Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Using graphs to interrogate the atomic structure of polymer blends OLGA WODO, State Univ of NY - Buffalo, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University — The nanomorphology of polymer blend thin films critically affects performance especially in electronic devices. However, many aspects of the underlying physics linking morphology to performance are still poorly understood. Furthermore, there is increasing evidence that atomic organization can hold the key to efficient charge transport within organic electronic devices. In this work, we take advantage of recent advances in molecular dynamic simulations and quantify atomic-scale morphological aspects of the thin films. Specifically, we present a graph-based technique that allows quantifying the point-cloud data. In our approach, we first convert the point cloud data from atomistic simulation into a labelled, weighted, undirected graph and then use standard graph-based algorithms to calculate and quantify morphology features. The conversion of the CGMD-data into a graph preserves all the topological and geometric information about the internal structure, and local connectivity between individual atoms/beads (along and across the polymer chains). Our method provides hierarchical information about the charge paths that a hole/electron needs to take to reach the electrode (path length, fraction of intra-molecular hops, path balance). We showcase capabilities of our approach by analyzing coarse grained molecular simulations, and quantifying effect of various thermal treatment as well as electrode materials on the P3HT:PCBM blend.

Olga Wodo
State Univ of NY - Buffalo

Date submitted: 13 Nov 2014 Electronic form version 1.4