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Design and optimization of antireflecting coatings from nanostructured porous silicon dielectric multilayers

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ABSTRACT

We report the design and fabrication of an optimized antireflecting structure with the maximum transmittance (T_{max}) and minimum reflectivity (R_{min}), based on a porous silicon dielectric multilayer (PS-DM). The structures consist of 50 layers of equal thicknesses with an increasing refractive index profile, $n(z) \sim z^k$. Numerical results based on the transfer matrix method, along with an average spectral analysis, were used to compute a certain range of thicknesses (with the optimal thickness of 235 nm) to obtain similar optical response (T_{max} and R_{min}). The average reflectivity spectrum of a PS-DM structure in the proposed optimal range was experimentally measured to be 1.3% from 300 to 1100 nm. Such structures can be used to enhance the efficiency of silicon solar cells and optoelectronic devices.

1. Introduction

Single antireflecting coatings (ARCs) are designed to attenuate the reflected light of certain wavelength by matching the condition $n_c^2 = n_0 n_s$, where n_c, n_0, and n_s are the refractive index of the coating, the incident medium, and the substrate, respectively [1]. However, in order to increase the antireflecting wavelength range, several groups have been theoretically designed [2,3] and fabricated multilayered dielectric ARCs from several materials such as MgF_2, ZnS, Ta_2O_5, [4], TiO_2 [5], SiN_x [6], and porous silicon (PS) [7–11]. In particular, PS-ARCs have been demonstrated to increase the short-circuit current and photovoltaic energy conversion efficiency of silicon-based solar cells [12–17], due to the reduction of reflectivity loss (around 40% [18]), which can limit the performance of the device.

Therefore, different PS refractive index profiles have been studied as multilayered ARCs; for example, Ma et al. reported a structure fabricated with 24 steps refractive index profile (varying from 1.7 to 3.0), resulting in a total thickness of 4.1 μm, which showed to have a reflectance less than 5%, from 350 to 800 nm [18]. In another work, Striemer et al. fabricated an approximately 100 nm thick structure, with a linearly increasing refractive index profile and measured an average reflectivity of 3.7% within 350–1000 nm wavelength range [19]. More recently, Lv et al. demonstrated the formation of porous pyramidal structure over silicon with an increasing refractive index gradient and an average reflectance of 2.7%, from 200 to 2000 nm wavelength range [20].

In spite of the fact that gradually increasing refractive index profile of PS structure has demonstrated a reduction in the reflectivity of the structure, some authors have proposed the optimization of the multilayered ARCs to further decrease the reflectivity. For example, Mahdjoub and Zighed proposed a refractive index profile which follows a Fermi distribution function for non-zero temperature, and considering the spectral irradiance of sunlight and the internal spectral sensitivity of a solar cell, they obtained a *weighted average* reflectance of 5.6% and theoretically estimated an enhanced short-circuit current of 52.79% [3]. Osorio et al., proposed the optimization of a *transference parameter* with a three layer system of 180 nm thickness, which produced a reflectance below than 4.2%, for a wavelength range from 400 to 900 nm and estimated 95.2% of energy transference to silicon substrate [21].

Additionally, Zhou et al. investigated a linearly graded porosity profile to minimize the averaged reflectivity as a function of thickness of multilayered structure [22]. Although they found an optimal averaged reflectance of 1.55% for a 400 nm thickness structure, we believe that the reported parameters have to be further investigated due to the fact that the explored thicknesses suggest the following: as the length of the structure is increased, the reflectivity tends to reduce. The rough model used in the above-mentioned work fails to describe a real optimization of

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a multilayered ARC for solar cell applications, where the absorption and the thickness of the structure play an important role in the optical transmittance, which has to be taken into account. In spite of the previously mentioned optimization works, the optimal thickness of the multilayered ARC, the number of layers of the structure, and the specific refractive index profile required to obtain the minimum reflectivity and maximum transmittance, is yet to be investigated. In this work, the refractive index profile of a multilayered ARC (of the form $n(z)\sim z^k$), to optimize the average reflectivity/transmittance, has been numerically analyzed. The electric field (EF) distribution within the multilayered ARC has also been calculated and compared to other previously reported structures of different thicknesses. The multilayered ARC structures were fabricated through electrochemical anodization of silicon wafers to experimentally demonstrate their reflectivity response.

2. System of study and numerical optimization

As the reflection of light from an interface is due to the relative difference of refractive indices (Δn) between two materials, a decrease in Δn reduces the reflectance [1]. Hence, in order to minimize the reflectance from an incident medium with refractive index n_0 (air) to certain substrate with refractive index $n_{Si} > n_0$, we propose a gradual variation of refractive index in a multilayered system from the first to the last layer (with index of refraction n_1 and n_N), according to the simple envelop function $n(z) = n_1 + (n_N - n_1)(z/L)^k$, where z is the depth from the first layer to the substrate, N is the number of layers, and L is the thickness of the multilayer structure.

