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The optimization of nano-scale multilayer structures by annealing algorithm

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Abstract: When the thickness of each layer is comparable or less than the wavelength of electromagnetic waves, the wave interference effects inside each layer become important to correctly predict the radiative properties of multilayer structure of thin films. The transfer-matrix method provides a convenient way to calculate the radiative properties of multilayer structures of thin films. Coating thickness and the optimal coefficients for the reflectance and transmittance can be achieved by the use of simulated annealing algorithm pattern in the required industry.

Key words: Radiation properties; Maximum reflectance; Maximum transmittance; Simulated Annealing (SA)

1. Introduction

At nanometer distances, near-field radioactive heat transfer could be orders of magnitude greater than that between two blackbodies, especially when surface plasmon polaritons (SPPs) or surface phonon polaritons (SPhPs) are excited (Joulain et al., 2005; Basu et al., 2010). A number of groups have experimentally demonstrated that near-field radiation can exceed the blackbody limit using plateplate or sphere-plate geometries (Hu et al., 2008; Shen, 2013).

The emissivity of the wafer is a function of wavelength and temperature and can vary over a large range due to dopant type and concentration, surface roughness, coating layers, and patterning (Timans, 1997; Ravindra et al., 1998). A reflective shield has been placed in the lower chamber of some RTP systems to enhance the effective emissivity of the wafer, thus reducing the temperature measurement uncertainty (Acharya and Timans, 1998; Tsai and DeWitt, 1999).

Under severe environmental conditions, radioactive properties degradation can be limited by using diffusion barriers (thin films of silicon oxide or dioxide), in order to prevent the diffusion of coating with substrate (which produces intermetallic compounds of low reflection), and/or using protective over coatings (thin transparent oxide layers), to prevent abrasions and oxide growth (Van Vliet, 1965).

No quantitative criterion has been presented to characterize the range of applications for the two methods; the choice depends on the thickness of the film and of the degree of coherence (Chen and Tien, 1992).

Presently accounting for about 0.1% of capital and operating costs in integrated circuit (IC) manufacture, RTP is projected to extend to applications such as integrated Nano scale devices and Nano-electro-mechanical systems (NEMS)(Fiory and Mater, 2005).

Rapid thermal processing (RTP) of silicon wafers is employed as a processing step whenever a short time at high temperature serves a critical need for a low thermal budget (loosely defined as a small temperature- time product)(Fiory, 2000, 2001).

The smallness of the penetration of gold (Au), copper (Cu) and silver (Ag) to the silicon substrate ratio, cause that the transmission coefficient by increasing the thickness of the gold would be faster closes to Zero(Rad et al., 2014).

Coating thickness is increased to reduce the reflection coefficient. The emission coating for optimum reduction rate of 0.669 at a wavelength equal to 0.65 μm , reduction of 0.68 at a wavelength equal to 0.8 μm , emission(Mirjalili et al., 2014).

The reflectivity coating for optimum reduction rate of 0.334 at a wavelength equal to 0.65 μm, reduction of 0.366 at a wavelength equal to 0.8 μm, respectively. Coating thickness and the optimal coefficients for the reflectance and transmittance can be achieved by the use of simulated annealing algorithm pattern in the required industry (Mirjalili et al., 2014).

The TGA spectrophotometer and TPP tests reveal that the basalt and glass fabrics exhibit good thermal stability, and the nonwoven fabrics present excellent thermal protective performance and thermal insulation properties for real exposure time applications (Weidong and Akram, 2014).

2. Materials and methods

2.1. Coherent formulation

When the thickness of each layer is comparable or less than the wavelength of electromagnetic waves, the wave interference effects inside each

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layer become important to correctly predict the radiative properties of multilayer structure of thin films. The transfer-matrix method provides a convenient way to calculate the radiative properties of multilayer structures of thin films (Fig.1). 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 (oloomi et al., 2009; Ellison and Moline, 1994; Fu et al., 2003).

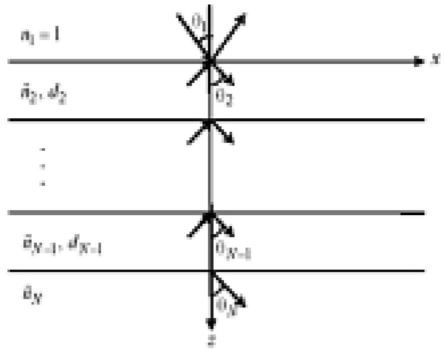

Fig.1: The geometry for calculating the radiative properties of a multilayer structure

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

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 (Li, 1980).

