MS24-P05

Structural and optical characteristics of non-polar ZnO epitaxial films grown by radio-frequency magnetron sputtering

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ZnO is recognized as an important wide band gap semiconductor material for its applications in UV and blue spectral range devices such as light emitting diodes (LEDs), laser diodes (LDs), and photodetectors. The non-centrosymmetric characteristics of its wurtzite structure gives rise to piezoelectric and spontaneous polarizations along the c-axis. The polarization across the interface of c-axis oriented quantum well structures results in the undesired effects such as quantum confined Stark effect and deteriorates the electronic and optical properties of devices. Therefore, many efforts have been put to grow and to characterize non-polar ZnO epitaxial films.

High-quality non-polar a-plane and m-plane ZnO epitaxial films were grown on r-plane and m-plane sapphire substrates, respectively, by radio-frequency magnetron sputtering. The structural characteristics, including strain and structural defects, of both non-polar ZnO films were studied by X-ray diffraction and transmission electron microscopy (TEM). Surface morphology and roughness of the ZnO samples was investigated by atomic force microscopy (AFM). The anisotropic optical properties of the non-polar ZnO films characterized by polarization-dependent photoluminescence (PL) are correlated with its structural features.

References:

Lin, B. H. et al. (2012). ACS Appl. Mater. Interfaces 4, 5333-5337

Keywords: non-polar ZnO, strain, structural defects

MS25- Combined approaches for the structure determination of new materials at the nanoscale

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MS25-P01

Structure of the conducting PANI/CSA polymer system as seen by XRD, neutron diffraction and advanced computer modeling

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The structure of the conducting polymer system of polyaniline (PANI) protonated with camphorsulfonic acid (CSA) remained unclear for several years and resisted attempts at solving by use of typical methods. This case may serve as an example of how different experimental and computational methods may impact each other and develop a successful, combined approach to structural study aimed at determining a reliable model and verifying its properties.

Molecular dynamics simulations may provide useful information concerning the studied system, even if the accuracy of such simulations is finite. These were performed for PANI/CSA [1] and allowed drawing important conclusions regarding the type of structure – alternating double layers of polymer chains and counterions. Additionally, they suggested the indexing of principle peaks observed in the X-ray powder diffraction pattern obtained for samples of this polymer. Finally, they were the basis for formulating a hypothesis regarding the preferred orientation of crystallites in thin film samples of this system cast from different solvents in agreement with grazing incident beam X-ray diffraction data.

The above described simulations were the foundation for the scope a crystallographic unit cell model. After taking advantage of artificial intelligence based methods aimed at optimizing the layout of the structural units of PANI/CSA within such a cell with respect to the powder diffraction pattern, a new model was found [2]. Apart from satisfying the optimization criteria, is allows explaining the differences observed in neutron diffraction patterns recorded for regular and partially deuterated samples of the studied system. It also has all the previously reported advantages of the principal structure obtained from molecular dynamics simulations and allows verifying the hypothesis regarding preferred orientation in thin films cast from different solvents.

Taking a generalized look at the process of obtaining this new structural model of PANI/CSA, it could be described as an example of a systematic approach in which various experimental (XRD, grazing incident beam X-ray scattering, neutron diffraction) and computational (molecular dynamics, artificial intelligence) techniques mutually inspire one another and allow developing and verifying a structural model of a polymer system. Each of the contributing pieces listed above by themselves are not enough to develop a good structural model, while combining insight into the studied problem provided by each of them leads to one which is reliable.

References:

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Keywords: polyaniline, crystalline structure, simulations

MS25-P02

Combination of GIWAXS and TEM study in understanding polymer-fullerene fibrillar network structure

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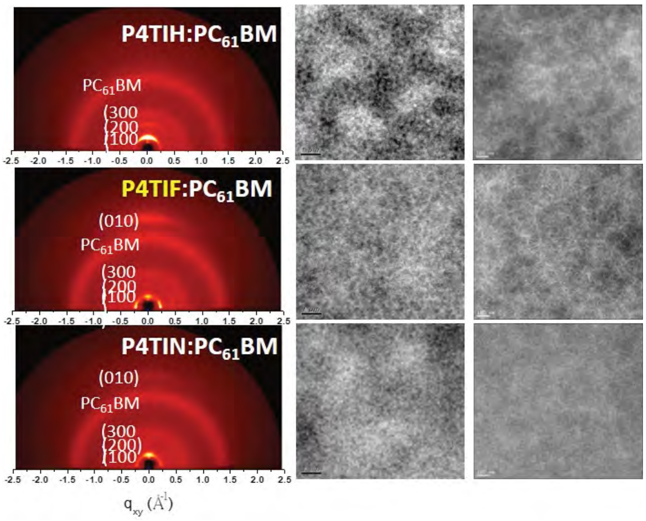
In addition to the larger absorption coefficient and longer absorption wavelength, high short-circuit current density can be associated to the high portion of face-on, in-plane crystallite orientation of **P4TIF**, which is evident by GIWAXS study. GIWAXS study reveals that the face-on (in plane) orientation is most pronounced, lamellar structure, (100), pi-pi stacking structure, (010), and crystallite correlation length are more significant or longer than those of **P4TIN**. Moreover, thin film morphology probed by TEM reveals the fibril network nanostructure, which is more pronounced in PC$_{61}$BM-blended **P4TIF** thin films than **P4TIN** ones. The chemical structure difference between **P4TIF** and **P4TIN** is the fluorine (F) and nitrile (CN) substituent. Such difference in fibrillary morphology, which is in turn due to the different molecular interaction of F or CN, promotes the photocurrent output and hence short-circuit current density of the polymer-based organic photovoltaics.



Keywords: GIWAXS, TEM, polymer-fullerene fibril