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Analysis of an anti-reflecting nanowire transparent electrode for solar cells

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Transparent electrodes are an important component in many optoelectronic devices, especially solar cells. In this paper, we investigate a nanowire transparent electrode that also functions as an anti-reflection coating for silicon solar cells, taking into account the practical constraints that the electrode is typically encapsulated and needs to be in electric contact with the semiconductor. Numerical simulations show that the electrode can provide near-perfect broadband anti-reflection over much of the frequency range above the silicon band gap for both polarizations while keeping the sheet resistance sufficiently low. To provide insights into the physics mechanism of this broadband anti-reflection, we introduce a generalized Fabry–Perot model, which captures the effects of the higher order diffraction channels as well as the modification of the reflection coefficient of the interface introduced by the nanowires. This model is validated using frequency-domain electromagnetic simulations. Our work here provides design guidelines for nanowire transparent electrode in a device configuration that is relevant for solar cell applications. Published by AIP Publishing.

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I. INTRODUCTION

Transparent electrodes are widely used in solar cells and many other optoelectronic devices.1 Traditional transparent electrodes typically consist of transparent conductive oxide coating such as tin-doped indium oxide (ITO). Recently, however, a number of other approaches have also been explored, including networks of metallic nanowires,2–8 metallic grids,9–14 carbon nanotubes,15,16 and graphene.17–21 The fundamental requirements of a high-performing transparent electrode are high electrical conductivity and high optical transparency.1 Moreover, for a transparent electrode to be used in a practical device, there are several additional general constraints: (1) The electrode must be in electric contact with the semiconductor to extract carriers; (2) The electrode is usually encapsulated to prevent it from damage and enhance durability.3,4 These two constraints should be considered when one performs optical design of the electrode.

In this paper, taking into account these constraints, we consider the optical properties of a silver nanowire transparent electrode in a geometry shown in Figure 1. The periodic silver nanowires are placed atop a high-index semiconductor and embedded in an anti-reflection coating (Figure 1). For demonstration, we choose silicon as the high-index semiconductor to analyze the optical properties of the electrode. This is motivated in part by recent experimental efforts that placed silver nanowire on top of silicon solar cell structures as the transparent electrode.22

Geometries similar to Figure 1 have been studied experimentally and numerically. Zeng et al. experimentally demonstrated the mechanical, thermal, and chemical robustness of a random silver nanowire network buried in a matrix.3 Massiot et al. theoretically and experimentally validated broadband multi-resonant absorption in thin film solar cells with 1D and 2D metallic gratings.6,12,23 The influence of adding an anti-reflection coating to plasmonic solar cells with metallic gratings was numerically studied by Munday and Atwater.24 Xie et al. numerically investigated the optical transparency of a circular and square nanowire network in different dielectric environments.13 Lee and Ahn studied the effects of substrates on the transmission of metal grids by simulation.25

Complementary to the existing numerical work on similar geometries, we provide a theoretical discussion on the physics of broadband anti-reflection in this system. As the main contributions of the paper, we show that this system can provide near-perfect broadband anti-reflection over much of the frequency range above the silicon band gap for...
both polarizations. We also introduce a generalized Fabry–Perot interference model for this class of structure and show that the anti-reflection arises because one can choose the radii of the nanowires that are sufficiently large such that the sheet resistance is low, and in the mean time still do not significantly affect the anti-reflection property of the coating. Our work highlights an opportunity for using the silver nanowire electrode for light management, and moreover points to the relevant physics when performing optical design of a transparent electrode in the actual electromagnetic environment of a solar cell.

The paper is organized as following: In Section II, we consider an exemplary structure, and show that the transmission of such nanowire electrode structure as shown in Figure 1 can be close to that of a single-layer anti-reflection structure without the nanowire. In Section III, we develop a generalized Fabry–Perot model to highlight the relevant physics of such a transparent electrode structure. In Section IV, we discuss the tunability and the angular dependence of such electrode, as well as aspects of physics related to plasmon excitation that is not captured by the generalized Fabry–Perot model. We conclude in Section V.

