Optimization of broadband omnidirectional antireflection coatings for solar cells

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Abstract: Broadband and omnidirectional antireflection coating is generally an effective way to improve solar cell efficiency, because the destructive interference between the reflected and incident light can maximize the light transmission into the absorption layer. In this paper, we report the incident quantum efficiency $\eta_{in}$ not incident energy or power, as the evaluation function by the ant colony algorithm optimization method, which is a swarm-based optimization method. Also, SPCTRL2 is proposed to be incorporated for accurate optimization because the solar irradiance on a receiver plane is dependent on position, season, and time. Cities of Quito, Beijing and Moscow are selected for two- and three-layer antireflective coating optimization over $\lambda = [300, 1100]$ nm and $\theta = [0^\circ, 90^\circ]$. The $\eta_{in}$ increases by 0.26%, 1.37% and 4.24% for the above 3 cities, respectively, compared with that calculated by other rigorously optimization algorithms methods, which is further verified by the effect of position and time dependent solar spectrum on the antireflective coating design.

Key words: antireflection coating; ant colony algorithm; incident quantum efficiency; SPCTRL2

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1. Introduction

Broadband and omnidirectional antireflection is one of the most desirable characteristics for high-efficiency solar cells to allow maximum light transmission into the absorption layer[1, 2]. Antireflection (AR) can be achieved by a few additional layers outside of Si solar cells that occupy about 80% of the photovoltaic market due to the mature technology and low price[3, 4]. As early as 1880 it was found that multilayer films with graded refractive-index increasing from top to bottom between air and the Si substrate have broadband transmittance both at normal and oblique incident angles[5-8]. Insect compound eyes are one of the typical graded refractive-index structures which have inspired the development of lots of nanostructure and fabrication techniques in recent years, such as SiO$_2$ microsphere arrays[9, 10], Si nanowires[11, 12], nanorods[13-15], Si nanostructure arrays[16], etc. The minimum refractive index reached 1.05 using oblique-angle deposition techniques, which are highly desirable for antireflective coatings[17-19]. In the view of the effective medium theory (EMT), light is bent progressively in the ARs with smoothly graded refractive index changing profile from air to substrate[20, 21]. Generally, different refractive index profile curves, such as linear, parabolic, cubic, quartic, exponential and exponential-sinusoidal, exhibit different antireflective performance. The optimization of the refractive-index profile experimentally is then changed to optimize the profile of the nanostructure and its filling factor[22, 23]. However, it is still a great challenge to obtain a high-performance optical structure compared with the optical performance characterization of a structure[24-26]. Recently, several rigorous optimization algorithms based on advanced global optimization techniques, such as the genetic algorithm[27, 28], simulated annealing algorithm[29, 30] and artificial immune algorithm[31] have been developed to optimize multilayer AR coating design. Recently, various swarm-based optimization algorithms have been successfully implemented in the design of multilayer AR coating to improve the existing numerical methods. These optimization methods are robust, stochastic and generally do not rely on the initial conditions. Among them, ant colony algorithm (ACA)[32] is a heuristic optimization algorithm that mimicks the way ants establish the shortest path from their nest to the food source and back by leaving their pheromones on the path as a communication medium among them[33]. A moving ant releases quantities of pheromone on the way, and the other ants detect and evaluate the choice of route according to the pheromone trail. Finally, the shortest path can be found after more and more ants select a more intense pheromone way. It has proved to be a powerful method to solve the optimization problems in basic and applied science[34]. It also demonstrated the best optimization result in the AR coating system. An average reflectance of 2.98% was obtained, which is much lower than 4.5% optimized by the genetic algorithm and 6.59% by the simulated annealing algorithm over the optimization range of $\lambda = [400, 1100]$ nm and $\theta = [0^\circ, 80^\circ]$[34].

There are two problems with the current optimization algorithms. The first problem is that it is the reflectance or transmittance, which is the concept of energy, that is utilized in the
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Fig. 2. (Color online) The dependence of the incident photon flux density on the wavelength and the incident angle on the day of the spring equinox for (a) Quito, (b) Beijing and (c) Moscow, respectively. At noon of the day of the spring equinox, the sunlight is vertically incident on the equator. The incident angle at noon of the day of spring equinox for Quito, Beijing and Moscow is 0, 40, and 55 degrees, respectively. At sunrise or sunset, the incident angles of these three cities are the same 90 degrees. (d) The comparison of the spectrum of the incident photon flux density of three cities at noon on the day of the spring equinox. The incident photon flux density spectra are totally different Earth due to the atmosphere scatter and absorption at different location with different incident angle and latitude.