Consequently, the radiative properties of the N-layer system are given by (Ellison and Moline, 1994) (Li, 1980).

$$\rho = \frac{B_1 B_1^*}{A_1^2} \quad (2)$$

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

$$\varepsilon = 1 - \varepsilon - \rho \quad (4)$$

2.2. Optical constants

The Jellison and Modine (J-M) expression of optical constants of silicon for a wavelength between 0.4 µm and 0.84 µm is given in (Timans, 1993). Li developed a functional relation, for optical constants of silicon that covers the wavelength region between 1.2 µm and 14 µm (Lee and Zhang, 2005). The J-M expression is used in this study to calculate the optical constants of silicon for the wavelength region from 0.5 µm to 0.84 µm but Li's expression is employed for wavelengths above 1.2 µm. For a wavelength range of 0.84 µm to 1.2 µm, we use a weighted average based on the extrapolation of the two expressions. The optical constants of silicon dioxide, silicon nitride and gold are mainly based on the data collected in Palik (Philip, 1998).

3. Simulated annealing

The word Simulated Annealing means molten the substance but in expression is a physical process to increase substance temperature up to molten point and then cool it during certain situation, that in this process substance energy became minimum. In 1953 Metro Police, presented an algorithm to evaluate solid substance temperature changes. First he increase substance temperature until it becomes melted, then in order to reduce substance internal energy, replace its atoms. This replacement is done between two atoms. Then, in vicinity of this atom, select another atom and replace with that one, atom selection for replacement is completely randomly and there is no order for this issue. In this temperature, several replacements are done, and whenever there is no change in energy, substance temperature decreased. Before decrease substance temperature, a balancing test is done. If due to placement, substance energy decreased, placement is accepted but if substance energy didn't decrease, placement is accepTable with a probability. Later in 1983, Crack Patrick, by equaling this algorithm, between minimizing cost function of a problem and cooling substance to reach basic energy state used to solve optimization problems. Through this substitution, he and his peers introduced an algorithm called Simulated Annealing to solve integrated optimization problems (Kirkpatrick et al., 1983).

3.1. Iterations at each temperature

One method is to do a constant number of iterations at each temperature. An alternative is to dynamically change the number of iterations as the algorithm progresses. At lower temperatures, it is important that a large number of iterations are done so that the local optimum can be fully explored. At higher temperatures, the number of iterations can be less.

General form of this algorithm is Fig.2:

In this algorithm, external segment of freezing process which reduce temperature and internal segment discussed reaching to balance in each temperature.

Select primary solution of I from possible solutions category. I □ s

Select primary temperature T_0. $T_0 > 0$

Select temperature reduction process.

Select relevant function to replacement numbers in each temperature.

Put zero the relevant numerator to temperature degree change t = 0.

Repeat this loop (freezing process).

Put zero the relevant numerator to replacement numbers in each temperature degree n = 0.

Repeat below loop

Create j solution in vicinity of I solution.

Calculate df = f (j) - f(i).

If df < 0, accept the solution.

Otherwise, select a random number between 0 and 1. x□ u(0,1)

If x< e ^ (-df / T), then i=j.

N= n + 1.

Repeat loop until n = N(t) established.

t = t + 1.

Calculate new temperature degree. T = T(t)

Repeat loop until establishment of stopping condition.

