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Minimize Radiative properties of Non Metallic Thin Films using Simulated Annealing Algorithm

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ABSTRACT

Semiconductor coatings play an important role in the many industries and micro electromechanical and nano electromechanical equipments. Accurate radiometric temperature measurements of silicon wafers and heat transfer analysis of rapid thermal processing furnaces require a thorough understanding of the radiative properties of the silicon wafer, whose surface may be coated with dielectric or absorbing films. In this research thin film multilayer has been investigated. The transfer matrix method is applied to calculate the radiative properties of multilayer structures. This method considers wave interferences in each layer. The empirical expression for the optical constants of lightly dopped silicon is used. Simulated annealing algorithm is used to achieve optimum radiative properties of thin films and their structures. In this study the layers at 25°C has been investigated. The electromagnetic wave with an angle of 10° to the multi-layered structure is applied. The reflectivity coating for optimum reduction rate of 0.334 at a wavelength equal to 0.65 , reduction of 0.366 at a wavelength equal to 0.8 , 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.

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INTRODUCTION

Nano-scale multilayer coatings have found use in a number of commercial applications where wear and corrosion resistance determine the service life of the components [1]. Silicon dioxide and silicon nitride coating act as anti reflector and these coatings reduce reflectance toward bare silicon. If thickness of non metal coating increases, reflectance of multilayer decreases and transmittance increases [2]. In visible wavelengths the reflectance increases as the temperature increases, because of decreasing emittance. As the film thickness increases, the free spectral range decreases, resulting in more oscillations with thicker silicon dioxide film, but interferences in the substrate are generally not observable in incoherent formulation [3].

Understanding the radiative properties of semiconductors is essential for the advancement of manufacturing technology, such as rapid thermal processing [4]. Because the major heating source in rapid thermal processing is lamp radiation, knowledge of radiative properties is important for temperature control during the process.

Optical and thermal radiative properties are fundamental physical properties that describe the interaction between electromagnetic waves and matter from deep ultraviolet to far-infrared spectral regions [5].

This work uses transfer-matrix method and the coherent formulation for calculating the radiative properties of lightly dopped silicon.

It is observed that the concentrations highly affect the radiative properties of doped silicon multilayer at temperatures below 600°K. At temperatures below 600°K the concentration and the type of impurities have important effects on the radiative properties of the film [6].

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. But this effect has not been shown at visible wavelengths [7].

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High emittance is needed for suitable thermal balance of the thin film solar cells for space applications. Optical coatings that provide high emittance must be formed on the solar cells to overcome that problem by increasing number of thin film layers. Radiative properties are complex function of wavelength [8].

The reflectance of multilayer coated with gold increases by increasing the thickness of coating. This study will benefit and enhance the value of nano coating technology in the semiconductor industries, particularly in the development of micro electromechanical and nano electromechanical devices [9].

When silicon dioxide thin film thickness increases to 300 nm, then reflectance of multilayer will decrease from 0.4553 to 0.0443. The layer thicknesses need to be optimized to achieve maximum transmittance for the given materials [10].

The large activity and stability for the pretreated route could be comparable with those of the advanced electrocatalysts. All these progresses lay a bottom-up approach for future electrocatalysts [11].

Jyoti describes the advancement of performance of simple SA applied upon the problem of graph coloring using a specially designed operator called random change operator instead of the general change operator [12].

Cretu applies the matrix method formalism in conjunction with a simulated annealing algorithm with the aim to design acoustical structures, especially acoustic filters [13].

Thermal stability and mechanical properties of zirconium tungsten nitride (Zr–W–N) thin films have been studied. Hardness and elastic modulus of annealed films increase with increasing strain [14].

The directional, spectral, and temperature dependency of the radiative properties for the Nanoscale multilayer structures are modeled consisting of silicon and related materials such as silicon dioxide, and silicon nitride. Results showed that maximum transmittance depends on the type of materials coatings and its temperature [15].

The TiN-Ni nanocomposite films were found to exhibit lower hardness than a TiN film deposited using similar conditions and were more ductile due to the presence of metallic Ni. The film deposited at room temperature and low bias was found to be highly elastic, exhibit reasonable hardness (~ 18 GPa) and low intrinsic stress [16].

