Determination of optical constants and phase transition temperatures in polymer fullerene thin films for polymer solar cells

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Date: 2 Jan 2012

Program topic: OR Presentation type: Poster
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Plastic photovoltaics combining semiconducting polymers with fullerene derivatives have the potential to become the first cost efficient solar cells able to compete with fossil fuels. The maximum power conversion efficiency is already 8.3%[1] , and new polymers arrive frequently in the search for efficiencies of 10%. As a first step in the screening of candidate materials, the optical constants of the pure polymer as well as the polymer blend with fullerenes are determined from Variable Angle Spectroscopic Ellipsometry (VASE), using Tauc-Lorentz oscillator models, throughout the solar spectrum. These models are then used to predict the upper limits to photocurrent generation in devices, in transfer matrix simulations of the multilayer thin film photovoltaic devices. This forms an essential step in the choice of materials for optimization in devices.

Materials optics measurements are also used to deduce the phase diagram of polymer and polymer blend films. The glass transition temperature is very important for plastic solar cells and must be higher than the 80°C a device can reach to avoid degradation during operation. Temperature dependent ellipsometric measurements has proven to be a feasible way to determine phase transitions in polymer thin films[2] . These transitions are displayed as a sudden change of the volumetric expansion coefficient, and are manifested by an abrupt increase of thickness at the phase transition temperature. For thickness determination a Cauchy model is applied to the transparent infrared part of the spectra.

References