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고 흡수율과 고방사율 다중 코팅 설계를 위한 전산모사 연구

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Computer Simulation Study for Higher Solar Absorptance and Lower Emittance Multilayer Coating Design

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Abstract

본 연구에서는 복층으로 구성된 $WSio_2Al$ 금속절연체의 상세를 보여주고 있는데, 금속과 절연체의 합성물질은 태양 흡수율의 설계와 열적인 현상을 보여주기 위해 종종 사용된다. 금속의 접착기면 위에 얇은 복층 코팅으로 구성되는 디자인은 태양 스펙트럼의 파장권역에서 선택적 흡수를 위함이다. 본 연구는 태양 복사의 열성능 평가를 위해 금속과 절연체 필름의 방사율, 태양흡수율, 코팅순서, 미 반사층(AR)의 두께, 코팅 두께와 코팅 면수, 전체 코팅 두께 등에 대해 시뮬레이션 하였다. 그 결과 네 겹의 코팅설계에서 Sio_2AR 75 nm 두께와 각각의 층에서 0.5~0.7의 가변 금속부분 구성이 가장 우수한 성능을 갖는 것으로 나타났다. 또한 시뮬레이션으로 금속과 절연체 합성물의 최적의 구성과 각각의 코팅 두께에 대한 예측이 가능했으며, 최대 태양흡수율은 0.94, 방사율은 0.115의 금속과 절연체의 합성물을 구성할 수 있었다.

Keywords : 흡수율(Absorptance), 방사율(Emittance), 컴퓨터 시뮬레이션(Computer simulation)
태양선택코팅(Solar selective coating), 무반사(Antireflection : AR)

1. Introduction

The effective utilization of solar energy derived from solar radiation requires efficient solar selective coatings. This is defined as simultaneously having high absorptance in the solar spectral region and low emittance in the thermal spectral region to reduce thermal radiative heat loss [1].

This is feasible due to large temperature difference between the sun and the surface exposed to them. The spectral irradiance of solar radiation and the thermal infrared spectrum of heated bodies do not over lap to any appreciable extent. The terrestrial solar spectral irradiance distribution curve start at 0.3m [2]. For temperatures below 773 K, almost all thermal radiation (98%) occurs at 2 m.

The main objective of this study was to analyze the solar absorptance and thermal emittance of a solar selective coating design. The effects of using metal and dielectric materials with different volume fractions of suitable metal contents were studied using computer simulation. The effect of other parameters such as coating layer, antireflection coating thickness and layer thickness have been studied on the base of simulation results to investigate the performance of the solar selective coating design.

2. Selective Materials

In practice any material, which exhibits selectivity, i.e. a significant change in optical properties across solar and thermal wavelength, is termed a spectrally selective material. The material may be single, alloy or composed of two or more compounds.

The spectral selectivity is a result of different processes in the observed material. The basic physical effects are intrinsic absorption, interference in a double layer (reflecting absorbing tandem), interference effects of alternating dielectrics and metals, geometrical trapping by surface roughness, and the size effect of metal particles in an insulating matrix [1,3,4]. The spectrally selective surfaces can be prepared by one of the most common method: applying a high solar absorptive layer on to the low-emitting metal substrate [5,6]. The layer must be transparent in the infrared region in order to support the low-emittance of the substrate. Such layer is called a selective solar absorber.

The efficiency of a particular selective solar absorber depends upon its thickness. This thickness is a compromise between high absorption of the solar radiation and low thermal emission. Solar absorptance can be increased by using a thicker coating, but unfortunately the thermal emittance also rises very rapidly. The maximum efficiency of a given spectrally selective material is achievable at the optimum layer thickness.

In the present study, tungsten has been chosen as metal and SiO_2 as dielectra for making composite films. This dielectra was also analyzed for the AR coatings study. The main purpose of using tungsten as a metallic volume fraction is that it is lustrous and silvery white in colour. It is relatively inert, resisting attack by oxygen, acid and alkalis, and also has a high resistance to temperature fluctuations. In the visible region tungsten has very low reflectance and a very high absorptance. In the whole solar thermal range, the high optical constants of tungsten make it feasible to use with a high refractive index dielectric.

The choice of these ($WSiO_2$) materials is therefore an important factor with regards to the refractive index criteria of composites in order to achieve a high optical performance. For high refractive metals, a high refractive index and dielectra are suitable. A mismatch will decrease the optical performance of the selective absorber.

3. Multilayer Coating Design

The solar selective paint design in this study is a multilayer metal-dielectric graded index coatings. These multilayer coatings are known as interference stacks. The metal-dielectric layers act like selective filters for energy absorption. The accuracy of layer thickness is very important for these types of coatings. The active film is divided in to number of layers of different thickness. The upper layer of active film covered by a dielectric (SiO_2) antireflection layer to decrease the front surface reflectance. The volume fraction in the active film increases from top (air-film interface) to bottom (film substrate interface).

