

Supporting Information

This document contains the cross-sectional FIB-SEM images of the BLiS solar cell device, the surface topography images of the back-reflectors, the FDTD simulation model and the calculated optical absorption of the flat and BLiS solar cell devices.

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Article Title: Nanomolded buried light-scattering (BLiS) back-reflectors using dielectric nanoparticles for light harvesting in thin-film silicon solar cells

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FDTD Numerical Simulation

The absorbed power per unit area (\mathbf{P}) was calculated from the divergence of the pointing vector:

$$\mathbf{P}(\mathbf{r}, \omega) = \frac{1}{2} \omega \varepsilon''(\mathbf{r}, \omega) |\mathbf{E}(\mathbf{r}, \omega)|^2 \quad (\text{S-1})$$

where $|\mathbf{E}(\mathbf{r}, \omega)|$ is the magnitude of the electric field, $\varepsilon''(\mathbf{r}, \omega)$ is the imaginary part of the dielectric permittivity, \mathbf{r} is the position vector and ω is the angular frequency of the incident light.

To obtain a solar-spectrum-weighted optical generation rate (\mathbf{G}), the simulated fraction of absorbed light in the intrinsic layer of a-Si:H was calculated. The generation rate, \mathbf{G} is calculated considering one electron-hole pair generation for every absorbed photon and using

$$\mathbf{G}(\mathbf{r}, \omega) = \frac{1}{2\hbar} \varepsilon''(\mathbf{r}, \omega) |\mathbf{E}(\mathbf{r}, \omega)|^2 \quad (\text{S-2})$$

where \hbar is the reduced Planck's constant. The net AM1.5 solar spectrum-weighted generation rate of the solar cells is determined using

$$\mathbf{G}(\mathbf{r}, \omega) = \frac{1}{2\hbar} \int \frac{I_{\text{AM1.5}}(\omega) \mathbf{P}(\mathbf{r}, \omega)}{I_{\text{Source}}(\omega)} d\omega \quad (\text{S-3})$$

where I_{Source} is the light source intensity, and $I_{\text{AM1.5}}$ is the intensity of the solar AM1.5 spectrum. Then, the ideal J_{sc} is calculated using

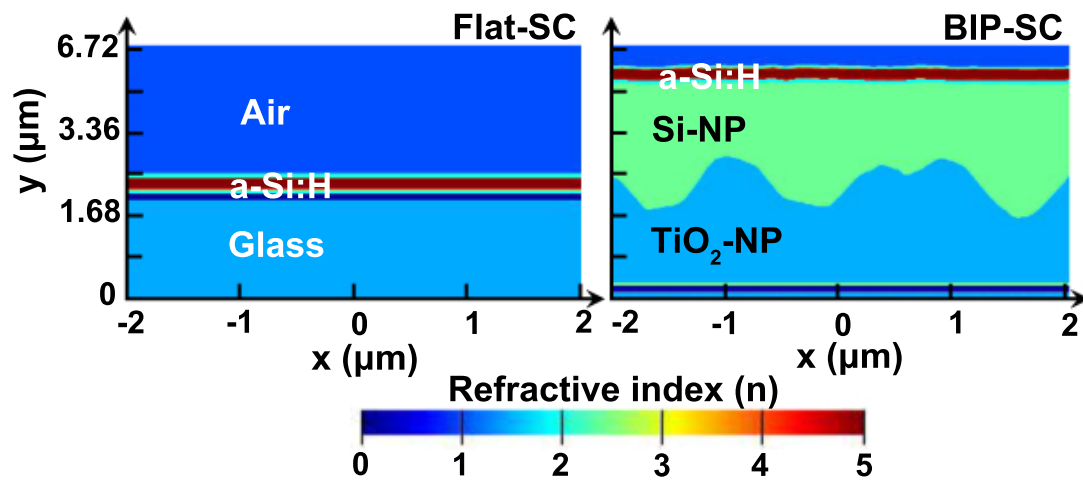
$$J_{\text{sc}} = \int \frac{e\mathbf{G}(\mathbf{r})}{A} d\mathbf{r} \quad (\text{S-4})$$

where e is the free electron charge and A is the solar cell area.

