Electronic Supplementary Material (ESI) for Nanoscale

Supporting Information

An efficient broadband and omnidirectional light-harvesting scheme employing the hierarchical structure based on ZnO nanorod/Si_3N_4-coated Si microgroove on 5-inch single crystalline Si solar cells

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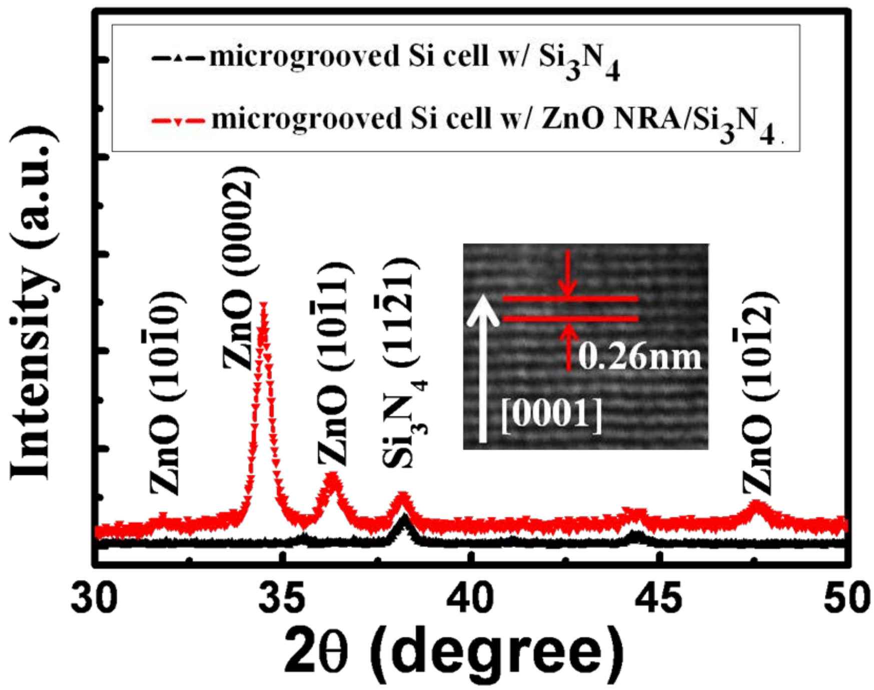


Fig. S1: The XRD pattern of the solar cells with Si_3N_4-coated Si microgrooves before and after the ZnO NRAs growth. The inset is the HRTEM image of a single ZnO nanorod.

The crystalline quality of ZnO NRAs was characterized by x-ray diffraction (XRD) with a fixed incident angle of 0.5˚. Figure S2 shows the XRD pattern of the NRAs. A strong peak locating at 34.48˚ corresponds to the diffraction from (0002) plane of ZnO.[S1] The recognizable peaks at 31.76˚, 36.22˚, 47.64˚ and 38.18˚ refer to (10-10), (10-11), (10-12) plane of ZnO and (11-21) planes of Si_3N_4, respectively. All of the ZnO diffraction peaks can be ascribed to the wurtzite ZnO structure with lattice constants of a = 0.3249 nm and c = 0.5205 nm. The inset in Fig. S1 shows a high-resolution transmission electron microscopy (HRTEM) image of the nanorod, indicating that the nanorod is grown along the [0001] direction. The interplanar spacing of approximately 0.26 nm measured from the fringe pattern of the HRTEM image corresponds to the (0002) lattice spacing of ZnO.