II. AN EXEMPLARY STRUCTURE

We consider a structure consisting of a periodic array of silver nanowires atop silicon. The silver nanowires are embedded in an anti-reflection coating assumed to be SiN (Figure 1). The frequency-dependent dielectric constants of Si, SiN, and Silver are taken from Ref. 26. The adjustable parameters in this structure are the periodicity of the array \( a \), the radius of the silver nanowires \( r \), and the thickness of the SiN layer \( h \). As the wavelength range of interest, we consider the wavelengths between 400 nm and 1100 nm, corresponding to photon energies above the silicon band gap. We set the periodicity \( a = 400 \text{ nm} \) such that at normal incidence within the wavelength range of interest, the diffraction order in air is limited only to the zeroth order, which is beneficial for anti-reflection purposes in transparent electrode design.\(^\text{27}\) As a representative set of parameters, the radius of the nanowire is chosen to be 20 nm. If we assume that the resistivity of silver is \( 1.59 \times 10^{-8} \text{ } \Omega \times \text{m} \),\(^\text{28}\) the corresponding sheet resistance of the nanowire electrode in the direction along the nanowire is \( 5 \text{ } \Omega/\square \). For very thin nanowires, the boundary scattering effect may be important. If we use the Fuchs and Sondheimer model and assume a 100% diffusive electron scattering at the nanowire surface,\(^\text{29,30}\) we obtain a sheet resistance of \( 12 \text{ } \Omega/\square \). These values are comparable to what is required for transparent electrode in solar cell applications.\(^\text{2}\) The thickness of the anti-reflection coating \( (h = 82 \text{ nm}) \) is chosen to maximize the average transmission in the considered wavelength range for an incident solar spectrum, with other parameters fixed.

We define the transmission of the electrode as the power transmitted into the silicon region divided by the incident power. It is equivalent to the absorption in silicon in our simulation because the silicon layer is set to be thick enough to absorb all light transmitted into silicon. We simulate the structure using two frequency-domain Maxwell’s equation solvers: a code based on the Fourier modal method, S4,\(^\text{31}\) and a code based on the finite-difference frequency-domain method, Maxwell FDFD.\(^\text{32}\)

The transmission spectrum of the electrode together with that of a bare air/silicon interface and that of an optimized single layer anti-reflection coating atop silicon are shown in Figure 2. The transmission of the flat air/silicon interface (blue curve in Figure 2) is around 60% over most part of the wavelength range of interest. Nearly 40% incident light is reflected due to impedance mismatch between air and silicon. A conventional approach to reduce the reflection is to place a single layer anti-reflection coating at the air/silicon interface. As an example we use a single layer of SiN as the anti-reflection coating with a thickness of 77 nm that is optimized to maximize the average transmission over the wavelength range of interest. The spectrum of transmission into silicon (green curve in Figure 2) shows significant improvement over the entire wavelength range of interest as compared with the bare air/silicon interface. The solid and dashed red curves in Figure 2 represent the spectra of the electrode shown in Figure 1 for the s (whose E field is parallel to the nanowires) and p (whose E field is perpendicular to the nanowires) polarizations, respectively. The transmission of the electrode for both the s- and the p-polarizations are far above the transmission of the bare air/silicon interface over almost the entire wavelength range of interest. The transmission of the electrode for the s-polarization approximates that of the single layer anti-reflection coating with a slight red shift in the transmission peak. Compared with the transmission of the s-polarization, the transmission of the p-polarization is higher in the longer wavelength and lower in the shorter wavelength within the wavelength range of interest.

