

Absorption Enhancement in Ultrathin Crystalline Silicon Solar Cells with Antireflection and Light-Trapping Nanocone Gratings

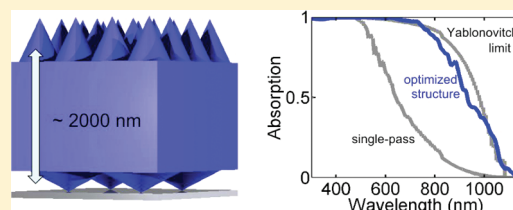
Ken Xingze Wang,[†] Zongfu Yu,[‡] Victor Liu,[‡] Yi Cui,^{§,||} and Shanhui Fan^{*,‡}

[†]Department of Applied Physics, [‡]Department of Electrical Engineering, and [§]Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, United States

^{||}Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California 94205, United States

ABSTRACT: Enhancing the light absorption in ultrathin-film silicon solar cells is important for improving efficiency and reducing cost. We introduce a double-sided grating design, where the front and back surfaces of the cell are separately optimized for antireflection and light trapping, respectively. The optimized structure yields a photocurrent of 34.6 mA/cm² at an equivalent thickness of 2 μm, close to the Yablonovitch limit. This approach is applicable to various thicknesses and is robust against metallic loss in the back reflector.

KEYWORDS: Solar cells, light trapping, antireflection, crystalline silicon, absorption enhancement, nanocone gratings



There is significant recent interest in designing ultrathin crystalline silicon solar cells with active layer thickness of a few micrometers.^{1–17} Efficient light absorption in such thin films requires both broadband antireflection coatings and effective light trapping techniques, which often have different design considerations. In this Letter, we show that by employing a double-sided grating design, we can separately optimize the geometries for antireflection and light trapping purposes to achieve broadband light absorption enhancement. The photocurrent generated by the proposed thin film absorber is able to reach the Yablonovitch limit.^{18–20}

We use nanocones as the basic building elements for the grating geometry because of their unique optical properties and compatibility with inexpensive fabrication techniques.^{21–23} The structure we consider, as shown in Figure 1a, contains a crystalline silicon thin film with nanocone gratings also made of silicon. The circular nanocones form two-dimensional square lattices on both the front and the back surfaces. The film is placed on a mirror. As a starting point, we assume the mirror is made of a perfect electric conductor (PEC). We will consider the more realistic silver mirror with metal loss toward the end of the paper.

The optimization process is as follows: For a given structure with two-dimensional nanocone gratings, using the rigorous coupled wave analysis (RCWA),^{24–26} we calculate the absorption spectrum from which we determine the short circuit current assuming an air mass 1.5 (AM1.5) incident solar irradiance. In a supercell of period 1000 nm, we optimize the geometry over six parameters, the numbers of primitive cells and the base radii and heights of the nanocones on both sides, for the greatest photocurrent generated from the structure. In the optimization, we adjust those geometrical parameters, as well as the thickness of the uniform layer sandwiched between the top and bottom gratings, while ensuring that the structures always consist of the same amount of silicon as a flat thin film structure with a predetermined

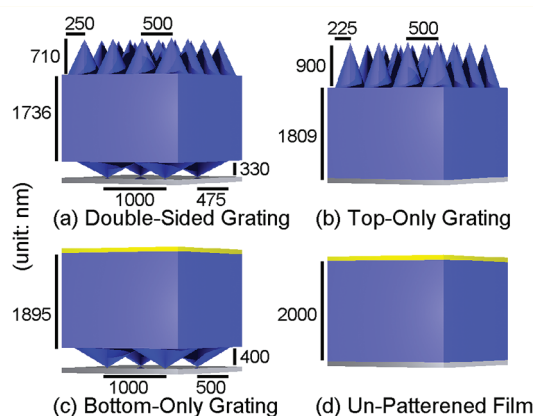


Figure 1. Three-dimensional silicon thin film structures in air. In all subfigures, blue represents silicon, gray represents a perfect electric conductor (PEC), and yellow represents nonabsorbing silicon nitride. The nanocones are made of silicon, as is the uniform layers, and they are placed in a two-dimensional square lattice either on the front or on the back surface of the film. (a) The optimized double-sided nanostructure. (b) The optimized top-only nanostructure. (c) The optimized bottom-only nanostructure with a thin layer of nonabsorbing silicon nitride on top. (d) The flat film with a thin layer of nonabsorbing silicon nitride on top.

thickness. We refer to this thickness as the equivalent thickness of our nanostructured thin film.