This category is called "Variable (layer) Thickness Absorber Coating (VTAC)".

The multilayer coating design of metal/dielectric composite($WSiO_2Al$) is shown in Fig 1.

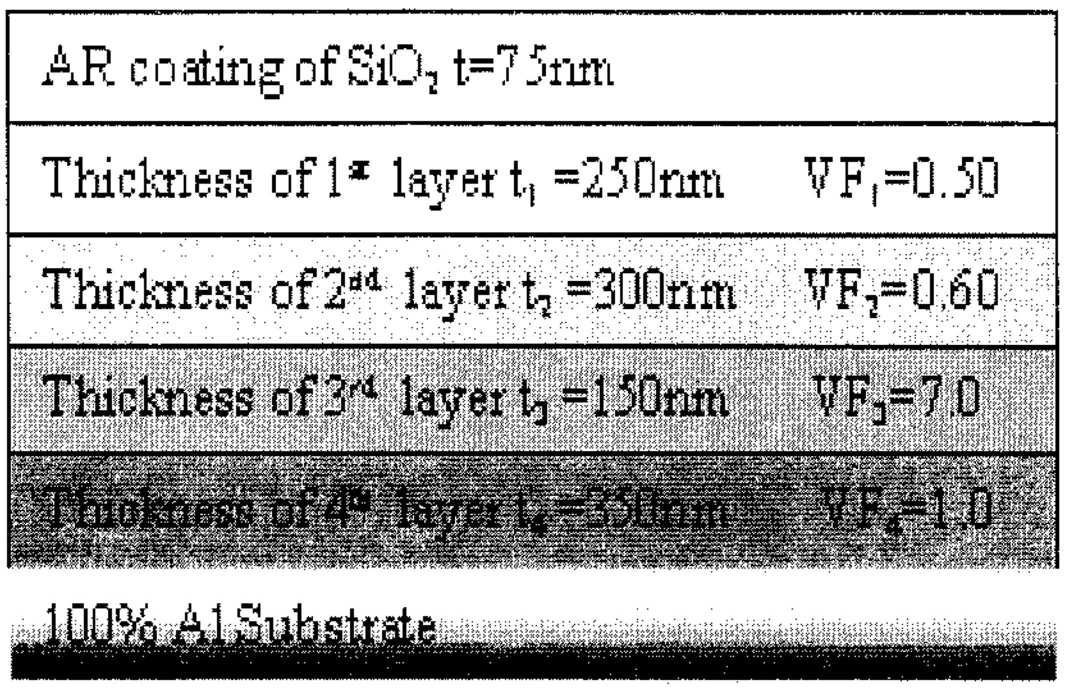

Fig 1. Multilayer metal/dielectric composite ($WSiO_2Al$) coating design

The metallic volume fraction for each layer varies from 0.5 to 0.7. The thickness of each layer is chosen to enhance the desired effect of optical interference between adjacent layers.

4. Computer Simulations

Computer simulations were performed by a program called CEMTAR, which was written in PASCAL. It calculates the solar absorptance and thermal emittance of composite spectrally selective coatings. The structure of the program is such that it reads the optical constants of both metal and dielectric constituents at specify wavelength points. The wavelengths are taken at the selected ordinates of the AM 2 solar spectrum and thermal spectrum at the required temperature of the black body.

It starts with input values of metal volume fraction (VF), thickness of the individual layers and the total number of layers of the film. The program calculates the dielectric constants of individual layers by using a Maxwell Garnet or Bruggeman formalism, dependent on the VF and then calculates the overall dielectric constants of the composite film by matrix multiplication. The antireflection (AR) coating has been assumed to be a smooth surface for the studied results, but in the program there is a provision that the AR layer can be a porous film of the air and dielectric. The porosity is assumed to be the VF of air in the dielectric.

4.1 Selective Materials : Theory

Any material, which exhibits selectivity, i.e. a significant change in optical properties across solar and thermal wavelengths, is termed a spectrally selective material. The material may be single, alloy or composed of two or more materials such as metals/semiconductors and insulators.

A material whose properties are intermediate between the properties of metals and insulators fulfills the requirements of a selective absorber and most widely used selective absorbers belong to this category. Effective medium models normally characterize the composite behavior of the ingredients. This model for composite absorbers is sophisticated due to the large number of influencing factors such as size, shape and binding of particles in the composite. A number of theoretical models are available for such mediums. The most important will be discussed below.

4.2 Maxwell Garnet Theory

This theory assumes that conducting particles embedded in an insulating material are spherical and much smaller than the incident wavelength of the radiation. Since the particle size is small, the conducting spheres can be considered as a system of interacting dipoles. The Maxwell Garnet theory gives the effective dielectric permeability of the composite materials by the following relation [7].

$$\frac{\varepsilon-\varepsilon_b}{\varepsilon+2\varepsilon_b}=\frac{f(\varepsilon_a-\varepsilon_b)}{(\varepsilon_a+2\varepsilon_b)} \tag{1}$$

Where is the dielectric function of the composite film.

