Si nanocrystal-based triple-layer anti-reflection coating for Si solar cells

Zhang, Jun; Chen, Tupei; Liu, Yang; Wong, Jen It

2013

Zhang, J., Chen, T., Liu, Y., & Wong, J. I. (2013). Si nanocrystal-based triple-layer anti-reflection coating for Si solar cells. *Journal of applied physics*, 114(5), 053109.

<https://hdl.handle.net/10356/98373>

<https://doi.org/10.1063/1.4817821>

© 2013 AIP Publishing LLC. This paper was published in *Journal of Applied Physics* and is made available as an electronic reprint (preprint) with permission of AIP Publishing LLC. The paper can be found at the following official DOI: [<http://dx.doi.org/10.1063/1.4817821>]. One print or electronic copy may be made for personal use only. Systematic or multiple reproduction, distribution to multiple locations via electronic or other means, duplication of any material in this paper for a fee or for commercial purposes, or modification of the content of the paper is prohibited and is subject to penalties under law.

Downloaded on 26 Apr 2023 23:35:06 SGT

Si nanocrystal-based triple-layer anti-reflection coating for Si solar cells

Jun Zhang, T. P. Chen, Yang Liu, and Jen It Wong

Citation: *J. Appl. Phys.* **114**, 053109 (2013); doi: 10.1063/1.4817821

View online: <http://dx.doi.org/10.1063/1.4817821>

View Table of Contents: <http://jap.aip.org/resource/1/JAPIAU/v114/i5>

Published by the AIP Publishing LLC.

Additional information on J. Appl. Phys.

Journal Homepage: <http://jap.aip.org/>

Journal Information: http://jap.aip.org/about/about_the_journal

Top downloads: http://jap.aip.org/features/most_downloaded

Information for Authors: <http://jap.aip.org/authors>

ADVERTISEMENT

The advertisement banner for AIP Advances features a green and yellow background with a pattern of thin, curved, wavy lines. The text "AIPAdvances" is prominently displayed in the center, with "AIP" in blue and "Advances" in green. To the right of the text is a circular seal that reads "Now Indexed in Thomson Reuters Databases". Below the main text, there is a blue bar with the text "Explore AIP's open access journal:" followed by a list of three bullet points: "• Rapid publication", "• Article-level metrics", and "• Post-publication rating and commenting".

AIPAdvances

Now Indexed in Thomson Reuters Databases

Explore AIP's open access journal:

- Rapid publication
- Article-level metrics
- Post-publication rating and commenting

Si nanocrystal-based triple-layer anti-reflection coating for Si solar cells

Jun Zhang,^{1,2} T. P. Chen,^{1,a)} Yang Liu,² and Jen It Wong¹

¹*School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore*

²*State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology, Chengdu, People's Republic of China*

(Received 29 May 2013; accepted 24 July 2013; published online 7 August 2013)

A triple-layer anti-reflection coating (TL-ARC) with Si nanocrystals (nc-Si)-dielectric nanocomposite thin film structure is proposed for Si solar cells. The TL-ARC has a graded refractive index (RI) profile of high RI, medium RI, and low RI. Such RI profile is achieved with the structure consisting of a Si_3N_4 layer embedded with high concentration of nc-Si and another Si_3N_4 layer embedded with low concentration of nc-Si and a SiO_2 layer. The design of the TL-ARC is carried out with the calculation of the effective indices of the high-RI and medium-RI layers with the Maxwell-Garnett effective medium approximation model. Due to the photoluminescence properties of nc-Si embedded in Si_3N_4 matrix, the TL-ARC has the inherent capability of down-converting ultraviolet photons to low-energy photons that are useful to Si solar cells. The deposition of the TL-ARC on Si solar cell is fabricated with plasma enhanced chemical vapor deposition in a single process step. The performance enhancement of Si solar cells by the TL-ARC has been demonstrated by experiments. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4817821>]

I. INTRODUCTION

Nowadays, solar cells have been used in large-scale commercial production of clean green electricity that is created from the unlimited solar energy. With the consideration of cost and output, most commercial solar cells are made of silicon (Si). Because the refractive index (RI) of Si is very high (e.g., RI is 3.88 at the wavelength of 632 nm), Si solar cells without any anti-reflection process reflect off over 30% of incident light in the wavelength range from 300 nm to 1100 nm, which significantly lowers the energy conversion efficiency of solar cells. To reduce the incident light loss, anti-reflection coating (ARC) is commonly deposited on the surface of Si solar cells.^{1,2}

Si_3N_4 is widely used as a single layer ARC in most commercial Si solar cells due to its low cost, good performance, and excellent surface passivation.³ Moreover, the RI of Si_3N_4 matches with the relationship $n_1^2 = n_0 n_2$ (where n_0 is the RI of air, n_2 is the RI of Si, and n_1 is the RI of Si_3N_4), and hence, the single layer ARC could reduce the reflection to zero at one specific wavelength. As a result, it could achieve low reflection in the wavelength range of 450 nm–750 nm which corresponds to the maximum radiation energy region of solar radiation. However, the single layer ARC could only reduce the reflection in a narrow spectrum region, whereas the solar radiation spans across a broad band spectrum. To maximize the usage of the solar energy, the wavelength range of low reflection must be extended.

