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Multilayer antireflection coatings model for red emission of silicon for optoelectronic applications

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Abstract

A model, based on the Transfer Matrix Method (TMM) of multilayer is used to evaluate the transmittance at the central wavelength 720 nm of Si when using Ge, SiO2 and Si as multilayer thin film coatings.In this study, the results indicate that the transmissivity of ~ (720-750) nm emission of Silicon as emitter is affected significantly by multilayer thin film coatings of Ge, SiO2 and Si. Si /SiO2/Air and Si /Ge/Si/SiO2/Air show high transmissivity 92% and ~100% at central wavelength design (720nm) respectively. Uncoated Si surface shows low transmissivity ~66%.The width of the high-transmittance region of Si/Ge/Si/SiO2/Air is less than Si/SiO2/Air .The origin of the red emission of Si has been investigated

Keywords: Antireflection coatings, Silicon active medium, transmissivity.

1. Introduction

Porous Silicon (PS) has been widely studied as a potential optoelectronic material, since its visible emission at room temperature was found. However, the luminescence mechanism of PS is still a controversial problem. Several types of models have been suggested for PS luminescence. In one type of model the quantum confinement effect is considered necessary, while luminescence materials other than pure Si are not necessary in another type of model, on the contrary, luminescence materials other than pure Si are necessary, while the quantum confinement in nanoscale silicon is not necessary. A third type of model, called the quantum confinement/luminescence center (QCLC) model postulates that electron-hole pairs are mainly excited inside the nanoscale Si and then recombine at luminescence centers (LCs) outside the nanoscale Si; for as-prepared PS, LCs are adsorbates at the surfaces of nanoscale Si, and for oxidized PS,LCs are impurities, defects, or self-trapped excitons in SiOx layers covering the nanoscale Si[1].

The transmissivity of Si emission at the Air-Silicon is low due to the large refractive index discontinuity that exists at the Air-Silicon range (Fig.1a).By placing a single layer AR(Antireflection coating) of intermediate refractive index on the Silicon surface, this large index discontinuity is broken into two smaller steps (Fig.1b), resulting in a lower broadband

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reflectivity. Further reduction in broadband reflectivity can be achieved by adding additional intermediate index layers, thus breaking the air-Silicon index discontinuity into smaller and smaller steps. Therefore, a gradient index AR is the limit of this progression, where a single index discontinuity is replaced by a continuous transition from a high to a low index material (air) as shown in Fig.1c. If this continuous index transition occurs over several wavelengths of optical path length, broadband reflectivity approaching zero can be achieved [2].

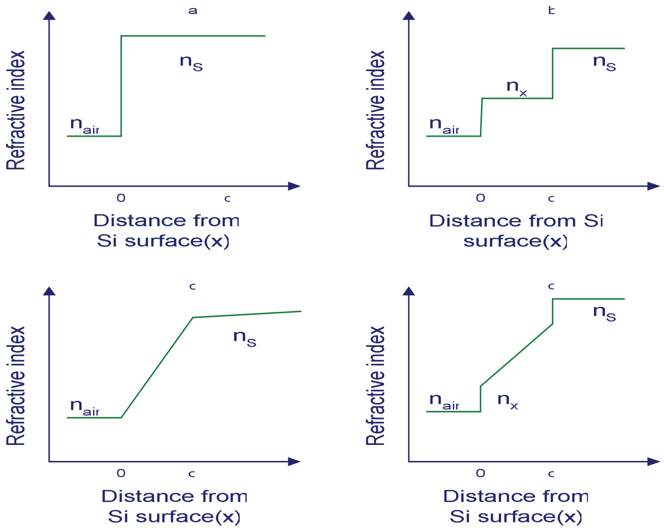

Fig. 1: Four basic spatial refractive index profiles of thickness d:
a)No AR film;b) Single layer AR film;c) Linear graded AR Film
d) AR film with a partial gradient (n($_x$) is arbitrary)

Graded index refractive index profile i.e. n=n (λ, d), where d is the depth from the surface, offer the best performance. Different kind of paraboloid or exponential refractive index profiles can give very broad transmission bands. Single-layer antireflections coatings are generally deposited with a thickness of λ/4, where λ is the desired wavelength for peak performance. Since the refractive index of air is 1.0, the thin antireflection film ideally should have a refractive index of √nsubstrate [3, 4, 5]. There is no ideal material that can be deposited in durable thin layers with a low enough refractive index to satisfy this requirement exactly [3].These coatings are still more theoretical than practical solution because refractive index gradients are difficult to control during fabrication.

In this paper, we explain the model and basic formula of single and multilayer antireflection coatings of Si, SiO2 and Ge for increasing the transmittance of Si as active medium in far red region (720-750) nm.This study reports the design and simulation of the transmissivity of single and multilayer coatings as well as results of each design at central wavelength (720 nm).

2. Modeling and Simulation

The knowledge of thickness and refractive index of antireflection (AR) coatings on semiconductor material surface is a key issue for increasing the performance efficiency of emitters such as output intensity, monohromaticity. Single and multilayer antireflection coatings are designed to increase material surface transmission and reduce surface reflection over a specific wavelength range. The transmittance curves can be calculated with the transfer matrix method for as many AR layers as desired using 'MATLAB', software.

In the case of Silicon as emitter, the radiation emits in all directions .The main loss mechanism of emitter is in the material (deffects, surface roughness..etc.) , contacts and the reflection (at emitter surface-air interface).This latter loss is very significant as Silicon has relatively high refractive index as shown in Fig. (2).