### Table 1. Input parameters used in SPCTRL2 program.

| Parameter | Latitude (°) | Longitude (°) | Aerosol optical depth | Alpha | Albedo (surface reflectance) | Total column ozone (cm) | Total precipitable water vapor (cm) | Surface pressure (mB) | Days of the year |
|-----------|-------------|---------------|-----------------------|-------|----------------------------|------------------------|-------------------------------------|---------------------|-----------------|
| Quito     | 0           | 78.5W         | 0.27                  | 1.14  | 0.2                        | 0.34                   | 1.42                               | 1013.25             | 79              |
| Beijing   | 39.9N       | 116.3E        | 0.77                  | 1.14  | 0.16                       | 0.34                   | 0.95                               | 1040                | 79              |
| Moscow    | 55.3N       | 37.5E         | 0.35                  | 1.14  | 0.1                       | 0.36                   | 1.36                               | 750                 | 79              |

### Table 2. Detail structures of two-layer antireflective coating optimized by ant colony algorithm with and without SPCTRL2 incorporated.

| Optimization method      | 1st layer | 2nd layer | 1st layer | 2nd layer |
|--------------------------|-----------|-----------|-----------|-----------|
| No SPCTRL2               | 1.41      | 1.1209    | 2.41      | 58.89     |
| SPCTRL2 at Quito         | 1.44      | 113.66    | 2.55      | 60.46     |
| SPCTRL2 at Beijing       | 1.27      | 165.29    | 2.29      | 76.10     |
| SPCTRL2 at Moscow        | 1.17      | 221.62    | 2.15      | 80.80     |

changes from 90° to 39.9° and then to 90° for Beijing from sunrise to sunset, as shown in Fig. 2(b). For the same reason, the minimum incident angle is 55.3° for Moscow, as shown in Fig. 2(c). Therefore, the boundaries of the incident angle in Eq. 1 will change with the actual location of the solar cells. Fig. 2(d) compares the incident photon flux density spectra for the solar cell will receive over the day of the spring equinox when placed in Quito, Beijing and Moscow, after integrating over the entire incident angle range. The incident photon flux density spectra are totally different on Earth due to the atmosphere scatter and absorption at different locations with different incident angle and latitude.

### 3. Results and discussion

Table 2 presents the detailed structures of two AR coating films optimized by the ACA method with and without SPCTRL2 incorporated. Fig. 3(a) shows the optimized optical transmittance spectrum optimized by ACA without considering SPCTRL2 with \( \lambda = [300, 1100] \) nm and \( \theta = [0°, 90°] \), where the area of the contour plot with the transmittance above 80% and 98% are 76.12% and 27.51%, respectively, which are marked by white lines. Figs. 3(b)–3(d) presents the optimized optical transmittance spectrum, wherein \( \eta_{in-Q}, \eta_{in-B} \) and \( \eta_{in-M} \) represent the \( \eta \) of Quito, Beijing and Moscow, respectively. The \( \eta \) are 95.74%, 92.27%, and 86.78% for Quito, Beijing and Moscow, respectively. Obviously, the area with higher transmittance redshifts and moves up to larger incident angle in order to adapt to the effect of the city location and time in the optimization, which can be distinguished from the contour lines of the transmittance. The area of the contour plot with the trans-
mittance above 80% and 98% are 73.72% and 35.99%, 71.32% and 27.12%, 69.92% and 17.43%, respectively. However, the $\eta_{in}$ for Quito, Beijing and Moscow are increased to 96.00%, 93.64%, and 91.02%, respectively. In other words, the incident quantum efficiency at Quito, Beijing and Moscow optimized by the ant colony algorithm with SPCTRL2 incorporated are...
0.26%, 1.37% and 4.24% larger than that optimized without SPCTRL2 incorporated for two-layer antireflective coating, respectively. Figs. 3(e)–3(g) show the omnidirectional incident quantum efficiencies $\eta(\lambda)$ of Quito, Beijing and Moscow with and without SPCTRL2 incorporated, respectively. It can be seen that, with SPCTRL2 incorporated, the quantum efficiency spectrum almost fits the actual solar spectrum very well for each city. While for the quantum efficiency spectrum optimized without SPCTRL2 incorporated, there is an obvious mismatch between the actual solar spectrum and quantum efficiency spectrum. Similar results are also obtained for three-layer AR coating optimization. The $\eta_2$ increases from 96.86% to 97.60% for Quito, from 95.72% to 97.03% for Beijing, and from 94.46% to 95.74% for Moscow, respectively.

