Monte Carlo simulation of electron transport through nanocrystalline TiO_2 in Dye Sensitized Solar Cells.

M.J.Cass[1], A.B.Walker[1] and L.M.Peter[2]
[1]Dept.of Physics, [2]Dept.of Chemistry, University of Bath, Bath BA2 7AY, UK

Dye sensitized nanocrystalline solar cells (Grätzel cells) have achieved solar-to-electrical energy conversion efficiencies of 12% in diffuse daylight. The cell is based on a thin film of dye sensitized nanocrystalline TiO_2 interpenetrated by a redox electrolyte. Photoexcitation of the dye is followed by fast (<100fs) electron injection into the conduction band of the TiO_2 nanoparticles. The injected electrons travel through the nanocrystalline TiO_2 to the anode. Electron transport is slowed by trapping in surface and/or bulk states. Detrapping from these states competes with the back reaction of electrons with I_3^- ions in the electrolyte. The back reaction causes electrons to be removed from the circuit and so reduces efficiency. The morphology of the film can also act to slow the electron transport, increasing the likelihood of back reactions occurring. We employ a Monte Carlo simulation to investigate the effects of the size of the inter-grain necks, trapping and back reaction on the electron transport. It is assumed that traps are located on the surface of the particles.

The passage of a large number of electrons through a 3 dimensional network of interconnected spherical grains, 20nm in diameter, is simulated. We use a fine scale simulation, where the electrons move a few grains along the chain. By repeating such a walk many times, we have obtained probabilities for the number of grains moved and the likelihood of trapping. These can then be used in a coarse scale simulation, in which the position of each electron is recorded only in terms of which grain it occupies, and at each time interval the electron moves or is trapped according to these probabilities. This allows us to model the transient current in response to a pulse of optical illumination. We quantify our results where possible in terms of an effective electron diffusion coefficient.

We simulate a 2μm thick film with an initial electron density between 10^{23} and 10^{24} m^{-3}. Figure 1 shows the affect of varying the inter-grain neck size on the transient photocurrent of a system with no traps. We see that for small inter-grain necks transport through the film is slowed considerably: This effect is expected to be more pronounced when traps are present, as grain to grain transfer will be in competition with trapping.

Figure 2 shows the effect of changing the density of traps in the system, namely to slow the electron transport.

Further work is in progress to relate these simulations to experimental current transients.

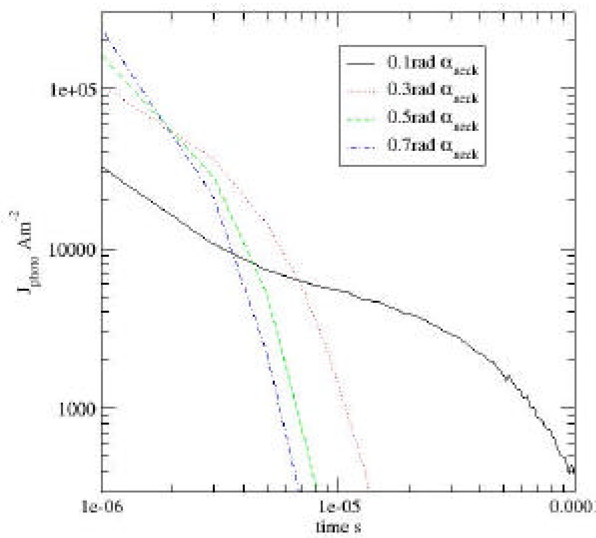

Figure 1, The effect of changing inter-grain neck size on the photo current J_{photo} in a film with no traps. The neck size is specified by α_{neck} (the angle between the line connecting the centres of the grains and a line from the edge of the neck to the grain centre). The initial density of electrons is between 1×10^{23} and $2\times10^{23} m^{-3}$ depending on the neck size.

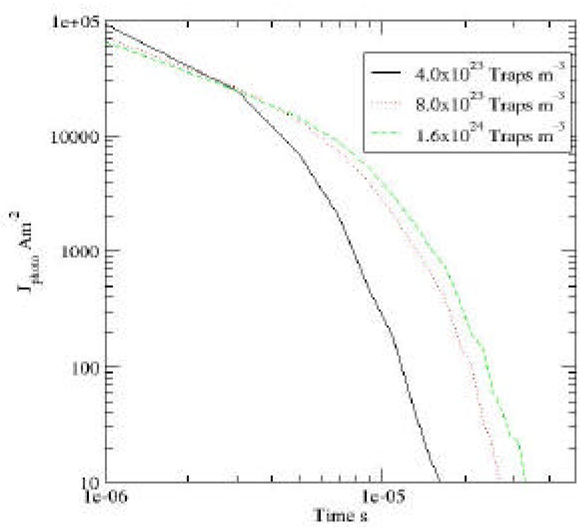

Figure 2, The effect of changing the density of traps. The initial electron density is 8×10^{23} m^{-3} and the inter-grain neck size is set to α_{neck}=0.475rad.