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Advanced TEM characterisation of nanoparticle based solar cells.

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α-Fe_2O_3 nanoparticles (NPs) were embedded into a p-i-n amorphous silicon (a-Si) solar cell as a model system for NP-based solar cells, in which the NPs promote the photogeneration of charge carriers as a result of their high absorption coefficient and suitable band gap. The a-Si p-i-n structure is expected to provide a low defect density matrix, as well as the electric field that is required for charge carrier separation. Key issues for the solar cell performance are the quality of the NP absorber layer, which should have a low recombination rate, as well as effective charge extraction from the NP to the p and n contacts.

α-Fe_2O_3 NPs were synthesized in a wet chemical process without using organic ligands [1]. NP layers were prepared by spin coating on p doped layers, followed by further PECVD growth of intrinsic and n-type layers. All of the silicon layers in the a-Si solar cells were deposited using plasma-enhanced chemical vapour deposition [2].

Although a working solar cell was achieved a comparison of our prototype solar cell with a reference p-i-n junction deposited without NPs showed a significant deterioration of the I-V characteristics and no contribution of the NPs to the quantum efficiency.

In order to study the influence of the deposition process on the NPs, we investigated the structural and electronic properties of Fe_2O_3 NPs before and after embedding. We performed conventional transmission electron microscopy (TEM) using an FEI Tecnai F20 microscope operated at 200 kV and advanced scanning TEM (STEM) and electron energy-loss spectroscopy (EELS) using an FEI Titan TEM operated at 300 kV equipped with a condenser lens aberration corrector.

Figure 5a shows a bright-field TEM image of α-Fe_2O_3 NPs embedded in a p-i-n a-Si solar cell structure, examined in cross section. The NPs form a two-dimensional array and are separated from each other by a-Si. The a-Si contains voids both beneath and near to the NPs, which appear dark in the STEM image shown in Fig. 1b.

The chemical compositions and bonding states of the NPs were investigated using the StripeSTEM EELS technique [3], both before and after embedding. Figure 6a shows line scans of background-subtracted Fe L and O K edge intensities recorded across the surface of an α-Fe_2O_3 NP that was not embedded. No indication of an O-rich shell is observed. Figure 2b shows similar results after embedding, from the interface between a NP and the surrounding a-Si as indicated in Figure 5b. An O-rich shell of thickness (1 ± 0.3) nm is observed around the embedded NP. In Figure **7**, the O K edge onset energy of the shell is compared with that of α-Fe_2O_3. The pre-peak at 532 eV, which is characteristic for α-Fe_2O_3, is missing in the O-rich shell. This missing peak is consistent with the O being bonded to silicon. Moreover, the Fe L_2 and Fe L_3 edge energies and ratios stay constant, providing no indication of changes in the bonding state of iron. We conclude that the shell around the embedded α-Fe_2O_3 NPs consists of O-rich Si.

The observed O-rich shells around the NPs may inhibit carrier extraction and may therefore explain the lack of a contribution from the NPs to the quantum efficiency. A possible reason for the formation of the shell is the presence of a remaining surface layer of water after spin coating, which may lead to the formation of a thin O-rich Si layer during the early stages of growth of the intrinsic a-Si matrix.

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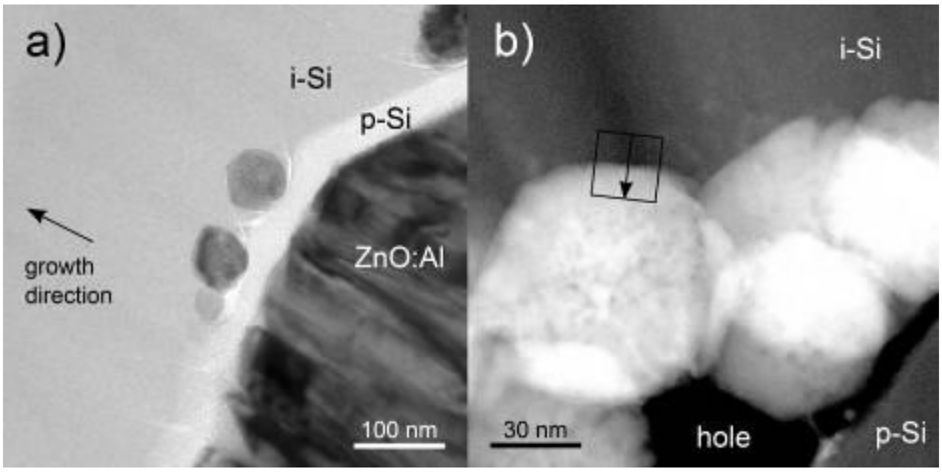