Fig. 1 shows the refractive index profile $n(z)$ as a function of depth z (normalized to the length of the structure L) for different power values (k). When $k<1$, trajectories are over the linear curve (as an example dotted-dashed lines); for $k>1$, paths are below the solid line (showed as dashed lines). The inset of Fig. 1 shows the schematic of the multilayered structure along with the silicon substrate. Using the above-mentioned system, the optical reflectivity response is computed for a range of k values (from 0 to 10) to find an optimal value of L and k, revealing the minimum average reflectance at the surface along with the maximum average transmittance on the Si-multilayer interface. Numerical calculations of the reflectivity/transmittance spectra and the electric field distribution were performed using the transfer matrix method [23,24].

In order to fix the number of layers of the system that discretize the enveloped function and hold the optical properties of the continuous refractive index profile, the average reflectance as a function of the number of layers (N) has been computed for different values of k. The average of R is defined as

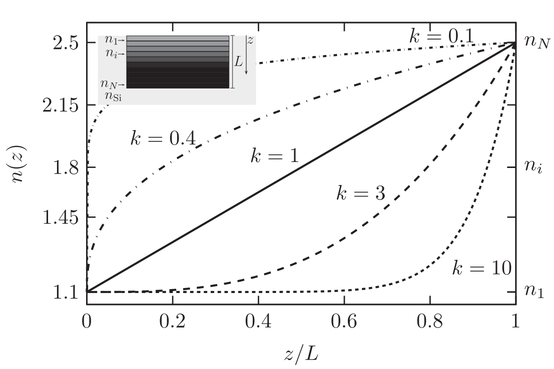

Fig. 1. Refractive index profile ($n\sim z^k$) as a function of the depth (normalized to the length of the structure, z/L) for different values of the k parameter. The inset shows the schematics of a graded multilayered PS structure.

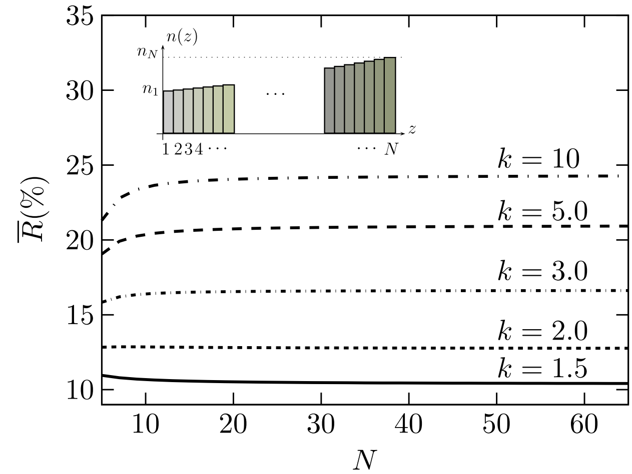

Fig. 2. Averaged reflectance ($\overline{R}$) as a function of the number of layers (N) for different values of k and $L=100$ nm. The inset shows the schematics of the number and position of each layer in the structure.

$$\overline{R}(k,L) = \frac{1}{\lambda_{max}-\lambda_{min}} \int_{\lambda_{min}}^{\lambda_{max}} R_{k,L}(\lambda)\, d\lambda, \quad (1)$$

where $R_{k,L}(\lambda)$ is the reflectance spectrum (for a defined value of k and L), and $\lambda_{max}/\lambda_{min}$ are the maximum/minimum wavelength values, respectively. Fig. 2 shows an example of the average reflectance value ($\overline{R}$) as a function of the number of layers for different values of k. A semi-constant behavior of the average reflectance is observed from $N\sim 20$ onwards. However, to ensure an adequate asymptotical convergence of the optical reflectivity, $N=50$ has been chosen in the present work. As compared to the number of layers (Fig. 2), the effect of the k value on the averaged reflectance is relatively high. The inset of Fig. 2 shows the schematic of the discretized refractive index profile as a function of the number/position of each layer through the structure.

To study the maximum/minimum values of the transmittance/reflectivity as a function of L and k, we defined the average function

$$\overline{F}(k,L) = \frac{100\% - \overline{R}(k,L) + \overline{T}(k,L)}{2}, \quad (2)$$

which is bounded between 0% (when $\overline{R}=100\%$ and $\overline{T}=0\%$) and 100% (when $\overline{R}=0\%$ and $\overline{T}=100\%$). Hence, we attribute the optimum value of L and k (minimum reflectance with maximum transmittance) when $\overline{F}$ is the maximum.

3. Experimental details

PS ARC's samples were fabricated through anodic etching of (100) oriented p-type crystalline Si wafers (resistivity 0.002–0.005 Ω cm) under galvanostatic conditions [25]. After an electrochemical polish (removal of the parasitic layer [26]), the Si wafer was anodized with an electrolyte mixture of HF (concentration: 48 wt %), glycerol (purity: 99.8 wt%), and ethanol (purity: 99.9 wt%) in 3:7:1 proportion of volume. The current density and the duration of the etching time of each layer were controlled by a computer interfaced electronic circuit, where the current density was varied from 0.4 to 70.4 mA/cm^2, corresponding to the refractive indices of 2.5 (porosity: 38%) and 1.1 (porosity: 92%). The refractive indices were calculated for 1500 nm using interferometric method and porosity through Bruggeman effective medium theory [27] and Palik refractive index database [28,29]. After the anodization process, the samples were rinsed in ethanol and dried with