Our optimized structure for an equivalent thickness of 2 μm is shown in Figure 1a. For the top nanocones, the period is 500 nm, the base radius is 250 nm, and the height is 710 nm; for the bottom nanocones, the period is 1000 nm, the base radius is 475 nm, and the height is 330 nm. The thickness of

Received: December 26, 2011

Revised: February 17, 2012

Published: February 22, 2012

the uniform layer of the thin film is 1736 nm. For this structure, the absorption spectrum is shown in Figure 2a. This structure

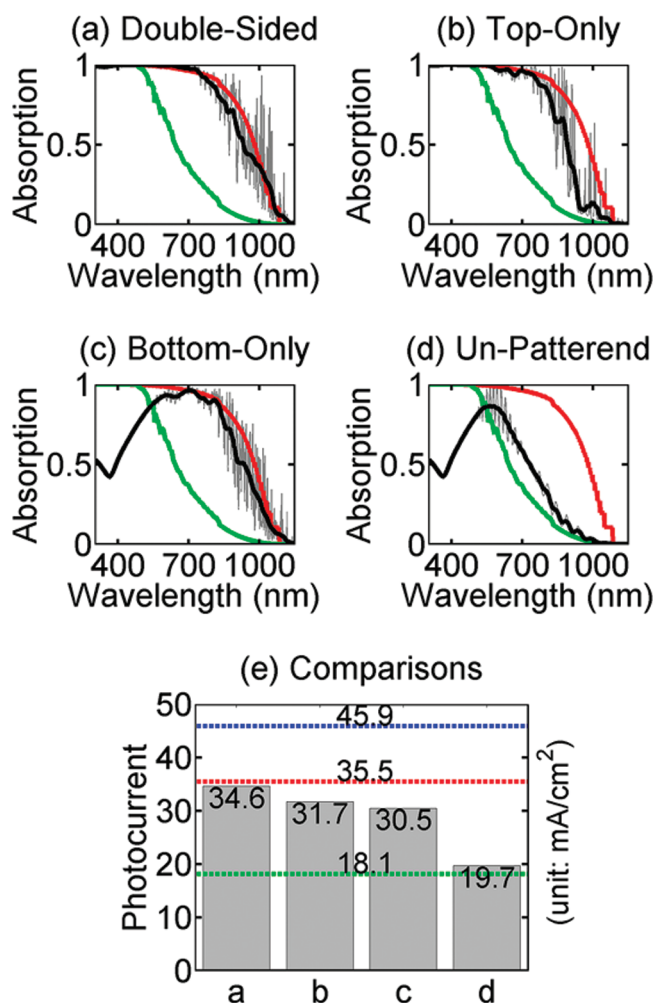


Figure 2. Absorption spectra under normal incidence from AM1.5 solar irradiance. The red curves represent the Yablonoitch limit given by eq 2, the green curves represent the single-pass absorption spectra given by eq 1, and the thick black curves are running averages of the absorption spectra for the corresponding structures in Figure 1. The kinks at the longer wavelength range in the curves are due to the discontinuity of the material constant from the reference book.³¹ (a) The absorption spectrum of the double-sided structure in Figure 1a. (b) The absorption spectrum of the “top-only” structure in Figure 1b. (c) The absorption spectrum of the “bottom-only” structure in Figure 1c. (d) The absorption spectrum of the flat thin film in Figure 1d. (e) Comparison of the short-circuit currents generated by the four structures (gray bars), the Yablonoitch limit (red line), the single-pass absorption (green line), and the full absorption (blue line).

generates a short circuit current of 34.6 mA/cm² assuming normal incidence from an AM1.5 solar spectrum.

In Figure 2, we compare the performance of our structure to both the single-pass absorption and the Yablonoitch limit of 2 μm thick film. Assuming perfect antireflection but no light trapping, that is, light passing through the material only once, and assuming normal incidence, the single-pass absorption spectrum (the green curves in Figure 2) in a thin film with thickness d is given by

$$A_{\text{singlepass}} = 1 - e^{-\alpha d} \quad (1)$$

where α is the absorption coefficient. Assuming perfect antireflection and perfect light trapping, the absorption spectrum (the red curves in Figure 2) in a thin film with thickness d is given by the Yablonoitch limit^{18–20}

$$A_{\text{Yablonoitch}} = 1 - \frac{1}{1 + 4n^2\alpha d} \quad (2)$$

where n is the real part of the refractive index. The absorption spectrum of our optimized structure is much higher than the single-pass absorption spectrum given by eq 1, and it is very close to the Yablonoitch-limit spectrum given by eq 2. The short circuit current of 34.6 mA/cm² in our optimized design is very close to 35.5 mA/cm², the short-circuit current corresponding to the Yablonoitch limit at the equivalent thickness of 2 μm.