ε_b is the dielectric function of the insulating material

ε_a is the dielectric function of the conducting particles.

4.3 Bruggemen Theory

Bruggeman supposes that the medium

is a random mixture of metal and insulating spheres and effective medium dielectric function is [8]:

$$\frac{f(\varepsilon_a-\varepsilon)}{\varepsilon_a+2\varepsilon}+\frac{(1-f)(\varepsilon_b-\varepsilon)}{\varepsilon_b+2\varepsilon}=0 \qquad (2)$$

The equation comes from assuming that a random unit cell of the medium has a probability "f" of being metallic and "1-f" of being insulating. The refractive index of a homogeneous composite layer is determined from effective medium theories. The refractive index of a graded film is calculated by dividing the film into a number of layers. Each layer is assumed to be homogeneous, for the purpose of determining the refractive index.

4.4 Optics of Multilayer Coatings

The composite film is divided into number of layers, each having a different composition. For multilayer composite absorbers, the E (electric) and H (magnetic) field factors should be continuous at any interface.

However, the matrix method is applied to calculate the reflectance and transmittance of the absorber coating.

The matrix in the equation characterizes one layer. Moreover its determinant is unity, which acts as a check on the calculations.

$$\begin{bmatrix} E_{m-1} \\ H_{m-1} \end{bmatrix} = \begin{bmatrix} \cos\phi_{mj} & \frac{i}{n_{cm}}\sin\phi_{mj} \\ in_{cm}\sin\phi_m & \cos\phi_m \end{bmatrix} \begin{bmatrix} E_m \\ H_m \end{bmatrix} \qquad (3)$$

For n number of layers we can rewrite as :

$$\begin{bmatrix} E_0 \\ H_0 \end{bmatrix} = \Pi_{m-1}^{N} M_{at\ N} \begin{bmatrix} E_m \\ H_m \end{bmatrix} \qquad (4)$$

$$\begin{bmatrix} E_N \\ H_n \end{bmatrix} = \begin{bmatrix} 1 \\ n_{sub} \end{bmatrix} E\Pi_{sub}^{+} \qquad (5)$$

$$M_N = M_j =$$

$$(\cos\phi j - (\frac{i}{N_i})\sin\phi j - i\,\overline{N_i}\,\sin\phi j\ \cos\phi j) \qquad (6)$$

Where, N_i is the complex refractive index of the composite "jth" layer, "i" is the square root of minus one ($\sqrt{-1}$), the phase shift, $\phi_i=\frac{2\pi N_i T_j}{\lambda}$, "$t_j$" is film thickness of "jth" layer, and λ is wavelength.

The composite films are analyzed on metallic substrates, so there is no transmission of radiation. The only parameter from which to deduce the absorptance and emittance of the system is reflectance, which can be calculated as:

$$R = \left|\frac{\cos\phi i-(-iNi\sin\phi i)+((-i/Ni)\sin\phi i-\cos\phi i)N_s}{os\phi i+(-iNi\sin\phi i)+((-i/Ni)\sin\phi i+\cos\phi i)N_s}\right| \qquad (7)$$

where R is the reflectance at a single wavelength point and Ns is the complex refractive index of the substrate. The reflectance at the selected ordinates of the solar spectrum is calculated to determine the solar absorptance. Similarly the emittance of the selective composite coatings is determined by calculating the reflectance at the selected ordinates of the thermal spectrum, for the required temperature. The solar absorptance and thermal emittance calculations are based on the assumption that the transmittance is zero.

5. Result and Discussion

The effect of metallic volume fraction, thickness variations in each layer, number of layers and AR coating on absorptance and thermal emittance have been discussed as follows on the basis of computer simulations.

5.1 Effect of Paint Layers on Absorptance and Emittance

The paint coating is a graded composite structure of metal (Tungsten) and dielectric (SiO_2) with gradation from top to bottom. Thickness of each layer is optimized on the basis of computer simulation study to achieve maximum solar absorptance for high refractive index material such as tungsten. The effect of 2-layer, 3-layer and 4-layer coating design on solar thermal absorptance and emittance with particular percentage of metallic volume distribution (0.7%) was studied. Fig 2 and 3 show the influence of the number of layers on the solar thermal absorptance and emittance.

It is clear from the results that the 4-layer coating design has higher values of absorptance and emittance as compare to 2-layer and 3-layer coating design (see Table 1). This high absorptance is due to the increase in the number of layers. The increase in the number of layers not only decreases the front surface reflection but also increases the metal gradation from top to bottom. The other reason for the high absorptance is that due to the large number of layers, multiple reflections and transmission of radiation occur in different coating layers, which causes the maximum absorption of solar thermal range radiation. Thus the interference effect in four layers coating design with volume fraction of 0.7% is high as compare to two and three layer coating system. The reason of increase in emittance with the increase of number of layer is due to variation in optical path of the coatings.