FDTD simulation model

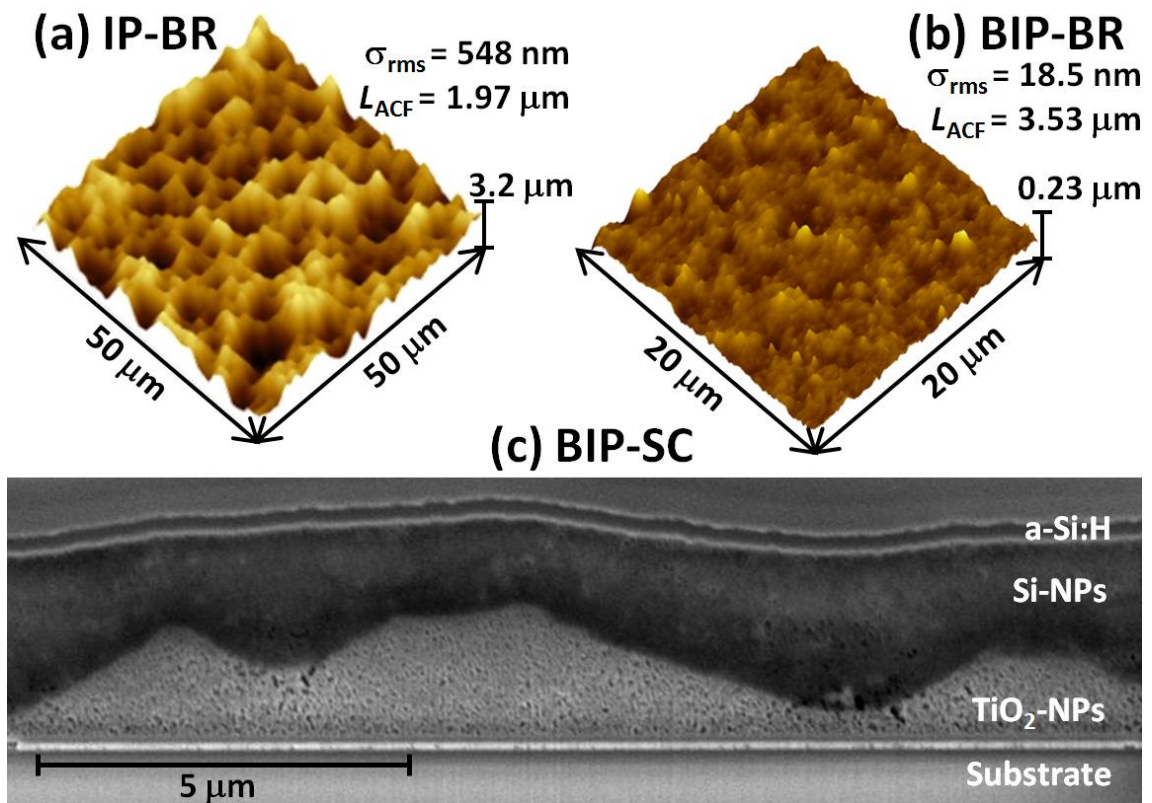
The structural parameter of the model, like the thicknesses of the TiO₂-NP and the Si-NP layers were taken from the cross-sectional FIB-SEM images of the fabricated devices (Supplementary Figure S2c). To obtain a realistic solar cell architecture, the AFM topographical data of the nanoparticle coated back-reflectors (Supplementary Figure S2a,b) were imported into the simulation to model. The layer thicknesses used for the constituent TCOs and a-Si:H (doped and intrinsic) thin films of the solar cell model architecture were estimated from the deposition time and their respective individual growth rates obtained from the reference samples. For simplicity, a conformal coating of these layers was considered.

A periodic boundary condition was set for a period of 4 μm in the x-direction and perfectly matched layer boundary conditions were applied in the y-direction (Supplementary Figure S1). A broadband plane wave (400–800 nm) was injected into the simulation region in the negative y-direction. The optical parameters like refractive indices and dielectric constants of all the layers except the Ag were obtained from spectroscopic ellipsometry measurements. The optical data for Ag was taken from literature.



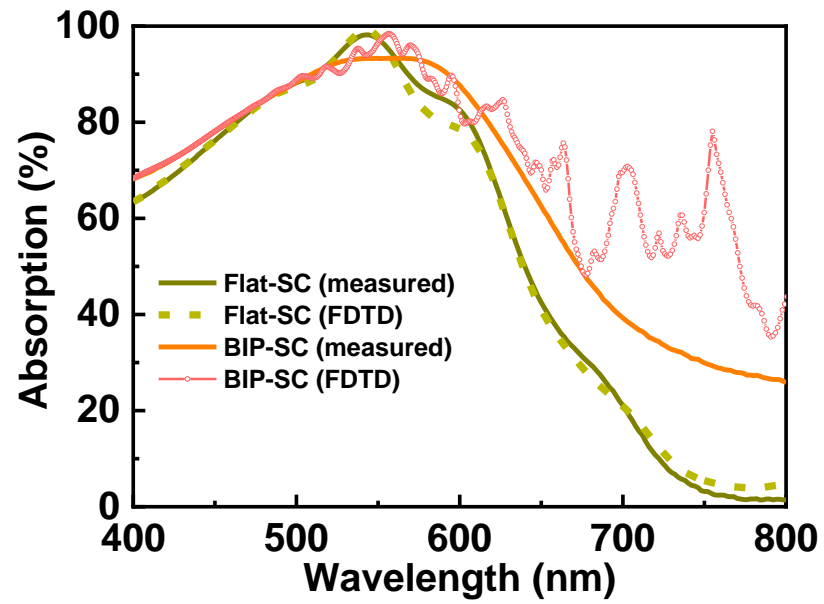
Supplementary Figure

Figure S1. Cross-sectional FDTD simulation models constructed for Flat-SC and BIP-SC devices. The color bar represents the refractive indices of the materials in the solar cell structures at $\lambda = 500$ nm.



Supplementary Figure

Figure S2. AFM images of the surface morphology of a) IP-BR and b) BIP-BR, and (c) FIB milled cross-sectional SEM image of an a-Si:H thin-film solar cell grown on BIP-BR (BIP-SC). σ_{rms} denotes the root mean square roughness and L_{ACF} denotes the length of autocorrelation function.



Supplementary Figure

Figure S3. Comparison of absorption of a-Si:H thin film solar cells (Flat-SC and BIP-SC devices) obtained from FDTD simulation (dotted lines) and experimental measurement (solid lines).