The device physics for the absorption enhancement strategy in our structure is as follows: The usable solar spectrum for a crystalline silicon cell extends from 300 to 1100 nm. To achieve significant absorption enhancement, one needs broad-band antireflection over the entire usable solar spectrum due to the strong impedance mismatch between silicon and air. One also needs efficient light trapping from roughly 800 to 1100 nm where a silicon cell with an equivalent thickness of a few micrometers is weakly absorbing. Our strategy is to use the front surface grating for the goal of antireflection, and the back surface grating for the goal of light trapping. Doing so allows us to separately address the different structural requirements in order to achieve these two separate goals. Below, we illustrate this strategy by comparing our optimized structure to optimized “top-only” and “bottom-only” grating structures. All these structures have an equivalent thickness of 2 μm. In the study of these optimized “top-only” or “bottom-only” structures, we will compare their performance to a flat thin film structure with the same equivalent thickness and with a nonabsorbing silicon nitride antireflection coating on top, as shown in Figure 1d.

The optimized “top-only” structure and its absorption spectrum are shown in Figures 1b and 2b, respectively. The periodicity of the nanocone grating is 500 nm, and the height is 900 nm, four times the base radius of 225 nm. The planar part of the structure has a thickness of 1809 nm. Comparing the absorption spectrum of such an optimized “top-only” structure (see Figure 2b) to that of the unpatterned flat thin film in Figure 2d, we observe substantial absorption enhancement over the entire usable solar spectrum. The short-circuit photocurrent for the “top-only” structure is 31.7 mA/cm², compared to 19.7 mA/cm² for the flat thin film. From 300 to 700 nm, the absorption curve closely follows the Yablonoitch limit.

The contribution for light absorption enhancement in Figure 2b, compared to the flat thin film absorption in Figure 2d, originates mainly from antireflection. Nanocone arrays suppress reflection because the cone geometry provides an averaged, graded index from air to silicon as the radius of its cross section increases from zero to its maximum at the planar film surface. The reflection suppression is broadband since the index-matching is largely independent of wavelength. To achieve effective antireflection, the periodicity of the array has to be in the subwavelength regime for the incoming light to see an effective averaged index. In addition, a high aspect ratio is preferred to provide a smooth index transition from air to silicon. These structural aspects are precisely what we see in the optimized “top-only” structure. However, for longer wavelengths, between 700 and 1100 nm, the absorption of the optimized “top-only” structure falls significantly below the Yablonoitch limit. Therefore, the structural feature of a nanocone that is optimal for antireflection purposes is suboptimal for light

trapping. Nevertheless, such a nanocone structure for antireflection has excellent performance in a wide range of light incident angles since the gradual change of refractive index is maintained over this range.^{21,23}

The optimized “bottom-only” grating structure and its absorption spectrum are shown in Figures 1c and 2c. The periodicity of the nanocone grating is 1000 nm. For an individual nanocone, the height is 400 nm, and the base radius is 500 nm. The planar part of the structure has a thickness of 1895 nm to ensure the total 2 μm equivalent thickness. We also place a 90 nm thick non-absorbing silicon nitride antireflection coating on top.⁵ This structure has a short circuit current of 30.5 mA/cm². Comparing the absorption spectrum of the optimized “bottom-only” structure to that of the planar structure in Figure 1d, we observe significant absorption enhancement beyond 600 nm, where the absorption of the optimized “bottom-only” structure closely follows the Yablonovitch limit. However, in the wavelength range below 600 nm, light absorption is below the Yablonovitch limit and even below the single-pass absorption spectrum due to optical loss from the reflection at the silicon-air interface. The nanocone grating structure on the bottom surface certainly does not contribute to antireflection.