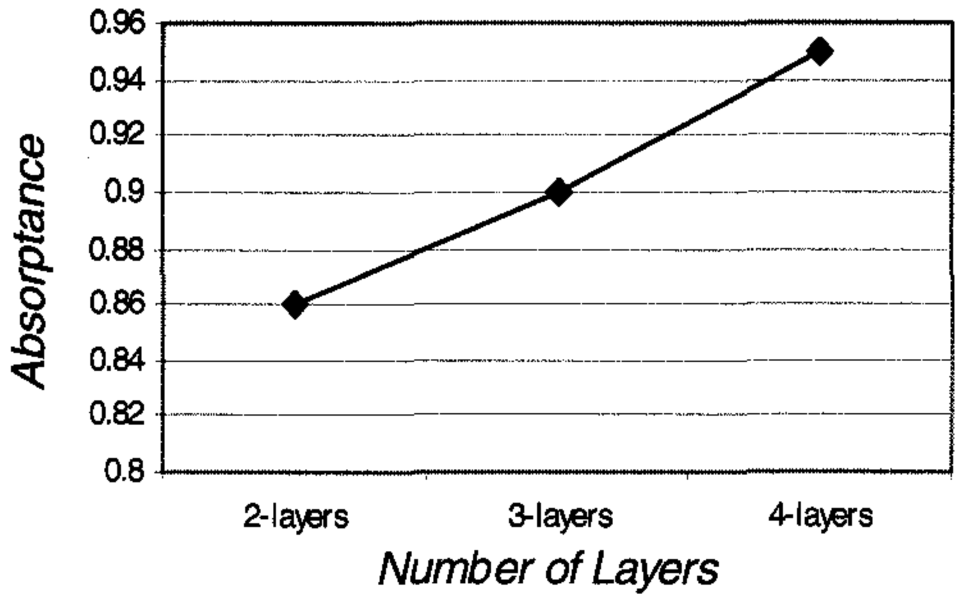

Fig 2. Effect of Gradation on absorptance

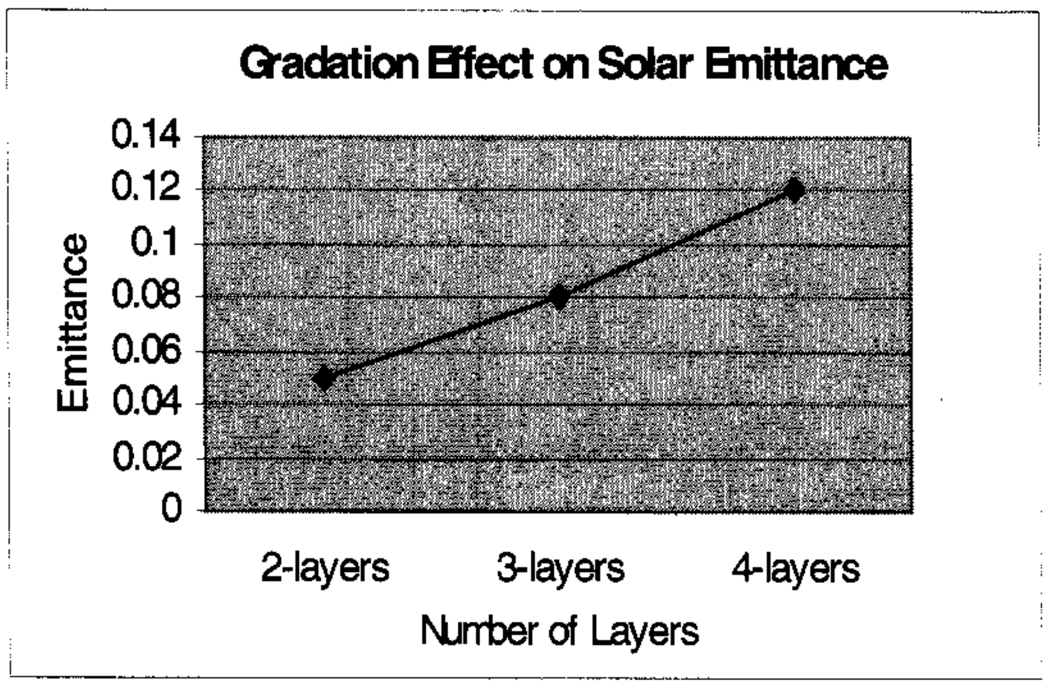

Fig 3. Effect of Gradation on emittance

Table 1. Gradation effect on solar absorptance and emittance

S.no	Number of Layers	Absorptance	Emittance
1	2-layers	.86	.05
2	3-layers	.90	.08
3	4-layers	.95	.12

5.2 Effect of Anti-reflection Layer Thickness on Absorptance and Emittance

A dielectric AR coating decreases the refractive index difference between the selective coating and air. The choice of material and thickness required in the AR coating can be determined by the optical properties of the absorber. In order to minimize front surface reflection in solar range, the boundaries of the upper and lower surfaces of the AR coating must have equal reflective properties. For selective absorbers, an AR coating that function over the whole range is desirable. Through computer modeling, the optimized thickness of AR coating was determined.

