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DESIGN OF THIN FILM'S GEOMETRY BY ANNEALING ALGORITHM AND COHERENT FORMULATION

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ABSTRACT

In this paper, the directional, spectral, and temperature dependence of the radiative properties including the reflection coefficient, transmission coefficient and emissivity for the multilayer structures consisting of silicon were examined. Optimum structures for different industrials requirement are obtained by Simulated Annealing Algorithm. The results show that the radiative properties of thin films depend on the wavelength strongly. It causes selective wavelength radiative properties. From the results, it may be concluded that industrial requirements are supported by selecting coating's material and thickness. It can analyze the specified wavelength by the Simulated Annealing Algorithm (SA). Coating thickness is increased to reduce the emittance coefficient. The emittance reduction is 0.628 at a wavelength of 0.5 μm and 0.673 at a wavelength of 0.7 μm, respectively. The appropriate structure with the appropriate number of layers, appropriate type and combination of thin film coating will be chosen by Simulated Annealing Algorithm.

Keywords: reflectance, transmittance, emittance, simulated annealing algorithm, optimization.

INTRODUCTION

The Silicon is semiconductor that plays a vital role in integrated circuits and MEMS/NEMS [1]. Semitransparent crystalline silicon solar cells can improve the efficiency of solar power generation [2]. In fact, surface modification by coatings can significantly affect the radiative properties of a material [3]. For lightly doped silicon the metal coating has higher reflectance than silicon nitride coating in visible wavelengths [3,4]. It is observed that the concentrations highly affect the radiative properties of doped silicon multilayer at temperatures below 600K [5]. The effect of wave interference can be understood by plotting the spectral properties such as reflectance or transmittance of a thin dielectric film versus the film thickness and analyzing the oscillations of properties due to constructive and destructive interferences [6].

The advancement of performance of simple SA is applied [7]. The matrix method formulation is used in conjunction with a simulated annealing algorithm with the aim to design acoustical structures, especially acoustic filters [8]. The reflectivity of a smooth surface coated with a thin film can be calculated with the ray-tracing method when ray amplitude and phase difference between rays undergoing multiple reflections within the film is considered [9].

This work uses transfer-matrix method for calculating the radiative properties. Light doped silicon is used and Coherent Formulation is applied. Simulated Annealing Algorithm used to optimize radiative properties of thin films for industry needs.

COHERENT FORMULATION

The transfer-matrix method provides a convenient way to calculate the radiative properties of multilayer structures of thin films (Figure-1 [10]). By assuming that the electromagnetic field in the j^{th} medium is a summation of forward and backward waves in the z-direction, the electric field in each layer can be expressed by [11]

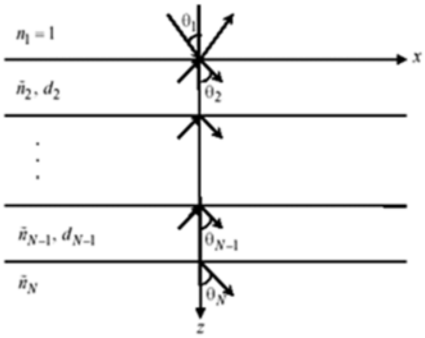

Figure-1. The geometry for calculating the radiative properties of a multilayer structure [10]

$$E_j = \begin{cases} \left[A_1 e^{iq_{1z}z} + B_1 e^{-iq_{1z}z}\right] e^{(iq_x x - i\omega t)}, & j = 1 \\ \left[A_j e^{iq_{jz}(z-z_{j-1})} + B_j e^{-iq_{jz}(z-z_{j-1})}\right] e^{(iq_x x - i\omega t)}, & j = 2,3,\ldots N \end{cases} \tag{1}$$

Where A_j and B_j are the amplitudes of forward and backward waves in the j^{th} layer. Detailed descriptions of how to solve for A_j and B_j is given in [12]. Consequently, the radiative properties of the N-layer system are given by ([12, 13])

$$\rho = \frac{B_1 B_1^*}{A_1^2} \tag{2}$$

$$\tau = \frac{\operatorname{Re}(n_N \cos\theta_N)}{n_1}\frac{A_N A_N^*}{A_1^2} \tag{3}$$

$$\varepsilon = 1 - \varepsilon - \rho \tag{4}$$

The optical constants of silicon dioxide, silicon nitride and gold are mainly based on the data collected in Palik [14]

SIMULATED ANEALING ALGORITHM [15, 16]

Simulated Annealing (SA) is motivated by an analogy to annealing in solids. The Table-1 shows how physical annealing can be mapped to Simulated Annealing. Using these mappings, any combinatorial optimization problem can be converted into an annealing algorithm.

