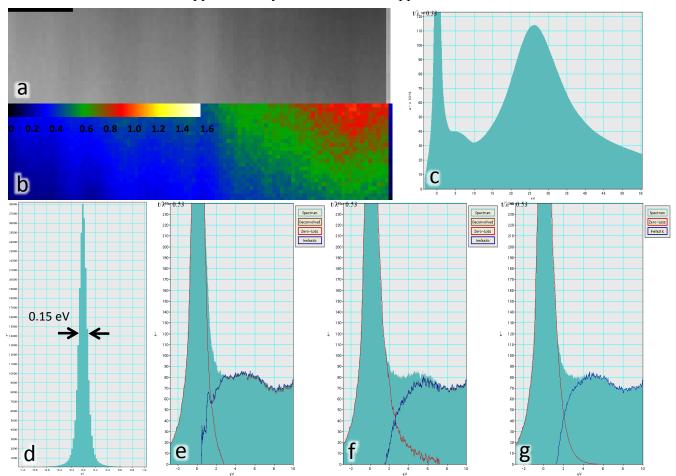


Figure 1.Low loss EELS of cross sectioned P3HT only layer in a BHJ OPV device: a) ZLP EELS SI; b) MFP thickness map; c) Low loss spectrum from (a); d) Vacuum ZLP; e) Reflected Tail ZLP extraction; f) Pre-Measured Zero-Loss (d) ZLP extraction; and g) Fitted Logarithm Tail ZLP extraction.