SiO_2 was used as an AR coating on a $WSiO_2Al$ composite. The above composite was graded with different metallic volume fraction (0.5 to 0.7 VF) into four layers.

Silicon has higher refractive index material so was used as an AR coating for higher refractive index composite like $W{:}SiO_2$. In order to determine appropriate AR coating thickness for 0.7 metallic gradation composites, 50 nm, 75 nm, 125 nm, 150 nm and 200 nm thick AR coating layers were studied. The variation in solar absorptance with the increase in AR coating thickness is shown in Table 2 and Fig 4 and 5. It is clear from the graph that by increasing the thickness of the AR coating the value of emittance and absorptance is also increases. The maximum absorptance and minimum emittance is observed for 75nm thick layer of AR coating i.e.=0.95%=0.115%.

Results shows that AR coatings thickness less than 75 nm and greater than 100 nm decrease the efficiency of the selective absorbers and latter adversely affect the thermal emittance as well. Results show that 75 nm thickness AR

Table 2. Antireflection layer thickness effect on solar absorptance and emittance

S.no	Thickness of AR Coating	Absorptance	Emittance
1	75 nm	.95	.115
2	125 nm	.94	.120
3	150 nm	.92	.122
4	200 nm	.90	.127

coating is feasible for selective absorbers studied. Deviation from this thickness reduces the absorptance of the coating slowly due to smaller phase change, which shifts the minimum reflectance from the visible spectrum where maximum solar energy lies to NIR or UV spectrum.