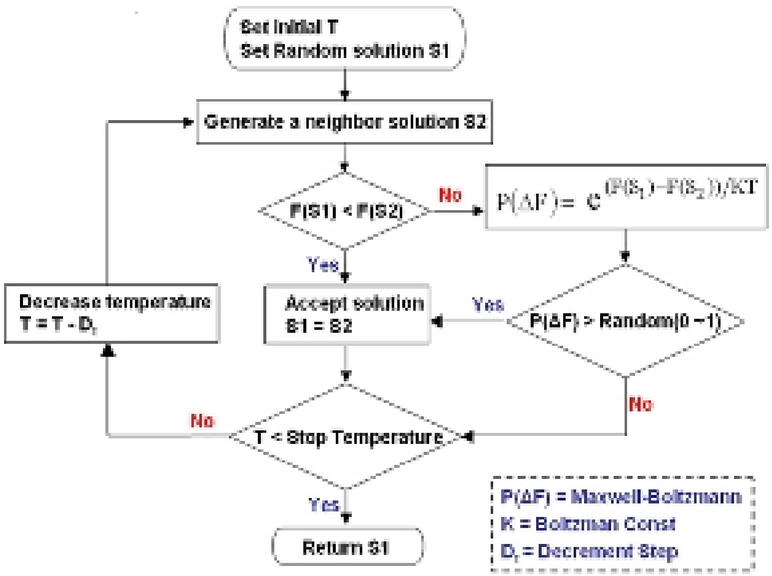

Fig.2: Simulated Annealing Algorithm

4. Results

Fig. 3 compares the reflectance and transmittance of thick silicon substrate with $700\ \mu m$ thickness and coated by silicon dioxide thin film with $300\ nm$ thickness in two different coating cases and two different temperatures with the results in. The Electromagnetic waves are incident at $\theta = 0^{\circ}$. The calculated results are in good agreement with results in (Lee and Zhang, 2005).

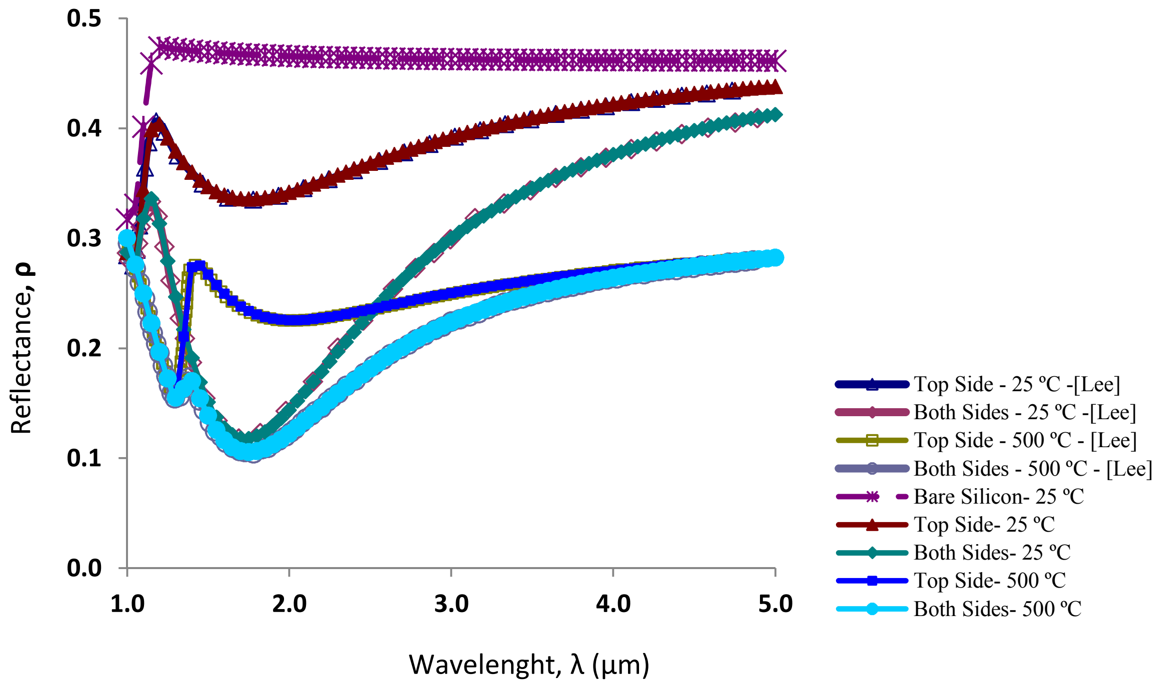

Fig.3: A comparison of the calculated reflectance with results of

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 (Fig. 3).

It is possible to choose the suiTable coating for minimum emittance, minimum transmittance and or minimum reflectance. It depends on industrial usages.

This paper considered the radiative properties of silicon coated with silicon dioxide and silicon nitride at room temperature for 9 layers with different coating procedures and coherent formulation is used.

Thin films play an important role in the semiconductor industry and micro electromechanical and Nano electromechanical equipment. 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 division of layer's materials and the thickness of each layer (according as micrometer) the outcome of optimization of Simulated Annealing Algorithm (SA) for maximum reflection coefficient in the Tables 1 and 2 and for the maximum transmittance in two wavelengths 0.65㎛ and 0.8㎛ in the Tables 3 and 4 are mentioned.