Figure 5. (a) Bright-field TEM image and (b) HAADF STEM image (inner detector angle 70 mrad) acquired from a cross-sectional specimen of α-Fe_2O_3 NPs embedded in a Si solar cell structure. The marked region and arrow in (b) indicate the area from which the STEM/EELS measurements in Fig. 2b were obtained.

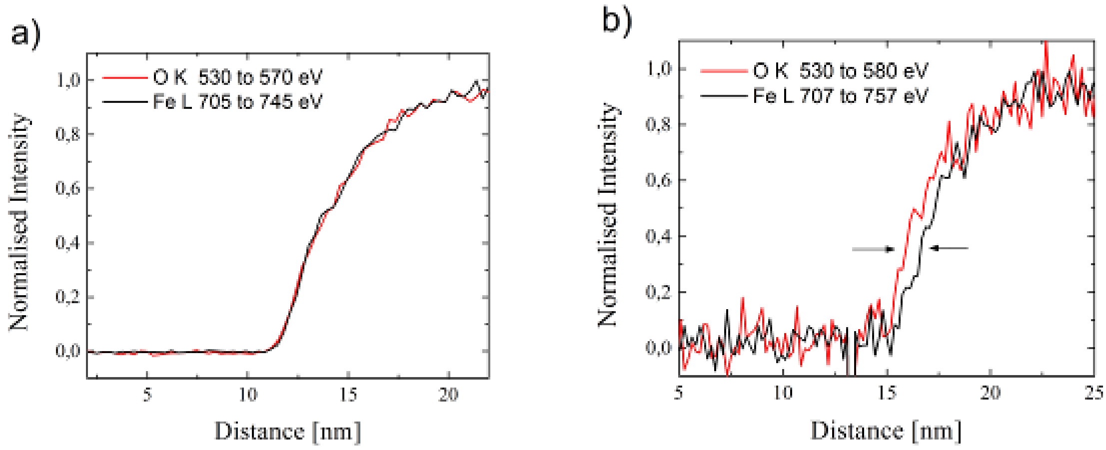

Figure 6. Integrated intensity profile determined from background-subtracted O K and Fe L EELS edges across the interface (a) between vacuum and a pristine NP and (b) between the a-Si interface and an embedded NP.

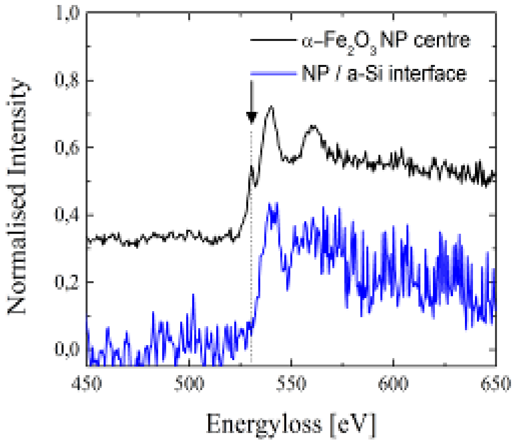

Figure 7. Background-subtracted EELS edges showing the O K edge onset recorded from an embedded α-Fe_2O_3 NP, both from its centre (black curve) and from the NP/a-Si interface (blue curve). The intensity was averaged over distances of 5 and 1 nm, respectively. The line and arrow mark a pre-edge peak at 532 eV that is characteristic for α-Fe_2O_3. The spectra have been shifted vertically for clarity.