Table-1. Relationship between physical annealing and simulated annealing.

Thermodynamic simulation	Combinatorial optimization
System States	Solutions Feasible
Energy	Cost
Change of State	Neighboring Solutions
Temperature	Control Parameter
Frozen State	Heuristic Solution

The starting temperature must be high enough to allow a move to almost any neighborhood state. If this is not done, the ending solution will be very close to the starting solution. It is usual to let the temperature decrease until it reaches zero. Therefore, the stopping criteria can either be a suitably low temperature or when the system is frozen at the current temperature.

RESULTS AND DISCUSSIONS

Figure-2 compares the reflectance of thick silicon substrate with $700\mu m$ thickness and coated by silicon dioxide thin film with $300nm$ thickness in two different coating cases and two different temperatures with the results in (Lee, 2005). The Electromagnetic waves are incident at $\theta = 0^\circ$. The calculated results are in good agreement with results in [13]. The calculated results are in good agreement with results of [13].

Because the refractive index of silicon dioxide (around 1.45) is smaller than that of silicon, the reflectance with a coating is always lower than that of bare silicon for non-metal thin film coatings (Figure-2). The oscillation in the reflectance is due to interference in the silicon dioxide coating.

The free spectral range is determined by $\Delta\lambda/\lambda^2 = (2n_f d_f)^{-1}$, where $\Delta\lambda$ is the separation between adjacent interference maxima and n_f and d_f are the refractive index and thickness of the thin film. The spectral separation $\Delta\lambda$ increases toward longer wavelengths. As the film thickness increases, the free spectral range decreases, resulting in more oscillations with the thicker silicon dioxide film. Therefore oscillations increased toward longer wavelengths. Interferences in the substrate are generally not observable in the incoherent formulation. This is the major difference between coherent and incoherent formulations [9].

Knowledge of the radiation properties of silicon and metal multilayered structures such as gold, silver and copper with different parameters is essential for small system applications. The maximum reflectance and the minimum of it are compared in Table-2 with Colonial Competitive Algorithm [17] and in Table-3 with Imperialist Competitive Algorithm [18] in two wavelengths $0.65\,\mu m$ and $0.8\,\mu m$. The maximum thickness of coating is considered constant. In this case, silicon thickness less than $500\,\mu m$ and a maximum thickness of each layer were considered equal to 400 nm.

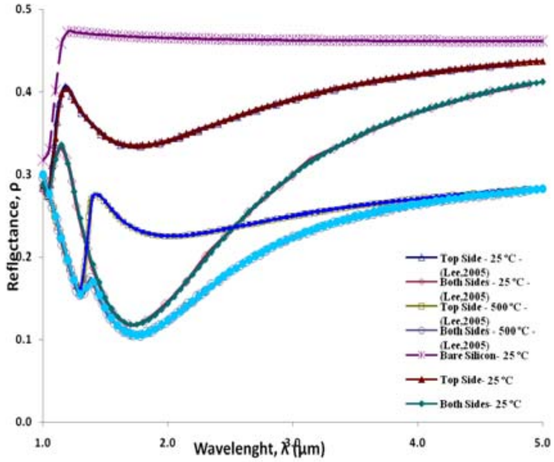

Figure-2. Comparison of the reflectance of thick silicon substrate coated by silicon dioxide thin film with the results in [13].

This paper considered the radiative properties of silicon coated with silicon dioxide and silicon nitride at room temperature for 11 layers with different coating procedures. Coherent formulation is used.

The division of layer's materials and the thickness of each layer can be analyzed by Simulated Annealing Algorithm (SA) for maximum reflectance in the Tables 4 and 5, and for the minimum emittance in two wavelengths 0.5 μm and 0.7 μm in the Tables-6-7 are mentioned.

Table-2. Comparison of the colonial competitive algorithm with the simulated annealing algorithm.

Wavelength (λ)	**0.65** μm **(Simulated annealing algorithm)**	**0.65** μm **(Colonial competitive algorithm)**
The number of layers	9	9
Layer 1	Si_3N_4	Si_3N_4
Layer 2	SiO_2	SiO_2
Layer 3	Si_3N_4	Si
Layer 4	SiO_2	SiO_2
Layer 5	SiO_2	Si_3N_4
Layer 6	Si	Si_3N_4
Layer 7	Si	SiO_2
Layer 8	SiO_2	Si
Layer 9	Si	Si_3N_4
Minimum of The Reflectance	0.296	0.31

Coating thickness is increased to reduce the emittance coefficient. The emittance reduction is 0.628 at a wavelength of 0.5 μm and 0.673 at a wavelength of 0.7 μm, respectively.