The average transmission of this electrode is 87.9%, which is slightly lower than the 91.6% transparency of the optimized single layer anti-reflection coating. Here the average is calculated by integrating over the solar spectrum in

![FIG. 2. The solid and dashed red curves represent the transmission spectra of the electrode as illustrated in Figure 1 \((a = 400 \text{ nm}, r = 20 \text{ nm}, h = 82 \text{ nm})\) for the s and the p polarizations, respectively. Light in the s- or the p-polarization has its electric field parallel or perpendicular to the nanowires, respectively. For comparison, the transmission spectrum of a flat air/silicon interface is plotted in blue and that of an optimized single anti-reflection SiN layer on silicon is represented by the green curve. The single anti-reflection layer (SiN) has a thickness of 77 nm. The complex refractive index \((n_{Ag} - ik_{Ag})\) of silver is shown in the inset at the right bottom corner. \(n_{Ag}\) and \(k_{Ag}\) are, respectively, plotted in solid and dashed black curves over the wavelength range from 400 nm to 1100 nm.](image)
the wavelength range of 400–1100 nm, where the solar spectrum is approximated by blackbody radiation spectrum at 5800 K \(^{33}\) for simplicity. For the electrode, we also average over both polarizations. The results here show that a nanowire electrode can be placed at the interface between the silicon region and the anti-reflection layer, without significantly degrading the performance of the anti-reflection layer.

### III. GENERALIZED FABRY–PEROT MODEL

In this section, we develop a theoretical model to account for the numerical results for the transparent electrode as discussed in Sec. II. For a typical anti-reflection layer consisting of a single layer of SiN, its physics can be simply described by a Fabry–Perot model which takes into account the interference effect as a plane wave of light bounces back and forth between the SiN/silicon interface and the SiN/air interface. This model has also been previously used to analyze the multi-resonant absorption in a thin film solar cell with a metal-grating on top.\(^{23}\) Our system differs in that we consider a thick silicon cell to focus primarily on the anti-reflection properties of the nanowire array, as opposed to the light trapping properties in a thin film cell as considered in Ref. \(^{23}\).

In our system, the anti-reflection effect can also be accounted for by considering similar interference effects. However, the presence of the nanowire array at the SiN/silicon interface introduces two new aspects that need to be taken into account in the Fabry–Perot model: (1) The silver nanowires may diffract light into higher order diffraction channels inside the SiN layer; (2) The reflection coefficient of the zeroth-order is different from that of a flat interface.

We generalize the Fabry–Perot model to take into account the two modifications as mentioned above. For simplicity, we study the normal incidence. With our choice of the periodicity \(a = 400\) nm, for the entire wavelength range, there is only the zeroth-order diffraction in air. On the other hand, both the SiN and the Si layers have indices substantially larger than 1, and hence these layers can support multiple diffraction channels as shown in Figure 3.

Our model describes the amplitudes for the waves in all the channels as shown in Figure 3. In the notation in our model, we denote the complex amplitudes of the forward and backward propagating waves as \(a\) and \(b\), respectively. Their subscripts represent the diffraction order of the wave. When the subscript is absent, the label represents a vector that consists of the complex amplitudes of all the diffraction orders. The SiN/silicon interface is located at \(y = 0\) and the air/SiN interface is located at \(y = h\). We set the incident light along the \(-\hat{y}\) direction.

At each interface, the outgoing waves are related to the incoming waves by a scattering matrix \(S\). For example, the scattering matrix \(S_1\) of the air/SiN interface has the form

\[
\begin{pmatrix}
  b(y = h^+) \\
  a(y = h^-)
\end{pmatrix} = S_1 \begin{pmatrix}
  a(y = h^+) \\
  b(y = h^-)
\end{pmatrix} = \begin{pmatrix}
  R_{1,ai}^h & T_1^h \\
  T_1 & R_{1,si}^h
\end{pmatrix} \begin{pmatrix}
  a(y = h^+) \\
  b(y = h^-)
\end{pmatrix}. \tag{1}
\]

![Figure 3. Schematic illustrating the various diffraction channels in the generalized Fabry–Perot model used to describe the electrode structure shown in Figure 1. Shown here is a single unit cell of the electrode structure. The forward and backward propagating channels are represented as black arrows. The complex wave amplitudes in each channel are denoted as \(a\) or \(b\) with subscripts specifying the diffraction order and superscripts specifying the layer.](https://example.com/figure3.png)