A nanocone structure that is optimal for light trapping, as shown in Figure 1c, has very different structural characteristics, compared with the optimal nanocone structure for antireflection in Figure 1b. The spectrum in Figure 2c shows that the absorption enhancement due to light trapping is primarily in the longer wavelength range where the silicon absorption is weak. Light trapping relies on the excitation of guided resonances,^{27–29} and therefore a careful choice of periodicity is important. The requirements on periodicity depend on two considerations. On one hand, more guided resonances lead to higher absorption, for which a large period is preferred. On the other hand, each of the guided resonances should not couple and leak to many external channels, that is, diffraction directions, for which a small period is preferred. Considering the trade-off between these two requirements, the optimal periodicity for light trapping should be close to the targeted wavelength.^{27,28} For silicon, light trapping is most important for the 800 to 1100 nm wavelength range. We therefore expect that the optimal periodicity is approximately 1000 nm, the wavelength at which the normally incident plane wave is efficiently coupled to guided resonances.

Taking into account the significant difference in the structural requirements for antireflection and light trapping, our optimized design with a double-sided grating structure significantly increases light absorption over the entire solar spectrum, and provides a performance that approaches the theoretical limit (see Figure 2e). Furthermore, the double-sided strategy is a generic approach that can be applied to a range of thicknesses. Figure 3 shows that for ultrathin films, our approach can consistently outperform both the “top-only” and “bottom-only” grating designs. The photocurrents from the optimized double-sided grating structures are very close to the theoretical Yablonovitch limit for a range of thicknesses in the few micrometers range.

To characterize the loss of real mirror, we replace the PEC mirror by a flat silver layer for the optimized structure in Figure 1a. A thin layer of silicon dioxide is placed between the silicon film and silver as a spacer to reduce metallic loss. We observe only a small reduction in short-circuit photocurrent from 34.63 to 33.86 mA/cm² (see Figure 4a). Since the grating at the bottom of the silicon layer is sufficiently far from the silver surface, there is no surface plasmon excitation (see Figures 4b,c).

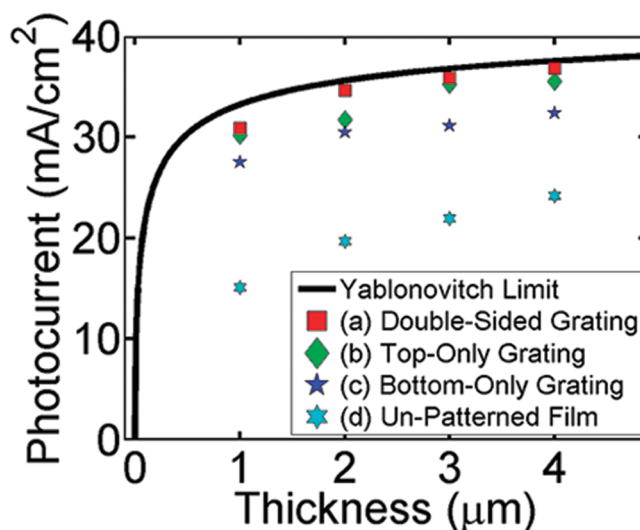


Figure 3. Photocurrents generated by structures as a function of their equivalent thicknesses. The black curve is the Yablonovitch limit calculated by integrating eq 2 over the AM1.5 solar spectrum.

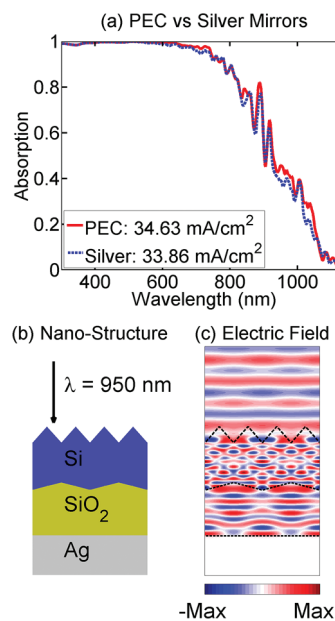


Figure 4. (a) Comparison of the absorption spectra with PEC and with silver (plus a spacer between the nanostructure and the silver back-reflector). The red curve is the absorption spectrum of the structure in Figure 1a, and the blue curve is the absorption spectrum of the same structure, except that the PEC is replaced with real silver,³¹ and a silicon dioxide layer of thickness 2 μm is placed between silicon and silver as a spacer. (b,c) The double-sided grating structure and the electric field profile at the wavelength of 950 nm.

