Optical and Electrical Modeling of Three Dimensional Dye Sensitized Solar Cells

P. Guo[1]

[1]Northwestern University, Evanston, IL, USA

Abstract

Dye sensitized solar cells (DSSCs) have received tremendous attention as alternative photon harvesting devices due to their cost-effectiveness and high throughout manufacturing. While the sintered TiO2 nanoparticle network attached with dye molecules achieve efficient photon absorption, the electrons have to diffuse through the long TiO2 network to reach the contact, resulting in a high electron density and thus increased recombination. Extensive research efforts have focused on the development of three-dimensional (3D) DSSCs. TiO2 nanotube and ZnO nanowire array based electrodes have been investigated as efficient photoanodes because they provide straight channels for photo generated electrons.

In this work, we used COMSOL Multiphysics® to simulate the photon absorption and photo generated electron diffusion within the DSSCs, based on either 2D or 3D photoanodes. In the first step, scattered field formulation enabled by the RF Module is applied to model the absorption profile through the photo active layer. Then in a second step electron diffusion equation is used to model the diffusion of photo generated electrons within the TiO2 network. The short circuit current and open circuit voltage can be calculated from a frequency sweep of the solar spectrum. The advantage of the coupled simulation is that 3D transparent conducting electrodes can be straightforwardly incorporated in the model. Using the model, we first compare the performance of DSSCs made of 2D and 3D based photoanodes. A photon conversion efficiency enhancement is found by using the 3D based photoanodes, with TiO2 network that has low electron diffusion length. We then optimized the photoanode geometry by varying the nanorod spacing and height. The underlying physics of the DSSC, such as absorption profile, electron density and recombination rate can be simultaneously extracted from the simulation results, which provides the design guidelines for high efficiency DSSC.