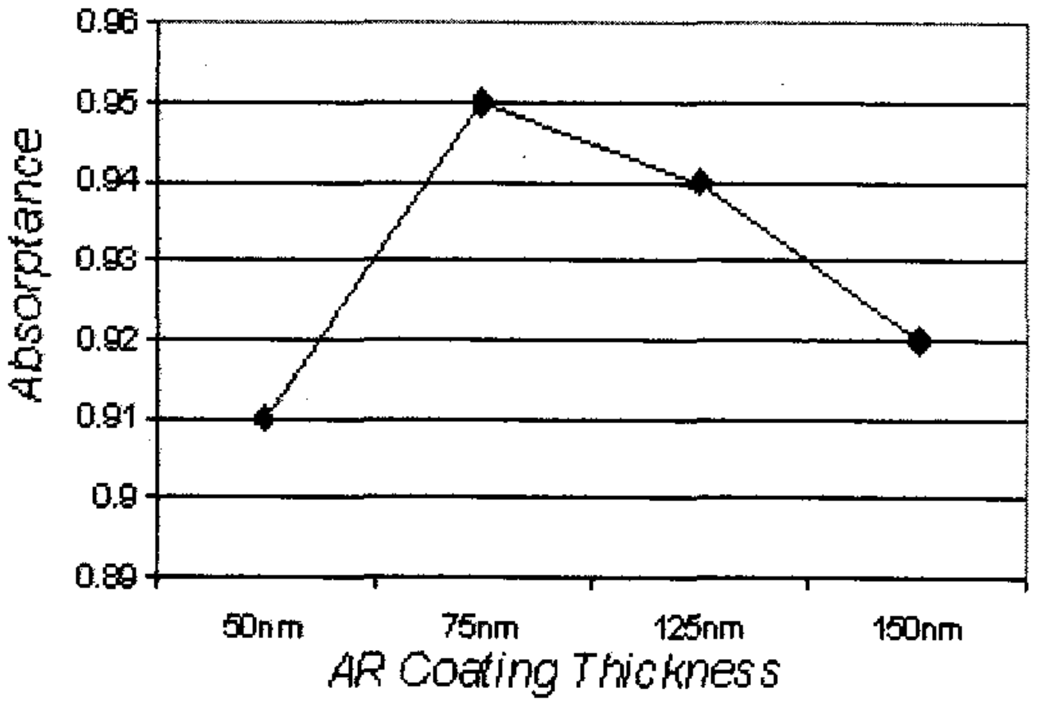

Fig 4. AR layer thickness effect on absorptance

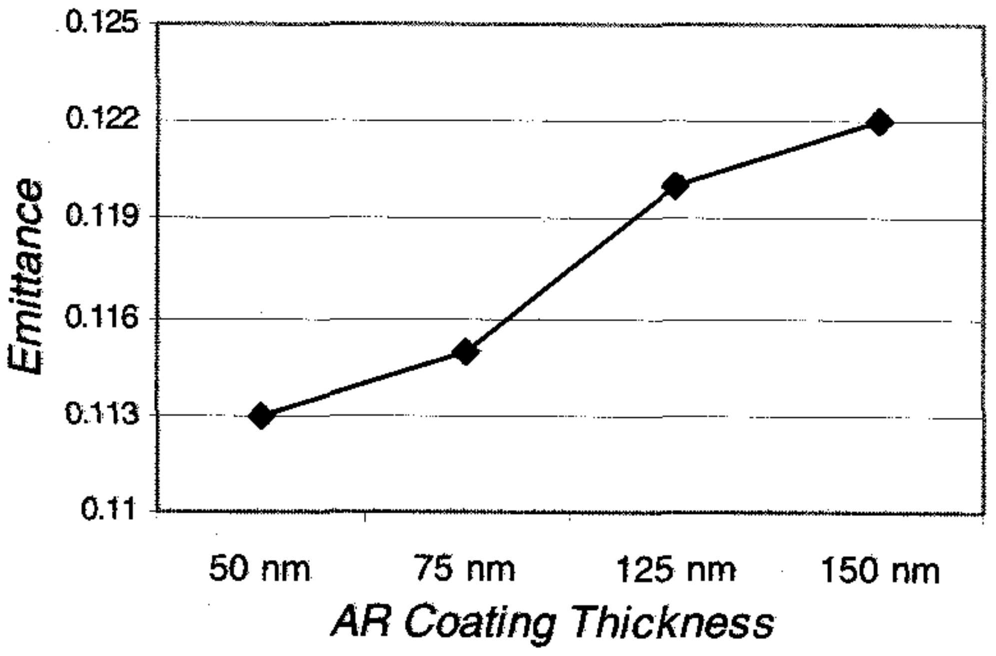

Fig 5. AR layer thickness effect on emittance

5.3 Layer Thickness Effect on Absorptance and Emittance

The effective dielectric constants of metal/insulator composite ($WSiO_2$) strongly depend upon the metal volume fraction and optical properties of the individual materials. The $WSiO_2$ is a comparatively high refractive index composite. A change in volume fraction significantly changes the refractive index of the composite and the performance of coating. The effect of metallic volume fraction on the absorptance of tungsten "W" based selective coating at VF〈〉0.70 has been investigated on the basis of computer simulation results. The metallic concentration and its effect on absorptance and emittance are presented in table 3. It is clear from the results that coating design with higher value of metallic volume fraction can improve the absorptance as compare to lower volume fraction coating design.

The results show that solar absorptance has increased by 4% with an increase of volume fraction from 0.6 to 0.7 and thermal emittance was also reduced to 3%. It is clear from result (Fig 6) that further increase in volume fraction did not improve the absorptance The 0.8 metallic volume fraction film decrease the solar absorptance by 3%, though the emittance was reduce by 2% relative to 0.7 metallic active films. The main reason for this reduction of absorptance is that 0.8-volume fraction composite film exhibited metallic behavior in the infrared, so the metallic characteristic

Table 3. Volume fraction effect on absorptance and thermal emittance

S.no	Volume fraction	Absorptance	Emittance
1	.60	.90	.15
2	.70	.94	.12
3	.80	.91	.10

dominates and reduces the absorptance. Result shows that 0.7 volume fraction coating is better than 0.6 and 0.8 volume fraction coating.