Wavelength range can be analyzed with the help of simulated annealing algorithm, the number of layers, the thin film coating, form and select the appropriate coating composition.

It can analyze the specified wavelength by the simulated annealing Algorithm (SA). The appropriate structure with the appropriate number of layers, appropriate type and combination of thin film coating will be chosen by simulated annealing Algorithm.

Table-3. Comparison of the imperialist competitive algorithm with the simulated annealing algorithm.

Wavelength (λ)	**0.65** μm **(Simulated annealing algorithm)**	**0.65** μm **(Imperialist competitive algorithm)**
The number of layers	9	9
Layer 1	Si	1
Layer 2	Si	4
Layer 3	SiO_2	1
Layer 4	SiO_2	1
Layer 5	Si_3N_4	3
Layer 6	SiO_2	2
Layer 7	Si_3N_4	3
Layer 8	SiO_2	2
Layer 9	Si_3N_4	3
Maximum of The Reflectance	0.863	0.8875

Table-4. Layers distribution for the maximum of the reflectance.

Wavelength (λ)	**0.5 μm**	**0.7 μm**
The number of layers	11	11
Layer 1	Si	SiO_2
Layer 2	SiO_2	Si
Layer 3	SiO_2	Si_3N_4
Layer 4	SiO_2	Si_3N_4
Layer 5	SiO_2	SiO_2
Layer 6	Si_3N_4	SiO_2
Layer 7	Si	SiO_2
Layer 8	Si	Si_3N_4
Layer 9	SiO_2	SiO_2
Layer 10	SiO_2	SiO_2
Layer 11	SiO_2	Si_3N_4
Maximum of the Reflectance	0.335	0.328

Table-5. Layers thickness the maximum of the reflectance.

Wavelength (λ)	**0.5 μm**	**0.7 μm**
The number of layers	11	11
Layer 1 Thickness	0.305 μm	0.741 μm
Layer 2 Thickness	0.1 μm	500 μm
Layer 3 Thickness	0.109 μm	0.71 μm
Layer 4 Thickness	0.109 μm	0.114 μm
Layer 5 Thickness	0.302 μm	0.221 μm
Layer 6 Thickness	0.528 μm	0.7 μm
Layer 7 Thickness	500 μm	0.751 μm
Layer 8 Thickness	500 μm	0.733 μm
Layer 9 Thickness	0.102 μm	0.786 μm
Layer 10 Thickness	0.399 μm	0.272 μm
Layer 11 Thickness	0.119 μm	0.126 μm
Total Thickness of the Multilayer	1002.073 μm	505.154 μm

Table-6. Layers distribution for the minimum emittance.

Wavelength (λ)	**0.5 μm**	**0.7 μm**
The number of layers	11	11
Layer 1	Si_3N_4	Si_3N_4
Layer 2	Si	SiO_2
Layer 3	Si_3N_4	Si
Layer 4	Si_3N_4	SiO_2
Layer 5	Si	SiO_2
Layer 6	Si	SiO_2
Layer 7	Si	SiO_2
Layer 8	Si_3N_4	SiO_2
Layer 9	Si	SiO_2
Layer 10	SiO_2	Si
Layer 11	SiO_2	SiO_2
Minimum of the Emittance	0.628	0.673

Table-7. Layers thickness the minimum of the emittance.

Wavelength (λ)	**0.5 μm**	**0.7 μm**
The number of layers	11	11
Layer 1 Thickness	0.694 μm	0.229 μm
Layer 2 Thickness	500 μm	0.172 μm
Layer 3 Thickness	0.106 μm	500 μm
Layer 4 Thickness	0.439 μm	0.701 μm
Layer 5 Thickness	0.709 μm	0.190 μm
Layer 6 Thickness	0.666 μm	0.747 μm
Layer 7 Thickness	0.365 μm	0.374 μm
Layer 8 Thickness	0.284 μm	0.166 μm
Layer 9 Thickness	0.189 μm	0.351 μm
Layer 10 Thickness	0.641 μm	0.771 μm
Layer 11 Thickness	0.115 μm	0.568 μm
Total Thickness of the Multilayer	504.208 μm	504.269 μm

CONCLUSIONS

In this paper, the directional, spectral, and temperature dependence of the radiative properties including the reflection coefficient, transmission coefficient and emissivity for the multilayer structures consisting of silicon were examined.

Optimum structures for different industrials requirement are obtained by Simulated Annealing Algorithm. Simulated Annealing (SA) is motivated by an analogy to annealing in solids.

The results show that the radiative properties of thin films depend on the wavelength strongly. It causes selective wavelength radiative properties. From the results, it may be concluded that industrial requirements are supported by selecting coating's material and thickness.

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