In order to reduce reflection over a wider band, two layers or multi layers ARC structures have been proposed, which usually contain high RI materials (CeO_2 , TiO_2 , etc) followed by lower RI materials (MgF_2 , SiO_2 , etc).^{3,4} However, these special materials (CeO_2 , TiO_2 , and MgF_2) incur higher cost and the refractive indices of these materials

are fixed hence the only optimizable parameter is the thickness. Besides, some ARC structures require a separate thermal deposition of SiO_2 or Si_3N_4 for surface passivation, which complicates the fabrication process and increases the cost. As a result, an ARC that can be produced at lower cost while maintaining good anti-reflection performance over a wide spectral range is highly desirable.

A low cost triple-layer anti-reflection coating (TL-ARC) is proposed in this work. As shown in Figure 1, the TL-ARC has a graded RI profile of high RI, medium RI, and low RI. The RI profile is achieved with the structure consisting of a Si_3N_4 layer embedded with high concentration of Si nanocrystals (nc-Si) and another Si_3N_4 layer embedded with low concentration of nc-Si and a SiO_2 layer. The TL-ARC also has the capability of down-converting the harmful ultraviolet light of the solar spectrum into low energy photons that are useful to Si solar cells.

II. METHODOLOGY

In order to construct the TL-ARC, three layers with different refractive indices are needed. With the advantages of low cost and high scratch resistance, SiO_2 is a good candidate as a low-RI layer on the top of the ARC. Based on the Maxwell-Garnett effective medium approximation (EMA) model, the high-RI and medium-RI layers can be achieved

FIG. 1. Schematic diagram of the TL-ARC.

^{a)}E-mail: echentp@ntu.edu.sg

by distributing different amounts of nc-Si in a Si_3N_4 layer.^{5,6} To determine the effective RI of the Si_3N_4 layer embedded with nc-Si (the layer is denoted as nc-Si/ Si_3N_4), the nc-Si/ Si_3N_4 layer is treated as an effective medium, where Si_3N_4 is the host matrix and nc-Si is the inclusion. The dielectric function (ϵ_{eff}) of the nc-Si/ Si_3N_4 layer can be calculated with the Maxwell-Garnett EMA as given below

$$\frac{\epsilon_{\text{eff}} - \epsilon_{\text{matrix}}}{\epsilon_{\text{eff}} + 2\epsilon_{\text{matrix}}} = \frac{\epsilon_{\text{nc}} - \epsilon_{\text{matrix}}}{\epsilon_{\text{nc}} + 2\epsilon_{\text{matrix}}} f_{\text{inclu}}, \quad (1)$$

where ϵ_{matrix} is the dielectric function of Si_3N_4 , ϵ_{nc} is the dielectric function of nc-Si, and f_{inclu} is the nc-Si volume fraction in the Si_3N_4 layer. As the dielectric function of Si_3N_4 is well documented and the dielectric function of nc-Si is also available from our previous studies,⁵ ϵ_{eff} of the nc-Si/ Si_3N_4 layer can be calculated with Eq. (1) for a given f_{inclu} . Thus, the effective refractive index (n_{eff}) and extinction coefficient (k_{eff}) of the nc-Si/ Si_3N_4 layer can be determined with $\epsilon_{\text{eff}} = (n_{\text{eff}} - ik_{\text{eff}})^2$.

The Maxwell-Garnett EMA model is only valid at low nc-Si volume fraction since it is assumed that the nc-Si are spatially separated in the Si_3N_4 layer.⁷ In this work, the maximum nc-Si volume fraction in Si_3N_4 is about 33% at which the EMA is still valid. To realize the ARC structure shown in Figure 1, the high-RI layer and medium-RI layer are formed by a Si_3N_4 layer embedded with 33% nc-Si and another Si_3N_4 layer embedded with 5% nc-Si, respectively. The refractive indices of the high-RI layer and the medium-RI layer can be calculated with Eq. (1). Figure 2 shows the refractive indices of the nc-Si, Si_3N_4 with 33% nc-Si and Si_3N_4 with 5% nc-Si and pure Si_3N_4 .