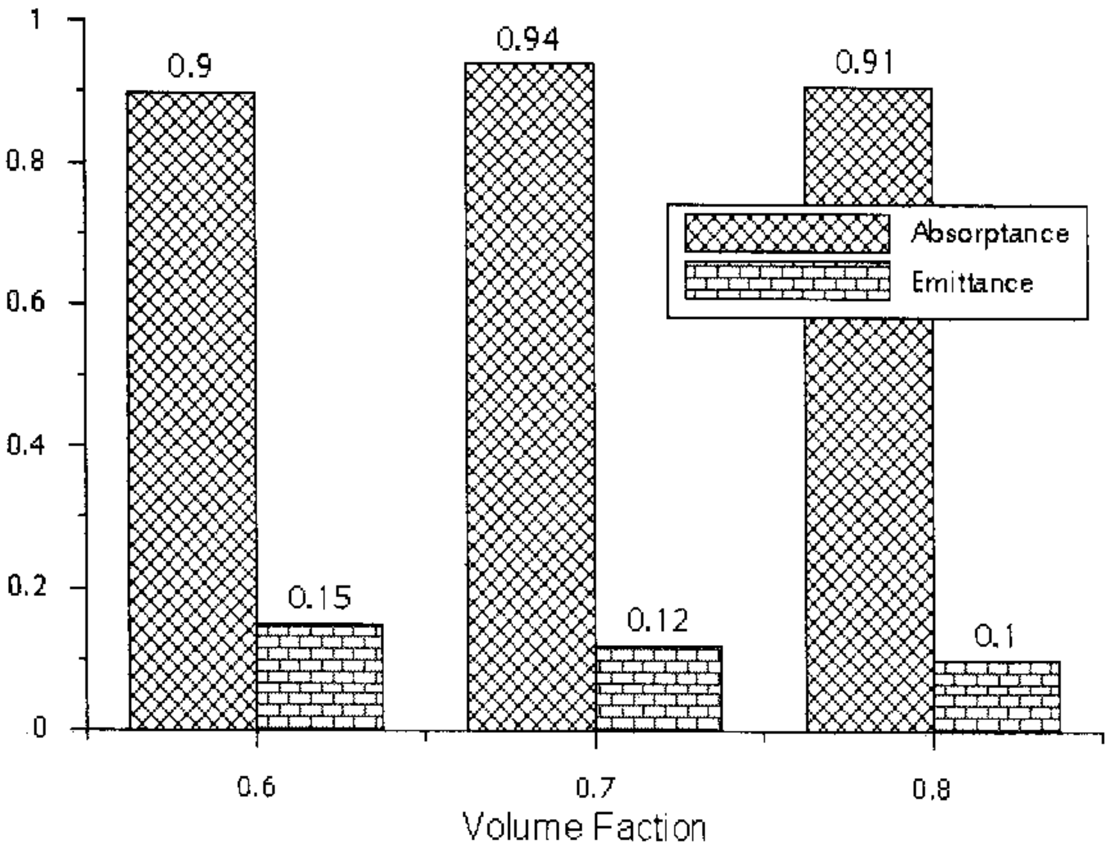

Fig 6. Volume fraction effect on absorptance and thermal emittance

The interference effects in the coatings depend on the optical thickness of the individual layers. The reflection and transmission of the dielectric change periodically as the film thickness is increased. The internal reflection in the film is negligible for a highly absorbing media, but its absorptance and transmittance are dependent on the film thickness. The solar radiation comprises a wide range of wavelengths, which cause interference effects in different geometrical thickness of films fabricated on a metal substrate. In general the solar absorptance and emittance increases with thickness. At a certain thickness the absorptance reaches to maximum and further increase in the thickness increase only the emittance for any volume fraction.

Table 4. Layers thickness effect on absorptance and emittance

Thickness	Film 1	Film 2	Film 3
first layer	200 nm	250	300
second layer	250	300	350
third layer	100	150	200
fourth layer	300	350	400
Absorptance	0.91	0.95	0.93
Emittance	0.102	0.115	0.133

The effect of layer thickness on 70% metallic graded 4-layer coating design has been studied on the base of computer simulated program. The simulated results show that solar absorptance has increase by 4% with increase in thickness of each layer (from film-1 to film-2) and also there is an increase of 2% in thermal emittance. It is clear from results (see Table 4) that further increase in thickness of each layer did not improve the absorptance. The results of film3 show that solar absorptance decreases to 2% with further increase in thickness. The main reason for this reduction in absorptance is that beyond the optimum thickness for a specified volume fraction, the solar absorptance decreases due to higher visible reflectance caused by constructive interference. The best result of absorptance =0.95 and =0.115 has been obtained for film-2 (see Fig 7 and 8). In order to investigate the optimum thickness of various volume fraction composites, the maximum absorptance is the best estimate to consider.