MATERIALS AND METHODS

Coherent Formulation:

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 (Figure. A.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

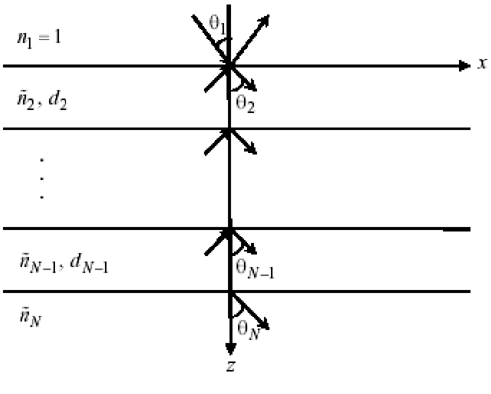

Fig. A.1: The geometry for calculating the radiative properties of a multilayer structure [5].

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

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 [5].

Optical Constants:

The optical constants of silicon dioxide are mainly based on the data collected in Palik's handbook [17].

Simulated annealing:

Simulated Annealing (SA) is motivated by an analogy to annealing in solids. The idea of SA comes from a paper published by Metropolis et al. Metropolis algorithm simulated the material as a system of particles. The algorithm simulates the cooling process by gradually lowering the temperature of the system until it converges to a steady, frozen state. In 1982, Kirkpatrick et al [18, 19, and 20] took the idea of the Metropolis algorithm and applied it to combinatorial (and other) optimization problems. 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. SA's major advantage over other methods is an ability to avoid becoming trapped at local minima. The algorithm employs a random search, which not only accepts changes that decrease objective function, f, but also some changes that increase it. The latter are accepted with a probability:

$$p = \exp(-\Delta f / T) \qquad \text{Eq. (B.1)}$$

where Δf is the difference in f and T is a control parameter.

And,

Δ = the change in objective function

T = the current temperature

Acceptance criteria:

In each step of Metropolis algorithm, a particle is given a small random displacement and the resulting change, δf, in the energy of the system is computed. If $\delta f \leq 0$, the displacement is accepted. The case $\delta f > 0$ is treated probabilistically. The probability that the configuration is accepted is given in equation (B.1). A certain number of iterations are carried out at each temperature and then the temperature is decreased. This is repeated until the system freezes into a steady state. This equation is directly used in simulated annealing. The probability of accepting a worse state is given by the equation (B.2):

$$p = \exp(-\Delta f / T) > r \qquad \text{Eq. (B.2)}$$

(Where r is a random number uniformly distributed between 0 & 1).

The probability of accepting a worse move is a function of both the temperature of the system and of the change in the objective function. As the temperature of the system decreases, the probability of accepting a worse move is decreased. If the temperature is zero, then only better moves will be accepted [20, 23].

Table A.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

Starting temperature:

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. However, if the temperature starts at too high a value, then the search can move to any neighbor and thus transforms the search (at least in the early stages) into a random search. Effectively, the search will be random until the temperature is cool enough to start acting as a simulated annealing algorithm [21, 22]. A method which is suggested by Dowsland is to rapidly heat the system until a certain proportion of worse solutions are accepted and then slow cooling can start.

Final temperature:

It is usual to let the temperature decrease until it reaches zero. However, this can make the algorithm run for a lot longer. In practice, it is not necessary to let the Temperature reach zero because as it approaches zero, the chances of accepting a worse move are almost the same as the temperature being equal to zero. Therefore, the stopping criteria can either be a suitably low temperature or when the system is frozen at the current temperature (i.e. no better or worse moves are being accepted).

Temperature decrement:

Once we have our starting and stopping temperatures, we need to get from one to the others. Theory states that we should allow enough iteration at each temperature so that the system stabilizes at that temperature. The theory also states that at each temperature, the number of iterations might be exponential to the problem size in order to achieve the system stability. As this is impractical, we need to compromise. We can either do this by performing a large number of iterations at a few temperatures, a small number of iterations at many temperatures or a balance between the two [21, 22, and 23].

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 [20]. 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.

Results:

Figures B.1 and B.2 compare the reflectance and transmittance 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 tow different temperatures with the results in [24]. The Electromagnetic waves are incident at $\theta = 0^\circ$. The calculated results are in good agreement with results in [24].

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 (Figures.B.1).

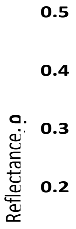

Fig. B.1: A comparison of the calculated reflectance with results of [24].

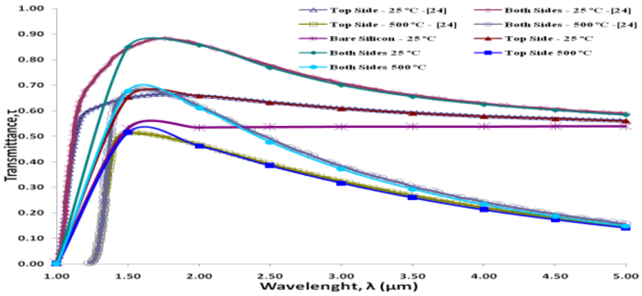

Fig. B.2: A comparison of the calculated Transmittance with results of [24].