Here the “+” and “−” superscripts are used to represent a position immediately above and below an interface, respectively. \(S_1\) is a symmetric matrix by reciprocity and can be determined analytically. The incoming and outgoing waves with respect to the SiN/silicon interface with silver nanowires are related by a scattering matrix \(S_2\) in the following form:

\[
\begin{pmatrix}
  b(y = 2r^+) \\
  a(y = 0^-)
\end{pmatrix} = S_2 \begin{pmatrix}
  a(y = 2r^+) \\
  b(y = 0^-)
\end{pmatrix} = \begin{pmatrix}
  R_{2,si}^h & T_2^h \\
  T_2 & R_{2,ai}^h
\end{pmatrix} \begin{pmatrix}
  a(y = 2r^+) \\
  b(y = 0^-)
\end{pmatrix}. \tag{2}
\]

The scattering matrix \(S_2\) can be numerically obtained. The number of simulations to obtain \(R_{2,si}^h\) and \(T_2\) is the number of diffraction channels in the SiN layer. Under normal incidence, the +\(i\)th diffraction order is a mirror of the −\(i\)th diffraction order. Thus, one simulation is sufficient to obtain the corresponding columns in the scattering matrix for a mirror pair.

In the situation that the silicon is thick enough to absorb all the transmitted light, the backward propagating waves in the silicon are zero, i.e., \(b(y = 0^-) = 0\). The relation between the incoming waves in SiN and the outgoing waves with respect to the SiN/silicon interface with silver nanowires can be simplified as

\[
\begin{pmatrix}
  b(y = 2r^+) \\
  a(y = 0^-)
\end{pmatrix} = \begin{pmatrix}
  R_{2,si}^h & T_2^h \\
  T_2 & R_{2,ai}^h
\end{pmatrix} \begin{pmatrix}
  a(y = 2r^+)
\end{pmatrix}. \tag{3}
\]

\(a(y = h^-)\) and \(a(y = 2r^+)\) \((b(y = 2r^+)\) and \(b(y = h^-)\)) are related by a propagation matrix \(M_P\) that describes the propagation phase shift between the two interfaces

\[
a(y = 2r^+) = M_P a(y = h^-), \tag{4}
\]
The reflection and transmission power, normalized to the incident power, are \( R = |r|^2 \) and \( T = \alpha^2 \). Here the transmission coefficient \( \alpha \) is a vector, with each of its component corresponding to the transmission coefficient into one of the diffraction channels inside the silicon region. The first term of \( \alpha \) in Equation (6) corresponds to the direct pathway where light is directly reflected from the air/SiN interface, and the second term corresponds to the indirect pathway where light is trapped in the SiN layer for a little while before being reflected back. The expression of the reflection coefficient becomes the same as that in the standard Fabry–Perot interference model if only one channel exists in the SiN layer. When multiple channels exist in the SiN layer, the complex amplitude of the indirect pathway should be calculated using the propagation matrix and the scattering matrices of the two interfaces.

The above model takes into account the multiple propagating channels that exist in the SiN layer (Figure 3), but neglects channels that are evanescent along the y-direction. With this model, the transmission of the electrode can be immediately calculated once the scattering matrices of the two interfaces are known. Since the scattering matrices of the interfaces have no dependence on the thickness \( h \) of the anti-reflection coating, this model helps to find the optimized thickness of the anti-reflection coating given the radii of the array, and the refractive index \( n \) of the anti-reflection coating.