The anti-reflection performance of the ARC not only depends on the RI of each layer, but also is determined by the thickness of each layer. To minimize the reflection in the wavelength range from 300 nm to 1100 nm, a simulation is carried out to optimize the thickness of each layer in the TL-ARC.⁸ The optimized thicknesses of the high-RI layer (33% nc-Si/ Si_3N_4), medium-RI layer (5% nc-Si/ Si_3N_4), and

low-RI layer (SiO_2) yielded from the simulation are 33 nm, 17 nm, and 81 nm, respectively. For comparison, reflectance of the Si substrate without any ARC and the Si substrate with a single layer (Si_3N_4) ARC are also simulated in the wavelength range of 300 nm–1100 nm. The comparison of reflectance among the structures is shown in Figure 3. The arithmetical average reflectance over the wavelength range is 37.5%, 15.1%, and 6.3% for the Si substrate without ARC, the Si substrate with the single layer (Si_3N_4) ARC, and the Si substrate with the TL-ARC, respectively. Figure 3 clearly shows that the TL-ARC has excellent anti-reflection performance in the wavelength range of 300 nm–1100 nm.

III. DEPOSITION OF THE TL-ARC

The TL-ARC can be easily deposited on Si substrate with plasma enhanced chemical vapor deposition (PECVD). The required material compositions and layer thicknesses of the TL-ARC are achieved by controlling the reactant gases, gas flow rates, pressure, RF power, temperature, and the deposition time in the PECVD process. To deposit the high-RI layer of Si_3N_4 with high concentration of nc-Si, SiH_4 and N_2 are chosen as the reactants. The nc-Si can be generated on a cold substrate *in-situ* in a PECVD chamber.⁹ NH_3 is added as one of the reactants to deposit the medium-RI layer of Si_3N_4 with low nc-Si concentration. To deposit the low-RI layer of SiO_2 , the reactants include SiH_4 , N_2 , and N_2O . Detail parameters of the TL-ARC deposition are tabulated in Table I. Because all the deposition parameters can be varied continuously, the deposition of the TL-ARC is completed in a single process in the same PECVD chamber. Therefore, it is a low cost process.

IV. RESULTS AND DISCUSSIONS

A. Refractive indices of the layers in TL-ARC

For the measurement of refractive indices of the three layers of the TL-ARC, each layer is deposited on Si substrate

FIG. 2. Refractive indices of nc-Si, Si_3N_4 with 33% nc-Si, Si_3N_4 with 5% nc-Si and Si_3N_4 .

FIG. 3. Calculated reflectance in the wavelength range of 300 nm–1100 nm of the Si substrate without ARC, Si substrate with a single layer (Si_3N_4) ARC, and Si substrate with the TL-ARC.

TABLE I. Process parameters used in the deposition of the TL-ARC.

	High-RI layer	Medium-RI layer	Low-RI layer
SiH ₄ flow rate (SCCM)	100	8	100
NH ₃ flow rate (SCCM)	0	50	0
N ₂ flow rate (SCCM)	700	400	600
N ₂ O flow rate (SCCM)	0	0	30
RF power (W)	40	40	60
Pressure (mTorr)	200	200	800
Temperature (°C)	50	200	300

separately. The RI of each layer is measured with ellipsometry in the wavelength range of 300 nm–1100 nm, and the results are shown in Figure 4. As can be observed in the figure, there is a large difference in the refractive index among the three layers, e.g., at the wavelength of 550 nm the refractive indices of the high-RI, medium-RI, and low-RI layers are 2.38, 2.01, and 1.48, respectively.

The refractive indices of the deposited layers as obtained from ellipsometric measurement are a little bit lower than the values of the simulations. For example, at the wavelength of 550 nm, the measured values for the high-RI layer and medium-RI layer are 2.38 and 2.01, respectively; while the corresponding simulated values are 2.52 and 2.10, respectively. One possible reason for the lower RI is that the actual nc-Si concentrations in the two layers (i.e., the high-RI and medium-RI layers) are lower than the values used in the simulations. The thicknesses of the high-RI layer, medium-RI layer, and low-RI layer optimized with the measured refractive indices are 55 nm, 6 nm, and 82 nm, respectively.

B. Photoluminescence from the TL-ARC

Photoluminescence (PL) from nc-Si embedded in a dielectric matrix such as SiO₂ and Si₃N₄ has been investigated intensively in the past decades.^{10,11} Under excitation of short-wavelength light such as ultraviolet light, the nc-Si/dielectric systems can emit photons of visible and near-

FIG. 4. Measured refractive indices of the high-RI, medium-RI, and low-RI layers.

