Effect of annealing on structural and optical properties of poly(3-hexylthiophene)/fullerene composite films for organic solar cells

Uladzimir Zhokhavets, Tobias Erb and Gerhard Gobsch
Institute of Physics, Ilmenau Technical University, D-98693 Ilmenau, Germany

Harald Hoppe and N. Serdar Sariciftci
Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University Linz, Altenbergerstr.69, A-4040 Linz, Austria

Pavel Schilinsky, Christoph Waldauf and Christoph Brabec
Konarka Technologies GmbH, Paul-Gossen-Str. 100, 91052 Erlangen, Germany

Composite films of P3HT/PCBM (poly[3-hexylthiophene-2,5-diyl]/ [6,6]-phenyl C_{61} butyric acid methyl ester) are widely used as active layers in plastic solar cells. We have studied the influence of thermal annealing on nano-structural and optical properties of thin spin-coated P3HT/PCBM-films.

X-ray diffraction in grazing incidence geometry shows that the untreated samples are non-crystalline, whereas the annealed samples are partially crystalline (see fig. 1). In not annealed P3HT/PCBM-films the PCBM seems to suppress the formation of polymer crystallites. Most likely, PCBM is very finely dispersed on a molecular basis between P3HT chains, thus preventing P3HT aggregation or crystallization. Whereas for annealed samples the detected peak at $2\theta=5.4°$ originates from P3HT-crystallites with *a*-axis orientation (backbone parallel and side-chains perpendicular to the substrate, as shown in the inset of fig. 1). The mean size of the polymer crystallites L=9 nm was obtained from the full width half maximum of the peak. No PCBM crystallites were detected. So we conclude that the main effect of annealing is the redistribution of PCBM, under enhanced temperature isolated molecules of PCBM begin to diffuse into larger aggregates. In these PCBM free regions, the P3HT aggregates can become converted into P3HT crystallites (see fig. 2).

With spectroscopic ellipsometry, a significant increase of optical absorption (especially in the energy region below 3 eV) and optical anisotropy upon annealing was observed. We assume that the increase of optical absorption is related to the change of the state of aggregation of P3HT from amorphous (not annealed) to crystalline (annealed). The increase of the optical anisotropy can be also explained by formation of the polymer crystallites. From the XRD-measurements it follows that such crystallites have a pronounced *a*-axis orientation. Thus the polymer chains become more parallel oriented to the substrate resulting in a higher optical anisotropy.

The increase of optical absorption together with reduced recombination losses leads to improved solar cell performance. An increase of solar cell efficiency from 1.0 % for the not annealed sample to 3.6% for the annealed sample was observed.

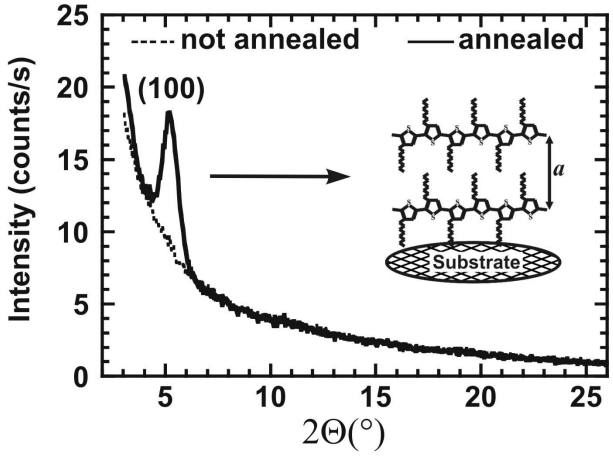

FIG. 1. Diffractogram of the untreated (dashed line) and the annealed (solid line) P3HT/PCBM-films. The orientation of the P3HT-domains with respect to the substrate is shown in the inset.

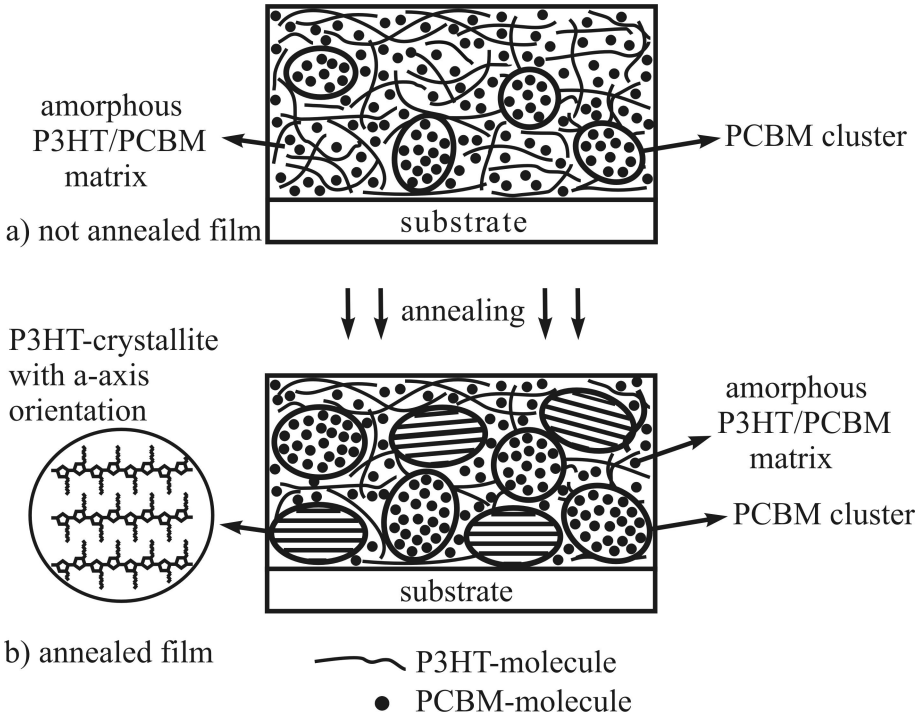

Fig. 2: Structural changes of P3HT/PCBM-films upon annealing (schematically).