Supporting Information:

Comparison of Ag and SiO₂ Nanoparticles for Light Trapping Applications in Silicon Thin Film Solar Cells

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METHODS

Fabrication of Nanoparticle Substrates. 30 nm of Al and 50 nm of Ag were electron beam evaporated on flat glass substrates (Schott AF 32 eco) as a metallic back contact. Then, a monolayer of PS nanospheres (ordered from microParticles GmbH Berlin in an aqueous dispersion of 10 wt%) with a diameter of 700 nm was deposited on top of the substrate as an evaporation mask (Figure 1b). Therefore, we diluted the PS dispersion with one part of H₂O and two parts of ethanol. The substrates and a sacrifice glass slide of similar height were stored in a petri dish filled with H₂O, covering the substrate's surface. The NP dispersion was poured dropwise onto the sacrifice sample until the entire water surface was covered with a monolayer of PS beads. The water was then removed with a Pasteur pipette and the samples dried under incandescent light. To obtain the different types of NPs, 140 nm of Ag or SiO₂ were electron beam evaporated on the PS beads, followed by a lift-off in toluene (Figure 1d) and a cleaning step by sonication in ethanol and blow drying with N₂. A 70 nm layer of ITO was deposited by DC magnetron sputtering on top of the NPs, serving as a diffusion barrier and optical spacer between the metallic/dielectric NPs and the a-Si:H (Figure 1e).

Solar Cell Fabrication and Characterization. Solar cells were fabricated on all substrates in n-i-p configuration (deposition order: n-doped / intrinsic / p-doped) by plasma-enhanced chemical vapor deposition and in a shared process to ensure comparability. SiH₄, H₂ and PH₃ were used as precursors for the n-doped layer (30 nm), SiH₄ and H₂ for the intrinsic layer (400 nm) and SiH₄, H₂ and B₂H₆ for the p-doped layer (20 nm), respectively. An ITO layer of 70 nm thickness was used as a transparent front electrode. All solar cells were annealed for 30 min at 160°C before characterization. The active cell area of the solar cells was defined by the size of the front contact to a square opening of 0.25 cm² using a marker pen and a lift-off process. Short

circuit current densities (J_{SC}) were obtained from external quantum efficiency (EQE) measurements by convolution with the AM1.5G spectrum. Open circuit voltage (V_{OC}), fill factor (FF) and PCE were measured with a solar simulator under standard test conditions. Solar cells were attached to a spectrophotometer (Varian Cary 5000) using an integrating sphere for the reflectivity characterization. A Hitachi FB-2100 FIB was used to cut the cross section and a Hitachi S4800 FESEM was used to obtain scanning electron micrographs with an in-lens secondary electron backscattering detector and an accelerating voltage of 5 kV.

Simulation Method. Optical material parameters were obtained by spectroscopic ellipsometry and subsequent modeling except for the Ag parameters, which were taken from the reference book¹. The software Sentaurus TCAD by Synopsys Inc. was used for the finite-difference time-domain (FDTD) simulation. To speed up the computation, calculations were partly performed on graphics processing units using the CUDA platform by Nvidia Inc. and the corresponding implementation from Acceleware Ltd. The simulation domain as shown in Figure 4a was designed according to the experimental structure using basic geometrical shapes. For the electromagnetic field calculation a discretization (tensor mesh) of 6 nm in x and y directions and of 3 nm in z direction was applied. Individual simulations for each wavelength (step size 5 nm) were carried out with plane wave excitation. For the EQE calculation, only the absorption in the intrinsic layer and not in the doped layers was taken into account. The absorbed photon flux was related to the incident photon flux to obtain an absorption spectrum. The simulated EQE spectrum equals this absorption spectrum under the assumption that each absorbed photon generates one charge carrier pair which is perfectly extracted from the absorber layer.

Reference:

(1) Palik, E. D., Handbook of optical constants of solids. Acad. Press: Boston u.a., 1997.