Therefore, our flat silver back-reflector induces no significant local or long-range surface plasmon excitation and its resultant substantial parasitic loss.¹⁵ When we extend our optimization to include nanocone gratings made of nonabsorbing dielectric materials instead of silicon, we observe similar geometrical configurations and absorption enhancements. Therefore, the strategy has great flexibility in the nanocone grating design regarding material choice for either the grating or the back-reflector.

As a final remark, the doubled-sided structure could be fabricated by applying the Langmuir–Blodgett (LB) assembly method of silica nanospheres and the reactive ion etching

(RIE) to each side sequentially.^{21,22,30} One could use the size of the silica nanoparticles to control the periodicity, and the RIE to control the shapes of the nanocones. This fabrication process could also be applied to a large scale.^{22,30} Since our structure involves only a slight surface modification of a silicon film with nanocones of relatively low aspect ratio, the issues associated with surface recombination and degradation of electronic properties should be less severe than those of other high aspect ratio nanoscale structures. The double-sided nanocone grating design provides an experimentally realistic strategy in efficiency improvement and cost reduction for crystalline silicon solar cells.

AUTHOR INFORMATION

Corresponding Author

*E-mail: shanhui@stanford.edu.

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

This work is supported in part by DOE Grant No. DE-FG07-ER46426. The simulations were carried out using TeraGrid, and the National Nanotechnology Infrastructure Network's Computational Cluster at Stanford University, supported by the National Science Foundation.