In practice, the refractive index value of bulk material between 1.46 and 2.55 is available for common silicon solar cells, which limits the current commercial availability of low-refractive index materials in solar cell applications. Two-layer and three-layer AR coatings are optimized with the restriction of refractive index between 1.46 and 2.55. Compared with the refractive index ranging from 1.05 to 2.66, the $\eta_3$ of two-layer AR coating optimized with and without SPCTRL2 incorporated at Quito, Beijing and Moscow are 96.60% and 95.30%, 93.64% and 92.83%, 91.02% and 87.71%, respectively. For three-layer AR coating, it is 97.60% and 95.96%, 97.03% and 93.02%, 95.74% and 87.94%, respectively. The improvement is still obvious. It is necessary to perform careful optimization for AR coatings in practice even with restrictions on the refractive index selection, especially for the cities in the high latitude. Comparing the detailed structure parameters, it was found that the lower limit of the refractive index is more important for $\eta_3$, because the large discrepancy of the refractive index between the air and surface layer of the solar cells determines the reflection. Expanding the range of the refractive index for the practical material can be achieved by nano-technology and advanced deposition techniques, which has proven to be a useful technique to manipulate the light coupling in silicon photonics.

4. Conclusion

In this paper, the incident quantum efficiency $\eta_3$ is set as the evaluation function with SPCTRL2 program incorporated to optimize the broadband and omnidirectional AR coating by the ACA method for silicon solar cells for the purpose of practical applications. The solar spectrum on the day of the spring equinox was selected, which can simplify the optimization process to expand to whole year optimization. Two-layer and three-layer antireflective coatings are optimized over $\lambda = [300, 1100]$ nm and $\theta = [0°, 90°]$. The $\eta_3$ of two-layer AR coating optimized by the ACA method with SPCTRL2 incorporated increases by 0.26%, 1.37% and 4.24% over that without SPCTRL2 incorporated for Quito, Beijing and Moscow, respectively. While for three-layer antireflective coating, the $\eta_3$ are improved by 0.74%, 1.31% and 1.28%, respectively. The careful optimization for AR coatings in practice even with restrictions on the refractive index selection can further improve the efficiency of the solar cells, especially for high latitude locations.

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References

[1] Leem J W, Guan X Y, Choi M, et al. Broadband and omnidirectional highly-transparent coverglasses coated with biomimetic moth-eye nanopatterned polymer films for solar photovoltaic system applications. Sol Energy Mater Sol C, 2015, 134, 45
[2] Rahman A, Ashraf A, Xin H, et al. Sub-50-nm self-assembled nano-textures for enhanced broadband antireflection in silicon solar cells. Nat Commun, 2015, 6, 5963
[3] Tyagi V V, Rahim N A A, Rahim N A, et al. Progress in solar, PV technology: research and achievement. Renew Sust Energy Rev, 2013, 20, 443
[4] Louwen A, Sark W V, Schropp R, et al. A cost roadmap for silicon heterojunction solar cells. Sol Energy Mat Sol C, 2016, 147, 295
[5] Rayleigh L. On reflection of vibrations at the confines of two media between which the transition is gradual. Proc London Math Soc, 1879, 1(1), 51
[6] Carlson D E, Wronski C R. Amorphous silicon solar cell. Appl Phys Lett, 1976, 28(11), 671
[7] Zeng L, Yi Y, Hong C, et al. Efficiency enhancement in Si solar cells by textured photonic crystal back reflector. Appl Phys Lett, 2006, 89(11), 111111
[8] Xiong C, Xu W, Zhao Y, et al. New design graded refractive index antireflection coatings for silicon solar cells. Mod Phys Lett B, 2017, 31(19–21), 1740028
[9] Tao M, Zhou W, Yang H, et al. Surface texturing by solution deposition for omnidirectional antireflection. Appl Phys Lett, 2007, 91(8), 081118
[10] Bett A, Eisenlohr J, Höhn O, et al. Front side antireflection concepts for silicon solar cells with diffractive rear side structures. 29th European Photovoltaic Solar Energy Conference and Exhibition, 2014: 987.
[11] Yang J, Luo F, Kao T S, et al. Design and fabrication of broadband ultralow reflectivity black Si surfaces by laser micro/nano-processing. Light Sci Appl, 2014, 3(7), e185
[12] Huang Y F, Chattopadhyay S, Jen Y J, et al. Improved broadband and quasi-omnidirectional anti-reflection properties with biomimetic silicon nanostructures. Nat Nanotech, 2007, 2(12), 770
[13] Diedenhofen S L, Vecchi G, Algra R E, et al. Broad-band and omnidirectional antireflection coatings based on semiconductor nanorods. Adv Mater, 2009, 21(9), 973
[14] Wang Z S, Kawauchi H, Kashima T, et al. Significant influence of TiO$_2$ photoelectrode morphology on the energy conversion efficiency of N719 dye-sensitized solar cell. Coord Chem Rev, 2004, 248(13/14), 1381
[15] Keis K, Magnusson E, Lindström H, et al. A 5% efficient photoelectrochemical solar cell based on nanostructured ZnO electrodes. Sol Energ Mat Sol C, 2002, 73(1), 51
[16] Cai J, Qi L. Recent advances in antireflective surfaces based on nanostructure arrays. Mater Horiz, 2015, 2(1), 37
[17] X J Q, Schubert M F, Kim J K, et al. Optical thin-film materials with low refractive index for broadband elimination of Fresnel reflection. Nat Photonics, 2007, 1(3), 176
[18] Guter W, Schön J, Philipp S P, et al. Current-matched triple-junction solar cell reaching 41.1% conversion efficiency under concentrated sunlight. Appl Phys Lett, 2009, 94(22), 223504
[19] Liang Y, Feng D, Wu Y, et al. Highly efficient solar cell polymers developed via fine-tuning of structural and electronic properties. J Am Chem Soc, 2009, 131(22), 7792
[20] Hiramoto M, Fujiwara H, Yokoyama M. Three-layered organic solar cell with a photoactive interlayer of codeposited pigments. Appl Phys Lett, 1991, 58(10), 1062
[21] Spinelli P, Verschuuren M, Polman A. Broadband omnidirectional antireflection coating based on subwavelength surface Mie resonators. Nat Commun, 2012, 3, 692