To validate our model, we compare the transmission spectrum of the electrode predicted by our model with that obtained by direct simulation using the Fourier modal method. The comparison between the model-predicted (blue curve) and the simulated (red curve) transmission spectra is shown in Figure 4(a) for the s-polarization and Figure 4(b) for the p-polarization. The parameters are identical to that in Figure 1. For both the s- and the p-polarizations, the theoretically predicted spectrum and the numerically obtained spectrum agree very well, especially over the long wavelength. Such an agreement suggests that our model captures the main physics involved in the optical transmission of the electrode.
the larger thickness of the SiN leads to the red-shifted transmission peak for the s-polarization as shown in Figure 2.

To summarize this section, we find that the presence of the silver nanowires results in only modest change in both the phase and the amplitude of the reflection coefficient at the SiN/silicon interface. As a result, the capability of the SiN layer for anti-reflection purposes is largely preserved in the presence of the silver nanowires for both polarizations.

IV. DISCUSSION

In this section we provide further discussions of various properties of the transparent electrode structure as shown in Figure 1. In Figure 2 we observe that the transmission of the p-polarized wave for the transparent electrode degrades significantly in the shorter wavelength range, as compared with the single layer anti-reflection structure. Moreover, in Figure 4(b) we observe that such a degradation is not adequately captured in the generalized Fabry–Perot model—there is deviation of the generalized Fabry–Perot model as compared with the simulation in the shorter wavelength range. Both observations here are due to the excitations of the localized surface plasmons by the p-polarized incident wave, which is not accounted for by the generalized Fabry–Perot model since the localized surface plasmon represents evanescent waves along the y-direction. The evidence of the excitation of the localized surface plasmon can be seen in Figure 6, where we plot the spectra of the absorption by the silver nanowires for both the s- and the p-polarizations. The p-polarization exhibits a strong absorption peak inside the silver nanowires around the wavelength of 460 nm. In contrast, the s-polarization has negligible absorption throughout the entire wavelength range. Figure 7 shows the electric field amplitude for each polarization at 460 nm. We observe the concentration of the electric field inside the silver nanowire for the p-polarization due to the localized plasmon (Figure 7(b)). Such a field concentration effect is absent in the s-polarization (Figure 7(a)).

We also investigate the characteristics of this transparent electrode (Figure 1) when we vary the parameters. We can tune the transmission peak within a broad wavelength range by changing the thickness of the SiN layer. The mechanism is captured in our model since the propagation matrix \( M_p \) in Eqs. (4) and (5)) depends on the thickness of the SiN layer. Figure 8 demonstrates the transmission spectra of the s-polarization for different thickness of the SiN layer. By increasing the thickness from 60 nm to 100 nm, the transmission peak shifts from around 480 nm to 810 nm with a near 100% peak value.

In applications of a transparent electrode, understanding its angular response is important for certain applications. For example, it may be desirable for a solar cell to capture both diffuse and direct sun light. In Figure 9 we show the average transmission for the s- (solid) and p- (dashed) polarization under different incident angles, where we assume that the incident direction is in the plane perpendicular to the nanowires. Each polarization maintains high transmission until the angle of incidences exceeds 60°. The result suggests that the electrode considered here can operate over a range of angle of incidence.

In this paper, we choose a cylindrical nanowire since such nanowire can be created by chemical synthesis and has been previously used for transparent electrode applications. Experimentally, the SiN grown for anti-reflection coating purposes may not be stoichiometric. The main results of the paper are not strongly affected by the refractive indices of the SiN assumed. For example, using the optical constants of SiN from Ref. 34, we find that the optimum thickness of the SiN layer changes from 82 nm to 88 nm, and the change in the transmission of the electrode is within 1%.
Our numerical results also show that the 2D network of silver nanowires with same periodicity and sheet resistance has lower optical transmission compared with the 1D network.

**V. CONCLUSION**

In conclusion, we investigate the optical characteristics of a silver nanowire electrode atop silicon and embedded in a SiN anti-reflection coating. We show that such a structure can exhibit broadband anti-reflection characteristics over wide angular range. The physics of such electrode is well accounted for a generalized Fabry–Perot model. The results here provide design guidelines for nanowire transparent electrode in a device configuration that is relevant for solar cell applications.

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