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 minimum reflection coefficient in the tables , No (A.2) and (A.3) and for the minimum transmittance in two wavelengths 0.65 μm and 0.8 μm in the tables No (A.4) and (A.5) are mentioned.

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

The results are compared in Table (A.6) with colonial competitive algorithm [25].

Table A.2: Distribution Gender layers for Minimum reflectance.

Wavelength(λ)	0.65 μm	0.8 μm
The number of layers	9	9
Layer Genus 1	Si_3N_4	SiO_2
Layer Genus 2	SiO_2	SiO_2
Layer Genus 3	Si_3N_4	Si_3N_4
Layer Genus 4	SiO_2	Si_3N_4
Layer Genus 5	SiO_2	Si
Layer Genus 6	Si	Si_3N_4
Layer Genus 7	Si	SiO_2
Layer Genus 8	SiO_2	SiO_2
Layer Genus 9	Si	Si
Minimum reflection coefficient	0.296	0.308

Table A.3: layers thickness for Minimum reflectance.

Wavelength(λ)	0.65 μm	0.8 μm
Layer thickness 1	0.139	0.369
Layer thickness 2	0.389	0.319
Layer thickness 3	0.181	0.37
Layer thickness 4	0.312	0.02
Layer thickness 5	0.394	500
Layer thickness 6	500	0.04
Layer thickness 7	500	0.348
Layer thickness 8	0.396	0.18
Layer thickness 9	500	0.0009
Total thickness of the coating(μm)	1501.811	501.6469

Table A.4: Distribution Gender layers for Minimum Transmittance.

Wavelength(λ)	0.65 μm	0.8 μm
The number of layers	9	9
Layer Genus 1	Si_3N_4	SiO_2
Layer Genus 2	SiO_2	SiO_2
Layer Genus 3	Si_3N_4	SiO_2
Layer Genus 4	SiO_2	Si
Layer Genus 5	SiO_2	Si_3N_4
Layer Genus 6	Si	Si
Layer Genus 7	Si	Si_3N_4
Layer Genus 8	SiO_2	Si
Layer Genus 9	SiO_2	Si_3N_4
Minimization transmission coefficient	$8.48*10^{-58}$	$1.42*10^{-26}$

Table A.5: layers thickness for Minimum Transmittance.

Wavelength(λ)	0.65 μm	0.8 μm
Layer thickness 1	0.391	0.396
Layer thickness 2	0.005	0.38
Layer thickness 3	0.003	0.376
Layer thickness 4	0.382	500
Layer thickness 5	0.09	0.327
Layer thickness 6	500	500
Layer thickness 7	500	0.389
Layer thickness 8	0.312	500
Layer thickness 9	0.399	0.376
Total thickness of the coating(μm)	1001.582	1502.244

Table A.6: Comparison of the colonial competitive algorithm with an algorithm simulated annealing [25].

Wavelength(λ)	0.65 μm	0.65 μm [25]
The number of layers	9	9
Layer Genus 1	Si_3N_4	Si_3N_4
Layer Genus 2	SiO_2	SiO_2
Layer Genus 3	Si_3N_4	Si
Layer Genus 4	SiO_2	SiO_2
Layer Genus 5	SiO_2	Si_3N_4
Layer Genus 6	Si	Si_3N_4
Layer Genus 7	Si	SiO_2
Layer Genus 8	SiO_2	Si
Layer Genus 9	Si	Si_3N_4

Minimum Reflectance	0.296	0.31

Conclusions:

Coating thickness is increased to reduce the reflection coefficient. 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.

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.

By selecting the appropriate coating, It can be seen the reduction of 10.031 times in the 0.65 μm wavelength, and the reduction of 6.51 times in the 0.8 μm wavelength for the transmittance.

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.