REFERENCES

- (1) Park, Y.; Drouard, E.; Daif, O. E.; Letartre, X.; Viktorovitch, P.; Fave, A.; Kaminski, A.; Lemiti, M.; Seassal, C. Absorption enhancement using photonic crystals for silicon thin film solar cells. *Opt. Express* **2009**, *17*, 14312.
- (2) Lin, C.; Povinelli, M. L. In Guided-resonance induced absorption enhancement in silicon nanowire arrays for photovoltaic application. Proceedings of Optics and Photonics for Advanced Energy Technology, Cambridge, MA, June 24–25, 2009; MIT Center for Integrated Photonic Systems: Cambridge, MA, 2009; <http://www.opticsinfobase.org/abstract.cfm?URI=Energy-2009-ThC3>.
- (3) Nagel, J. R.; Scarpulla, M. A. Enhanced absorption in optically thin solar cells by scattering from embedded dielectric nanoparticles. *Opt. Express* **2010**, *18* (S2), A139.
- (4) Li, J.; Yu, H.Y.; Wong, S. M.; Zhang, G.; Lo, G.-Q.; Kwong, D.-L. Si nanocone array optimization on crystalline Si thin films for solar energy harvesting. *J. Phys. D: Appl. Phys.* **2010**, *43*, 255101.
- (5) Han, S. E.; Chen, G. Toward the Lambertian limit of light trapping in thin nanostructured silicon solar cells. *Nano Lett* **2010**, *10*, 4692–4696.
- (6) Kelzenberg, M. D.; Boettcher, S. W.; Petykiewicz, J. A.; Turner-Evans, D. B.; Putnam, M. C.; Warren, E. L.; Spurgeon, J. M.; Briggs, R. M.; Lewis, N. S.; Atwater, H. A. Enhanced absorption and carrier collection in Si wire arrays for photovoltaic applications. *Nat. Mater.* **2010**, *9*.
- (7) Mallick, S. B.; Agrawal, M.; Peumans, P. Optimal light trapping in ultra-thin photonic crystal crystalline silicon solar cells. *Optics Express* **2010**, *18* (6), 5691–5706.
- (8) Wang, W.; Wu, S.; Reinhardt, K.; Lu, Y.; Chen, S. Broadband light absorption enhancement in thin-film silicon solar cells. *Nano Lett* **2010**, *10*, 2012–2018.
- (9) Grandidier, J.; Callahan, D. M.; Munday, J. N.; Atwater, H. A. Light absorption enhancement in thin-film solar cells using whispering gallery modes in dielectric nanospheres. *Adv. Mater.* **2011**, *23*, 1272–1276.
- (10) Bhattacharya, J.; Chakravarty, N.; Pattnaik, S.; Slafer, W. D.; Biswas, R.; Dalal, V. L. A photonic-plasmonic structure for enhancing light absorption in thin film solar cells. *Appl. Phys. Lett.* **2011**, *99*, 131114.
- (11) Paetzold, U. W.; Moulin, E.; Michaelis, D.; Bottler, W.; Wachter, C.; Hagemann, V.; Meier, M.; Carius, R.; Rau, U. Plasmonic reflection grating back contacts for microcrystalline silicon solar cells. *Appl. Phys. Lett.* **2011**, *99*, 181105.
- (12) Dewan, R.; Vasilev, I.; Jovanov, V.; Knipp, D. Optical enhancement and losses of pyramid textured thin-film silicon solar cells. *J. Appl. Phys.* **2011**, *110*, 013101.
- (13) Sheng, X.; Johnson, S. G.; Michel, J.; Kimerling, L. C. Optimization-based design of surface textures for thin-film Si solar cells. *Opt. Express* **2011**, *19* (S4), A841.
- (14) Gjessing, J.; Sudbo, A. S.; Marstein, E. S. Comparison of periodic light-trapping structures in thin crystalline silicon solar cells. *J. Appl. Phys.* **2011**, *110*, 033104.
- (15) Biswas, R.; Xu, C. Nano-crystalline silicon solar cell architecture with absorption at the classical $4n^2$ limit. *O. Express* **2011**, *19* (S4), A664.
- (16) Fahr, S.; Kirchartz, T.; Rockstuhl, C.; Lederer, F. Approaching the Lambertian limit in randomly textured thin-film solar cells. *Opt. Express* **2011**, *19* (S4), A865.
- (17) Zhang, R. Y.; Shao, B.; Dong, J. R.; Zhang, J. C.; Yang, H. Absorption enhancement analysis of crystalline Si thin film solar cells based on broadband antireflection nanocone grating. *J. Appl. Phys.* **2011**, *110*, 113105.
- (18) Yablonovitch, E. Statistical ray optics. *J. Opt. Soc. Am.* **1982**, *72* (7), 899–907.
- (19) Yablonovitch, E.; Cody, G. D. Intensity enhancement in textured optical sheets for solar cells. *IEEE Trans. Electron Devices* **1982**, *ED-29*, (2), 300–305.
- (20) Green, M. A. Lambertian light trapping in textured solar cells and light-emitting diodes: analytical solutions. *Prog. Photovoltaics* **2002**, *10*, 235–241.
- (21) Zhu, J.; Yu, Z.; Burkhard, G. F.; Hsu, C.-M.; Connor, S. T.; Xu, Y.; Wang, Q.; McGehee, M.; Fan, S.; Cui, Y. Optical absorption enhancement in amorphous silicon nanowire and nanocone arrays. *Nano Lett.* **2009**, *9* (1), 279–282.
- (22) Zhu, J.; Yu, Z.; Fan, S.; Cui, Y. Nanostructured photon management for high performance solar cells. *Mater. Sci. Eng. R* **2010**, *70*, 330–340.
- (23) Zhu, J.; Hsu, C.-M.; Yu, Z.; Fan, S.; Cui, Y. Nanodome solar cells with efficient light management and self-cleaning. *Nano Lett.* **2010**, *10*, 1979–1984.
- (24) Li, L.; New formulation of the Fourier modal method for crossed surface-relief gratings. *J. Opt. Soc. Am. A* **1997**, *14*, (10), 2758–2767.
- (25) Tikhodeev, S. G.; Yablonskii, A. L.; Muljarov, E. A.; Gippius, N. A.; Ishihara, T. Quasiguided modes and optical properties of photonic crystal slabs. *Phys. Rev. B* **2002**, *66*, 045102.
- (26) Liu, V.; Fan, S. S^4 : A free electromagnetic solver for layered periodic structures. *Comp. Phys. Commun.*, submitted for publication **2011**.
- (27) Yu, Z.; Raman, A.; Fan, S. Fundamental limit of light trapping in grating structures. *Opt. Express* **2010**, *18* (S3), A366.
- (28) Yu, Z.; Raman, A.; Fan, S. Fundamental limit of nanophotonic light trapping in solar cells. *Proc. Natl. Acad. Sci. U.S.A.* **2010**, *107* (41), 17491–17496.
- (29) Yu, Z.; Fan, S. Angular constraint on light-trapping absorption enhancement in solar cells. *Appl. Phys. Lett.* **2011**, *98*, 011106.
- (30) Hsu, C.-M.; Connor, S. T.; Tang, M. X.; Cui, Y. Wafer-scale silicon nanopillars and nanocones by langmuir-blodgett assembly and etching. *Appl. Phys. Lett.* **2008**, *93*, 133109.
- (31) *Handbook of Optical Constants of Solids*; Palik, E. D., Ed.; Academic Press: New York, 1985.