FIG. 5. Photoluminescence spectrum of the TL-ARC deposited on Si substrate.

infrared light.^{12–14} Since there is nc-Si embedded in the high-RI and medium-RI layers, the TL-ARC should have the capability of light emission under the excitation of ultraviolet light. This indeed has been confirmed in our experiment. Figure 5 shows the PL spectrum of the TL-ARC deposited on Si substrate under the excitation of a 325 nm excitation light source.

As can be observed in the Figure 5, the PL spectrum extends from ~500 nm to ~1000 nm peaking at 778 nm. The emitted light in the visible and near-infrared region can be efficiently used by Si solar cells. Because of the stable and intensive PL, the TL-ARC can serve as a luminescent down-converter. The high energy photons in the ultraviolet region from the solar radiation are usually dissipated as heat in conventional Si solar cells, causing not only waste of solar energy, but also degradation of solar cells.^{15,16} Through the PL process, the high energy photons can be converted to visible and near-infrared photons that can be used by Si solar cells more effectively. Therefore, besides the advantage of very low reflectance for the visible and near-infrared solar radiation, the TL-ARC also has the capability of down-conversion to make use of the ultraviolet solar radiation, which can increase the energy efficiency of Si solar cells.

C. Anti-reflection performance

In order to verify the actual anti-reflection performance, the TL-ARC was deposited on polished blank Si substrate with the PECVD process described above. The anti-reflection performance of the TL-ARC was measured by PerkinElmer Lambda 950 UV-Vis-NIR spectrometer. For comparison, the single layer (Si₃N₄) ARC was also fabricated on polished blank Si substrate with PECVD.

As shown in Figure 6, the arithmetical average reflectance measured in the wavelength range of 300 nm–1100 nm of the Si substrate with TL-ARC is 5.6%, which is significantly lower than that of the Si substrate without ARC (38.8%) and the Si substrate with single layer ARC (16.3%). The actual anti-reflection performance of the TL-ARC is

FIG. 6. Measured reflectance in the wavelength range of 300 nm–1100 nm of the Si substrate without ARC, the Si substrate with a single layer (Si_3N_4) ARC, and the Si substrate with the TL-ARC.

consistent with the simulation result. This indicates that the EMA model can provide a very good estimation of the effective refractive indices of both the high-RI and medium-RI layers, and the ARC design methodology discussed above is realistic and reliable.

D. Application in Si solar cells

To demonstrate the application of the TL-ARC in Si solar cells, a commercial polycrystalline Si solar cell with standard ARC (single layer ARC) purchased from the market was used. The standard ARC existing on the solar cell was removed by reactive ion etching (RIE), and then the TL-ARC was deposited on the solar cell surface with PECVD. Current density-voltage (J-V) measurement was conducted on the solar cell covered by the TL-ARC. For comparison, the measurement was also conducted on the solar cell with the standard ARC (i.e., the original commercial Si solar cell) and the solar cell without the standard ARC (i.e., after the etching by RIE).

The J-V characteristic was measured by using a solar simulator which utilizes an air mass (A.M 1.5) filter with power of 1000 W/m^2 . The J-V characteristics of the above samples are shown in Figure 7. The short-circuit current densities of the solar cell without ARC, the solar cell with the standard ARC, and the solar cell with the TL-ARC are 29.8 mA/cm^2 , 42.6 mA/cm^2 , and 46.6 mA/cm^2 , respectively; and the corresponding open-circuit voltages are 0.57 V, 0.59 V, and 0.60 V, respectively. The calculated energy conversion efficiencies of the solar cell without ARC, the solar cell with the standard ARC, and the solar cell with the TL-ARC are 8.6%, 12.4%, and 13.6%, respectively.

The result indicates that the TL-ARC was able to increase the short-circuit photocurrent and the energy conversion efficiency by 56.4% and 58.1%, respectively, as compared to the solar cell without ARC. On the other hand, it should be pointed out that the removal of the standard ARC by RIE could have caused some damages to the Si solar

FIG. 7. J-V characteristics of the solar cell without ARC, the solar cell with standard ARC (i.e., the original commercial Si solar cell), and the solar cell with the TL-ARC.

cell as both the short-circuit current and the energy conversion efficiency of the solar cell without ARC are lower than expected. Nevertheless, the short-circuit photocurrent and the energy conversion efficiency of the solar cell with the TL-ARC are still 9.4% and 9.7%, relatively higher than that of the solar cell with standard ARC (i.e., the original solar cell), respectively. It is also worthy to mention that the TL-ARC leads to a slightly higher open-circuit voltage, which could be due to the passivation effect of the high-RI layer.

