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Investigation of titania thin film morphologies via GISAXS and SEM for hybrid solar cells

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As the need for sustainable energy sources is steadily increasing, the concept of photovoltaics has attracted both scientific and economic interest. Whereas conventional semiconductor-based solar cells are already well researched and their efficiencies are promising, their energy need for the mere production and their lack of versatility remain a major drawback. Therefore, concepts are needed, which combine competitive efficiencies with the possibility for energy-inexpensive large-scale production. Hybrid solar cells, which combine the mechanical stability of inorganic semiconductors and the versatility of organic semiconductors, meet these criteria. Titania thin films as an inorganic material in combination with a conjugated polymer as an organic semiconductor are common for application in hybrid photovoltaics. Excitons are generated via light absorption in the p-type conducting polymer and split at the interface of the two compounds due to the band offset. Afterwards, the electrons are transported in the titania and the holes in the p-type polymer respectively.
Due to the restriction of the charge separation to the interfacial area, a nanoscale structure of the active layer is necessary in order to enhance the charge separation. Therefore, mesoporous titania structures, which serve as a matrix for infiltration with the polymer are a promising concept for high-efficiency active layers. Challenges concerning this concept arise due to the difficulty of the infiltration with the polymer, since occlusion of the pores in the upper part of the layer can occur and prevent backfilling of pores in lower parts of the layers. Accordingly, ways to control the structure of mesoporous titania films are of major importance.
We focus on the tuning of the pore size of mesoporous. In our experiments, a solution composed of an amphiphilic block copolymer as a structure-directing agent and a precursor dissolved in an organic solvent is applied as a wet film. Immersion in an antisolvent after an evaporation step leads to a structure formation process in the composite film, so that the morphology depends both on the evaporation time and the immersion bath. By controlling the evaporation step, the porosity of the film can be tuned. After calcination, mesoporous titania films are obtained. The films are characterized concerning their suitability for photovoltaic application, which regards their morphology, crystallinity and thickness. Surface morphologies are experimentally investigated by scanning electron microscopy as well as atomic force microscopy. These methods are suited for the estimation of the porosities of the film and for showing the dependence of the morphology on the processing parameters. In addition to the surface morphology, also the inner morphology is investigated. Therefore, grazing incidence small angle X-ray scattering is applied as a non-destructive method to probe the deeper layers.

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