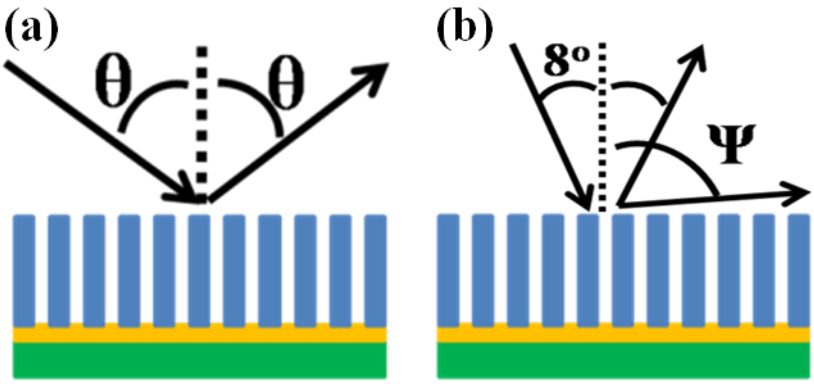
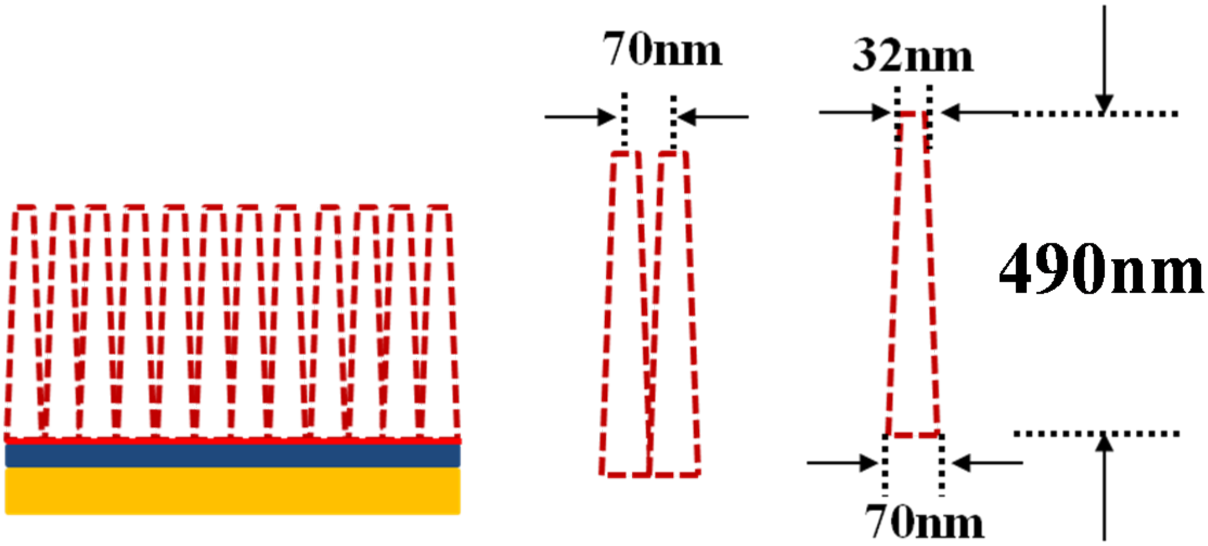


Figure S2: (a) Schematic of the AOI (θ)-dependent reflectance measurement. (b) Schematic of the AOD (Ψ)-dependent reflectance measurement.

Angles of incidence (AOI) and angles of detection (AOD) measurements: To demonstrate the omnidirectionality of ZnO NRA/Si_3N_4-coated Si microgrooved surfaces, the specular reflectance spectra on the solar cells with the three structured surfaces was measured at the AOI ranging from 0^o to 70^o. At every AOI, the incident wavelength was varied in the range of 300-850 nm. The AOD-dependent reflection is dominated by backward scattering. During the measurement, AOI was fixed at 8^o, while AODs and wavelengths were varied in the ranges of 8^o-80^o and 300-850 nm, respectively.

Total reflection measurements: The spectra of total reflectance were measured by a JASCO V-670 UV-visible spectrometer in the spectral range from 360 to 1100 nm. During the measurement, the reflected light in all directions was collected by the integrating sphere mounted on the spectrometer.



Layer	Material	Thickness (nm)	n at 500 nm	k at 500 nm	References
1	ZnO NRAs	490	2.0400	0	[S2]
2	dense ZnO	10	2.0400	0	[S2]
3	Si_3N_4	70	2.0494	0.0149	[S3]
4	Si	20000	4.3490	0.0156	[S4]

Figure S3: Schematic diagram of the Si solar cell with graded AR layers for FDTD simulations.

Steady-state filed distributions within the area of 3×22 μm^2 were calculated. The wavelength for the simulation is selected to be 500 nm, being close to the peak wavelength of solar irradiance. N and K are the wavelength-dependent refractive indices and extinction coefficients, respectively. Dimensions of the nanorods were the average values determined by SEM images shown in Fig. 2(d) in the manuscript. According to the magnified top-view image of Fig. 2(e), the area density of the NRAs, defined as the number of nanorods per unit area, is estimated to be 2.04 × 10^8 cm^{-2}. The diameter and the length of the ZnO NRAs are 70±5 nm and

500±15nm, respectively. For the device with ZnO NRAs, the linear density of nanorods on the surface (14.28 μm^{-1}) is estimated using SEM images. The grid sizes are $\Delta x \times \Delta z = 0.05 \times 0.002$ μm^2 in space domain, and the time step for every calculation is 0.0067 fs. Boundary in x direction is periodic extension layers. Boundary in z direction is surrounded by the 500-nm perfectly matching layers to absorb the electromagnetic waves.[S5] The 3-μm-wide excitation source is placed at Z=1 μm, i.e., around 1.2 μm away from the air/n-type-Si interface. Considering the close-packed NRAs with the line density of 14.28 nanorods on the 1-μm microgrooved surface were approximated to be evenly distributed. The electrodes and the regions below the 20-μm surface of the silicon were neglected. The effects of doping on N and K were also assumed to be negligible. All of the calculated values are normalized to the ones of the excitation source. The optical absorption is defined as the normalized E_y integrated over the region of 20-μm Si.

References

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