[22] Campbell W M, Burrell A K, Officer D L, et al. Porphyrins as light harvesters in the dye-sensitised TiO$_2$ solar cell. Coord Chem Rev, 2004, 248(13/14), 1363

[23] Krebs F C, Tromholt T, Jørgensen M. Upscaling of polymer solar cell fabrication using full roll-to-roll processing. Nanoscale, 2010, 2(6), 873

[24] Liao H H, Chen L M, Xu Z, et al. Highly efficient inverted polymer solar cell by low temperature annealing of Cs$_2$CO$_3$ interlayer. Appl Phys Lett, 2008, 92(17), 156

[25] Barkhouse D A R, Gunawan O, Gokmen T, et al. Device characteristics of a 10.1% hydrazine-processed Cu$_2$ZnSn(Se, S)$_4$ solar cell. Prog Photovolt: Res Appl, 2012, 20(1), 6

[26] Poxson D J, M F Schubert M F, Mont F W, et al. Broadband omnidirectional antireflection coatings optimized by genetic algorithm. Opt Lett, 2009, 34(6), 728

[27] Oh S J, Chhajed S, Poxson D J, et al. Enhanced broadband and omni-directional performance of polycrystalline Si solar cells by using discrete multilayer antireflection coatings. Opt Express, 2013, 21(101), A157

[28] Chang Y J. Suppressing lossy-film-induced angular mismatches between reflectance and transmittance extrema: optimum optical designs of interlayers and AR coating for maximum transmittance into active layers of CIGS solar cells. Opt Express, 2014, 22(101), A167

[29] Wang W. Design of nonpolarizing antireflection coating by using multiobjective optimization algorithm. Optik, 2013, 124(16), 2482

[30] Chang Y J, Chen Y T. Broadband omnidirectional antireflection coatings for metal-backed solar cells optimized using simulated annealing algorithm incorporated with solar spectrum. Opt Express, 2011, 19(104), A875

[31] Guo X, Zhou H Y, Guo S, et al. Design of broadband omnidirectional antireflection coatings using ant colony algorithm. Opt Express, 2014, 22(104), A1137

[32] Bird R E, Riordan C. Simple solar spectral model for direct and diffuse irradiance on horizontal and tilted planes at the earth’s surface for cloudless atmospheres. SPIE, 1993, 54, 171

[33] Asadollahbaik A, Boden S A, Charlton M D, et al. Reflectance properties of silicon moth-eyes in response to variations in angle of incidence, polarisation and azimuth orientation. Opt Express, 2014, 22(102), A402

[34] Chen Y, Bagnall D M. Sunrise to sunset optimization of thin film antireflective coatings for encapsulated, planar silicon solar cells. Prog Photovolt: Res Appl, 2009, 17(4), 241

[35] Holben B N, Eck T F, Slutsker I, et al. AERONET-A federated instrument network and data archive for aerosol characterization. Remote Sens Environ, 1998, 66(1), 1