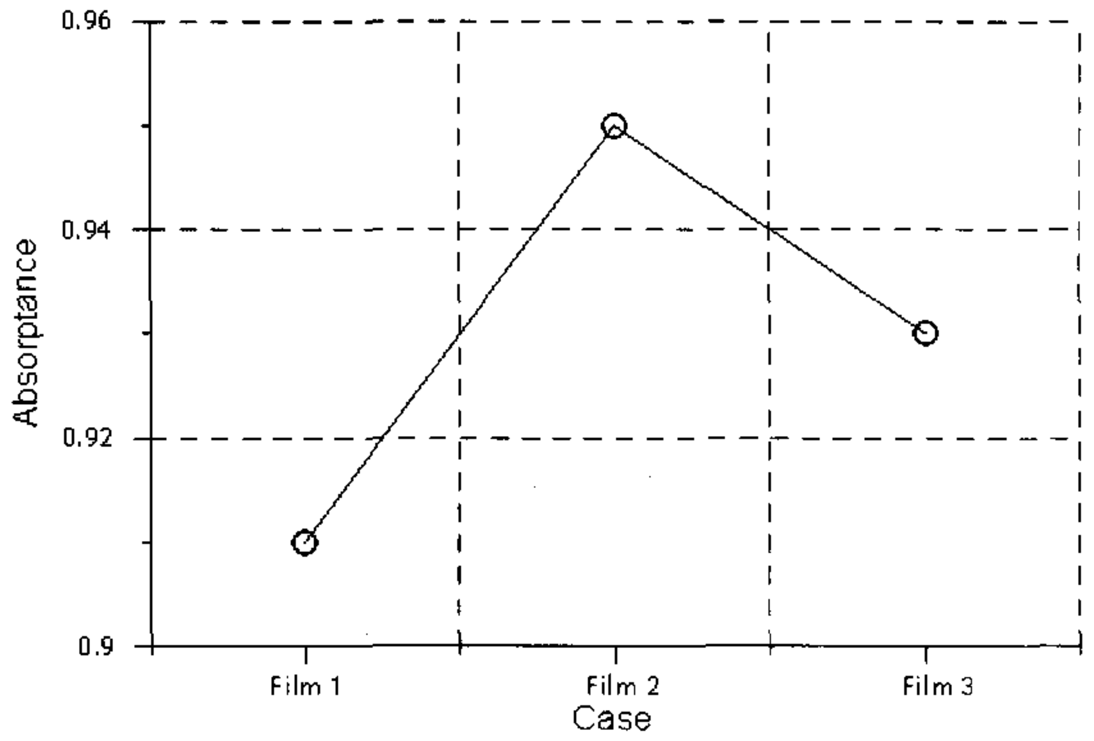

Fig 7. Layer thickness effect on solar absorptance

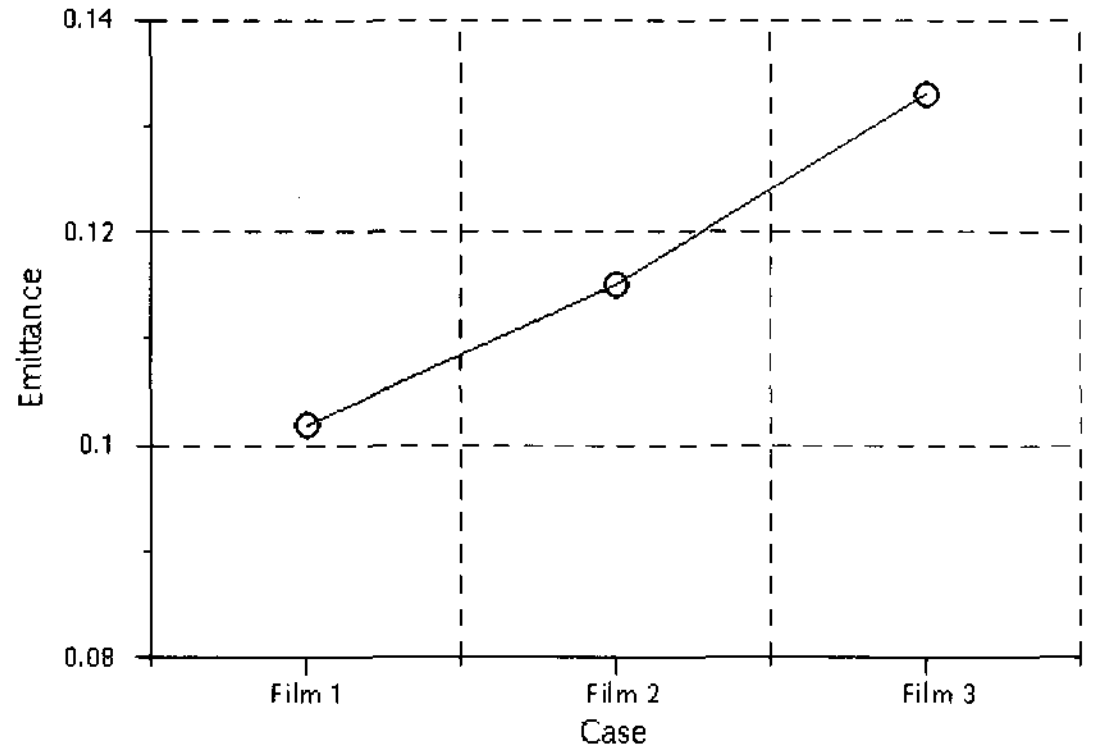

Fig 8. Layer thickness effect on solar emittance

6. Conclusion

This paper described a theory and parametric behavior of metal/dielectric composite ($WSiO_2Al$) film over solar absorption and emissivity values. A computer simulation logic has been included in this paper to analyze the performance of metal/dielectric multilayer composite film. This program operates under the check of unit matrix and is a value able tool to verify the key parameters of coatings. Different aspects of the selective coatings have been discussed with regards to solar absorptivity and emissivity, such as 1) the effects of the number of paint layers, 2) AR layer thickness, volume fraction and thickness of each layer. 3) The absorptance and emittance value increases as the number of paint layers incresed (Table 1) AR layer thickness should be optimized to maximize absortance (Fig 4). Four layer coating design with SiO_2AR layer of thickness 75nm and with variable metallic volume fraction of tungsten (0.5-0.7) in each layer produced the best results (Fig 6). These parameters are strongly interlinked in order to get the maximum performance of the coating. Results shows that a composite film with an appropriately metal/dielectric ($WSiO_2$) graded composition on a metal substrate of Al with optimum thickness (250 nm, 300 nm, 150 nm, 350 nm) of each layer plays an important role for maximum spectral selectivity (Table 4).

On the basis of computer simulation results the maximum solar absorptance =0.94 with low thermal emittance =0.115 has been obtained for four layer metal/dielectric multilayer composite film (Table 4).

Future study will focus on experimental verification of this model and program and application of solar single layered film available.

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