V. CONCLUSION

A high-performance TL-ARC consisting of a high-RI layer, a medium-RI layer, and a low-RI layer has been designed and demonstrated in this work. The high-RI layer and medium-RI layer are realized with Si_3N_4 layers embedded with high and low concentrations of nc-Si, respectively; while a SiO_2 layer serves as the low-RI layer. The deposition of the TL-ARC on Si solar cell can be carried out with PECVD in a single process step. The calculation of the refractive indices of the high-RI and medium-RI layers is based on the Maxwell-Garnett EMA model; and the best anti-reflection performance of the ARC over the wide spectral range of 300 nm–1100 nm is achieved by optimizing both the concentrations of nc-Si in the high-RI and medium-RI layers and the thicknesses of the three layers. Due to the photoluminescence property of nc-Si embedded in Si_3N_4 , the TL-ARC has the inherent capability of down-converting ultraviolet photons to lower-energy photons that are useful to Si solar cells. The excellent anti-reflection performance of the TL-ARC and the performance enhancement of Si solar cell by the TL-ARC have been demonstrated by experiment.

ACKNOWLEDGMENTS

This work has been supported by the SMART innovation grant under Project No. ING11027-ENG, MOE Tier 1 grant, and NTU Si COE program.

- ¹A. El amrani, I. Menous, L. Mahiou, R. Tadjine, A. Touati, and A. Lefgoum, *Renewable Energy* **33**, 2289 (2008).
- ²A. S. Zoofakkar, S. R. S. Othman, and M. H. Abdullah, in *Proceedings of International Conference on Information and Multimedia Technology* (IEEE Computer SOC, Cheju Isl, South Korea, 2009), p. 543.
- ³J. Ko, D. Gong, K. Pillai, K. S. Lee, M. Ju, P. Choi, K. R. Kim, J. Yi, and B. Choi, *Thin solid films* **519**, 6887 (2011).
- ⁴S. Y. Lien, D. S. Wu, W. C. Yeh, and J. C. Liu, *Sol. Energy Mater. Sol. Cells* **90**, 2710 (2006).
- ⁵L. Ding, T. P. Chen, Y. Liu, C. Y. Ng, and S. Fung, *Phys. Rev. B* **72**, 125419 (2005).
- ⁶T. P. Chen, Y. Liu, M. S. Tse, O. K. Tan, P. F. Ho, K. Y. Liu, D. Gui, and A. L. K. Tan, *Phys. Rev. B* **68**, 153301 (2003).
- ⁷P. U. Jepsen, B. M. Fischer, A. Thoman, H. Helm, J. Y. Suh, R. Lopez, and R. F. Haglund, *Phys. Rev. B* **74**, 205103 (2006).
- ⁸B. Harbecke, *Appl. Phys. B* **39**, 165 (1986).
- ⁹Y. Q. Wang, Y. G. Wang, L. Cao, and Z. X. Cao, *Appl. Phys. Lett.* **83**, 3474 (2003).
- ¹⁰V. Svrcek, I. Pelant, J. L. Rehspringer, P. Gilliot, D. Ohlmann, O. Cregut, B. Honerlage, T. Chvojka, J. Valenta, and J. Dian, *Mater. Sci. Eng., C* **19**, 233 (2002).
- ¹¹V. Svrcek, A. Slaoui, and J. C. Muller, *Thin Solid Films* **451**, 384–388 (2004).
- ¹²T. P. Chen and L. Ding, *Handbook of Nanostructured Thin Films and Coatings*, edited by S. Zhang (CRC Press, Boca Raton, 2010), Vol. 2, pp. 113–165.
- ¹³Z. H. Cen, T. P. Chen, L. Ding, J. D. Ye, Y. Liu, M. Yang, J. I. Wong, Z. Liu, and S. Fung, *Electrochem. Solid-State Lett.* **12**, H38 (2009).
- ¹⁴L. Ding, T. P. Chen, Y. Liu, C. Y. Ng, M. Yang, J. I. Wong, F. R. Zhu, M. C. Tan, S. Fung, X. D. Chen, and Y. Huang, *J. Nanosci. Nanotechnol.* **8**, 3555 (2008).
- ¹⁵W. R. Taube, A. Kumar, R. Saravanan, P. B. Agarwal, P. Kothari, B. C. Joshi, and D. Kumar, *Sol. Energy Mater. Sol. Cells* **101**, 32 (2012).
- ¹⁶B. H. Kim, C. H. Cho, T. W. Kim, N. M. Park, G. Y. Sung, and S. J. Park, *Appl. Phys. Lett.* **86**, 091908 (2005).