REFERENCES

[1] Savisalo, T., D.B. Lewis, P.E. Hovsepian, 2006. Microstructure and properties of novel wear and corrosion resistant CrON/NbON nano-scale multilayer coatings. Surface and Coatings Technology, 200:2731-2737.
[2] Oloomi, S.A.A., A. Saboonchi, A. Sedaghat, 2010. Effects of thin film thickness on remittance, reflectance and transmittance of nano scale multilayers. International Journal of the Physical Sciences, 5(5): 465-469.
[3] Oloomi, S.A.A., A. Saboonchi, A. Sedaghat, 2010. Comparison radiative properties of thin semiconductor films by coherent and incoherent formulation. World Applied Sciences Journal, 9(4): 372-379.
[4] Timans, P.J., 1996. The thermal radiative properties of semiconductors, Advances in Rapid Thermal and Integrated Processing. Academic Publishers. Dordrecht. Netherlands, 35-102.
[5] Fu, C.J., Z.M. Zhang, Q.Z. Zhu, 2003. Optical and thermal radiative properties of semiconductors related to micro/nanotechnology, Advanced in Heat Transfer, 37: 179-296.
[6] Oloomi, S.A.A., A. Saboonchi, A. Sedaghat, 2010. Parametric study of nanoscale radiative properties of doped silicon multilayer structures. World Applied Sciences Journal, 8: 1200-1204.
[7] Omidpanah, M., S.A.A. Oloomi, 2012. Effects of dopant concentrations on thin films with coherent formulation at visible wavelengths. Iranica Journal of Energy & Environment, 3: 284-290.
[8] Oloomi, S.A.A., A. Saboonchi, A. Sedaghat, 2010. Effects of thin films number on nano scale radiative properties. World Applied Sciences Journal, 11: 1398-1402.
[9] Oloomi, S.A.A., A. Saboonchi, A. Sedaghat, 2010. Effects of thin films effects of thin film thickness on emittance, reflectance and transmittance of nano scale multilayers. International Journal of the Physical Sciences, 5: 465-469.
[10] Omidpanah, M., S.A.A. Oloomi, 2012. Nanoscale radiative properties of thin films, middle-east Journal of Scientific Research,11: 727-733.
[11] Zhong shu, Y., H. Tian Hang, W. Jian Long, W. Cheng, L. Zhi Xiang, G. Jine Wei, 2014. Preparation of highly active and stable polyaniline-cobalt-carbon nanotube electrocatalyst for oxygen reduction reaction in polymer electrolyte membrane fuel cell, Electrochimica Acta, 119: 144-154.
[12] Jyoti Pal, A., B. Ray, N. Zakaria, S.S. Sarma, 2012. Comparative performance of modified simulated annealing with simple simulated annealing for graph coloring problem, Procedia Computer Science, 9: 321-327.
[13] Cretu, N., M.I. Pop, I.C. Rosca, 2010. Acoustic design by simulated annealing algorithm. Physics Procedia, 3: 489-495.
[14] Dubey, P., V. Arya, S.K. Srivastava, D. Singh, R. Chandra, 2014. Study of thermal stability and mechanical properties of fcc phase $Zr_{22}W_{19}N_{58}$ thin films deposited by reactive magnetron sputtering. Surface and Coatings Technology, 245: 34-39.
[15] Oloomi, S.A.A., A Saboonchi, A. Sedaghat, 2009. Parametric study of nanoscale radiative properties of thin film coatings. A Journal of Nanotechnology and its Applications, 7: 1-7.
[16] Pagon, A.M., E.D. Doyle, D.G. McCulloch, 2013. The microstructure and mechanical properties of TiN-Ni nanocomposite thin films. Surface and Coatings Technology, 235: 394-400.
[17] Palik, E.D., 1998. Silicon Dioxide (SiO2) Handbook of Optical Constants of Solids. San Diego.
[18] Kirkpatrick, S., C.D. Gelat, M.P. Vecchi, 1983. Optimization by simulated annealing. Science, 220: 671-680.
[19] Rutenber, R.A., 1989. Simulated Annealing Algorithm, IEEE circuits and Devices, 19-26.
[20] Szu, H., R. Hartley, 1987. Fast simulated annealing. Physics Letters A, 122: 157-162.
[21] Yang, G., D. Chen, G. Zhou, 2006. A new hybrid algorithm of particle swarm optimization. in Lecture Notes in Computer Science, 4115: 50-60.

[22] Aarts, E.H.L., J.H.M. Korst, 1991. Boltzmann machines as a model for parallel annealing. Algorithmica, 6: 437-465.
[23] Cerny, V.. 1985. A Thermodynamical approach to the travelling salesman problem; an efficient simulation algorithm. Journal of Optimization Theory and Applic, 45: 41-55.
[24] Lee, B.J., Z.M. Zhang, 2005. Modeling radiative properties of silicon with coatings and comparison with reflectance measurements. Journal of Thermo physics and Heat Transfer, 19: 558-565.
[25] Teymoorzadi, H., A. Shokrollahi, S.A.A. Oloomi, A. abedi, 2014. Optimum radiative properties of non-metallic nano-coatings using colonial competitive algorithm. Indian Journal of Scientific Research, 1: 752-758.