Supporting Information: Design of Nanostructured Solar Cells Using Coupled Optical and Electrical Modeling

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SOURCES OF PARASITIC ABSORPTION

This study highlights the importance of accounting for the spatial profile of optical absorption within the solar cell material (in this case, a-Si:H). Our method shows that light trapping structures can be chosen to direct light into the intrinsic region of the a-Si:H, thus increasing the efficiency with which charge carriers are collected when compared to structures which feature higher levels of absorption within the doped a-Si:H. We also note that materials other than the doped a-Si:H are sources of parasitic absorption in the structures considered here. These losses are accounted for in the optical simulation step of our method.

Figure S1 shows how each of the materials in the conformal AZO and conformal Ag structures contribute to the overall absorption of the device. Absorption in layers other than a-Si:H represents an optical loss in the device, as it cannot be expected to contribute to photocurrent. These losses depend on the details of the nanostructure, and are non-negligible in the Ag and ITO. They are an important consideration when designing light trapping structures.[1]

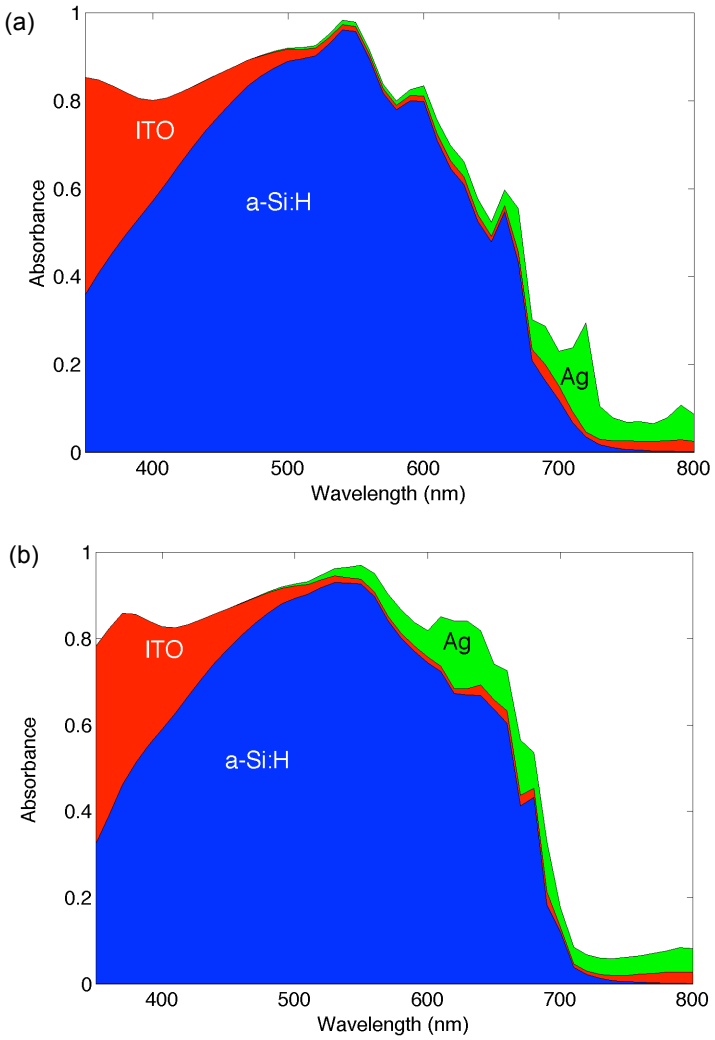

Figure S1. Spectral absorption, calculated from optical simulations, in each of the device layers of the "conformal AZO" device structure (a), and "conformal Ag" structure (b). Only the absorption in the a-Si:H can be expected to contribute to photocurrent. Absorption in the AZO layers is negligibly low.

ELECTRICAL SIMULATION DETAILS

The electrical parameters for a-Si:H used in the device physics model for this study were adapted from Schropp and Zeman[2] and are detailed here. It is important to note that there is no single agreed upon set of electrical parameters for a-Si:H, and that in general these will be dependent of on the details of material processing.

Basic a-Si:H electrical parameters

- Dielectric constant: 11.9
- Band gap: 1.78 eV
- Electron affinity: 4 eV
- Effective density of states in conduction band: 1×10^{20} cm^{-3}
- Effective density of states in the valence band: 1×10^{20} cm^{-3}
- Mobility (electron, hole): 20 cm^2 s^{-1}, 5 cm^2 s^{-1}
- Thermal velocity (electrons and holes): 4.27×10^4 cm s^{-1}

Traps

The device physics simulation software package used in this study allows for the explicit inclusion of traps accounting for their recombination statistics and electrostatic effects.[3] We include traps distributed in energy throughout the band gap as detailed in Table S1. These distributions are discretized into 15 levels in the band gap. Band tail ("BT") traps are distributed as a function of the energy, *E,* in the band gap according to an exponential:

$$N_0 e^{-\left|\frac{E-E_0}{E_s}\right|}.$$

Dangling bond traps ("DB") are distributed in the band gap according to a Gaussian:

$$N_0 e^{\frac{-(E-E_0)^2}{2E_s^2}}.$$

All the distributions are defined with respect to the conduction band edge with the exception of the donor/BT traps, which are defined with respect to the valence band edge.

All BT traps have capture cross-sections for both electrons and holes of 1.6×10^{-14} cm^2.

All DB traps have capture cross-sections of 7×10^{-14} cm^2.

Table S1. Trap Parameters

Layer	Type	N_o (cm^{-3})	E_o (eV)	E_s (eV)
Intrinsic	Acceptor/BT	8.00×10^{21}	0	0.032
	Donor/BT	4.00×10^{21}	0	0.047
	Donor/DB	2.00×10^{17}	0.89	0.144
	Acceptor/DB	2.00×10^{17}	0.69	0.144
P-type	Acceptor/BT	2.00×10^{21}	0	0.180
	Donor/BT	1.00×10^{21}	0	0.090
	Donor/DB	2.20×10^{19}	0.7	0.144
	Acceptor/DB	2.20×10^{19}	0.5	0.144
N-type	Acceptor/BT	1.00×10^{21}	0	0.070
	Donor/BT	2.00×10^{21}	0	0.160
	Donor/DB	5.54×10^{19}	1.4	0.144
	Acceptor/DB	5.54×10^{19}	1.2	0.144

REFERENCES

1. Ferry, V. E.; Polman, A.; Atwater, H. A. *ACS Nano* **2011,** 5, (12), 10055-10064.

2. Schropp, R. E. I.; Zeman, M., *Amorphous and microcrystalline silicon solar cells: modeling, materials and device technology*. Kluwer Academic Publishers: Norwell, Massachusetts 1998.

3. *TCAD Sentaurus*, (http://www.synopsis.com).