The maximum thickness of coating is considered constant. In this section, silicon thickness less than 500㎛ and a maximum thickness of each layer were considered equal to 400 nm.

The results are compared in Table 5 with colonial competitive algorithm (Teymoorzadi et al., 2014) and in Table 6 with Imperialist competitive Algorithm (Amiri Rad et al., 2014).

Table 1: Distribution Gender layers for maximum reflectance coefficient

Wavelength(λ)	The number of layers	Layer Genus 1	Layer Genus 2	Layer Genus 3	Layer Genus 4	Layer Genus 5	Layer Genus 6	Layer Genus 7	Layer Genus 8	Layer Genus 9	Maximum reflection coefficient
0.65 μm	9	Si	Si	SiO_2	SiO_2	Si_3N_4	SiO_2	Si_3N_4	SiO_2	Si_3N_4	0.333
0.8 μm	9	Si	SiO_2	Si_3N_4	Si	Si_3N_4	SiO_2	SiO_2	SiO_2	SiO_2	0.319

Table 2: Layers thickness for maximum reflectance coefficient

Wavelength(λ)	Layer thickness 1	Layer thickness 2	Layer thickness 3	Layer thickness 4	Layer thickness 5	Layer thickness 6	Layer thickness 7	Layer thickness 8	Layer thickness 9	Total thickness of the coating
0.65 μm	500	500	0.12	0.145	0.02	0.05	0.112	0.301	0.09	1008.8 μm
0.8 μm	500	0.215	0.331	0.07	0.384	0.117	0.116	0.214	0.393	501.8 μm

Table 3: Distribution Gender layers for maximum Transmittance

Wavelength(λ)	The number of layers	Layer Genus 1	Layer Genus 2	Layer Genus 3	Layer Genus 4	Layer Genus 5	Layer Genus 6	Layer Genus 7	Layer Genus 8	Layer Genus 9	Maximum Transmittance
0.65 μm	9	Si_3N_4	SiO_2	Si_3N_4	SiO_2	Si	SiO_2	Si_3N_4	SiO_2	SiO_2	$1.99 * 10^{-29}$
0.8 μm	9	Si_3N_4	Si_3N_4	Si_3N_4	Si_3N_4	Si	Si	SiO_2	SiO_2	SiO_2	$1.5 * 10^{-9}$

Table 4: Layers thickness for maximum Transmittance

Wavelength(λ)	Layer thickness 1	Layer thickness 2	Layer thickness 3	Layer thickness 4	Layer thickness 5	Layer thickness 6	Layer thickness 7	Layer thickness 8	Layer thickness 9	Total thickness of the coating
0.65 μm	0.387	0.296	0.084	0.374	500	0.367	0.163	0.163	0.239	502.07 μm

0.8 µm	0.33	0.36	0.306	0.3	500	0.399	0.08	0.001	0.392	502.1 µm

Table 5: Comparison of the colonial competitive algorithm with an algorithm simulated annealing

Wavelength(λ)	The number of layers	Layer Genus 1	Layer Genus 2	Layer Genus 3	Layer Genus 4	Layer Genus 5	Layer Genus 6	Layer Genus 7	Layer Genus 8	Layer Genus 9	Minimum Reflection Coefficient
0.65 μm	9	Si_3N_4	SiO_2	Si_3N_4	SiO_2	SiO_2	Si	Si	SiO_2	Si	0.296
0.65 μm (Teymoorzadi et al., 2014)	9	Si_3N_4	SiO_2	Si	SiO_2	Si_3N_4	Si_3N_4	SiO_2	Si	Si_3N_4	0.31

Table 6: Comparison of the Imperialist competitive Algorithm with an algorithm simulated annealing

Wavelength(λ)	0.65(Rad et al., 2014) μm	0.65 μm
The number of layers	9	9
Layer Genus 1	1	Si
Layer Genus 2	4	Si
Layer Genus 3	1	SiO_2
Layer Genus 4	1	SiO_2
Layer Genus 5	3	Si_3N_4
Layer Genus 6	2	SiO_2
Layer Genus 7	3	Si_3N_4
Layer Genus 8	2	SiO_2
Layer Genus 9	3	Si_3N_4
Maximum reflection coefficient	0.8875	0.333

It can analyze the specified wavelength and by the Algorithm simulated annealing (SA); it can choose the appropriate structure with the appropriate number of layers, appropriate type and combination of thin film coating.

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