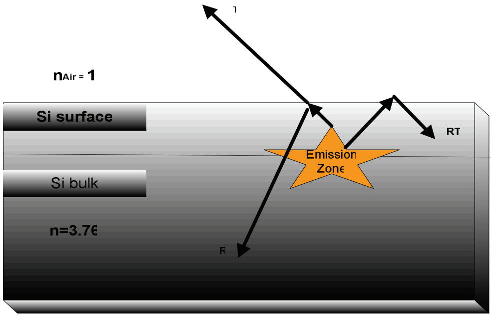

Fig.2: A schematic illustrating the main optical Losses mechanism of emission light at Si/Air interface.

Of the radiation emitted in the forward direction, that striking the front surface at an angle $\theta > \sin^{-1} (1/n)$ will suffer total internal reflection (ITR) . Hence, emission radiation which is emitted in a cone of half-angle less than this value will be capable of being emitted, that is $1/2n^2$ of the radiation emitted (IE) in the forward half-sphere. This radiation will suffer partial reflection (IR), given for near normal incidence by Fresnel's law as [6-8]:

$$\frac{I_R}{I_E} = \left(\frac{n-1}{n+1} \right)^2 , \tag{1}$$

The contribution of the single and multilayer antireflection coatings calculated by using transfer matrix method at central wavelength 720 nm ($\theta=0$, incident angle of emission light at Si/Air interface).We used theoretically determined optical thickness (d) of all materials ($n_{Si}=3.76$,$n_{SiO2}=1.455$,$nGe=4.897$).Single-layer antireflection coatings are generally deposited with a thickness of $\lambda/4$, where λ is the desired wavelength for peak performance, in our study λ is 720nm. In this study, we suppose Si is simple rectangular diode geometry in far red region ((720-750) nm).From Fig.2, we can explain our modeling by using Si/Air interface only or Si surface-antireflection coatings interface (Single or multilayer).A plain wave (emission wave from Si) interacting with a stack of thin layers is considered. So [9, 10]:

$$E = E_0\, e^{ikr-i\omega t}, \qquad H= H_0\, e^{ikr-i\omega t}, \tag{2}$$

Where E and H is the electrical fields and the magnetic field's strengths, respectively, E0 and H0 are their amplitude, k is a wave vector and ω is the frequency of the incident light. We let the thin layers have different refractive indexes.
Inside each layer, the Maxwell equations become [9-11]:

$$k \times E_0 =(- \omega/c)\times H0, \qquad k \times H_0 =(-\omega n^2/c)\times H_0 , \tag{3}$$

The boundary conditions at the interface of two layers having different refractive indexes n1 and n2 are:

$$(E_0)_{T1}= (E_0)_{T1} \;,\; n_1(e_k \times E_0)_{T1} = n_2(e_k \times E_0)_{T2} , \tag{4}$$

Where the subscript τ denotes the tangential component with respect to the boundary and ek shows the direction of the wave propagation. For simplicity we consider normal incidence of light with plane polarization (θ=0).
So,N layers of nj can be expressed in terms of the field (E) [9-11]:

$$\begin{pmatrix} E+ \\ E- \end{pmatrix}_{final} = (\hat{S}_a)^{-1}\hat{B}_N\hat{B}_{N-1}\hat{B}_{n-2}...\hat{B}_1\hat{S}_a\begin{pmatrix} E+ \\ E- \end{pmatrix}_{initial} , \tag{5}$$

Where: the subscript 'a' is related to the environmental area, $\hat{S}$ are the surface matrices:

$$\hat{\mathrm{S}}_{\mathrm{j}} = \begin{pmatrix} 1 & 1 \\ n_j & -n_j \end{pmatrix} , \tag{6}$$

where $\hat{B}$ is the layers' matrices:

$$\hat{B}_j = \hat{S}_j\hat{\Phi}_j(\hat{S}_j)^{-1} = \begin{pmatrix} \cos\varphi_j & i\dfrac{\sin\varphi_j}{n_j} \\ in_j\sin\varphi_j & \cos\varphi_j \end{pmatrix}, \tag{7}$$

Where Φ is the diagonal phase matrix connects the fields Ej (z) at the opposite surfaces of the layer j, φj is equal to [9-11] :

$$\varphi_j = n_j\frac{\omega}{c}d_j , \tag{8}$$

Where dj is the layer thickness and kj = njω/c is the wave number of j layers. Each layer is considered separately. Thus, the transmission can be expressed in term of field [9]:

$$T = \left|\frac{(E_+)_f}{(E_+)_i}\right|^2 = |t|^2, \tag{9}$$

Equation 9 can be expressed as written in ref. [12]:

$$Y = \frac{C}{B} , \tag{10}$$

Where, Y is the optical admittance. B and C are total magnetic and total electric amplitude of the light propagation in the medium, respectively. So, the transmittance (T) can be explained in term of Y as below:

$$T = \frac{4y_o\,\mathrm{Re}(y_{sub})}{(y_oB+C)(y_oB+C)^*} , \tag{11}$$

By increasing the transmissivity of visible emission of Si/Air interface can then cause an increasing in diode performance. The Quantum Confinement / Luminescence Center (QCLC) model is a good agreement with our simulation study to describe the origin visible emission of Si at surfaces Siactive medium/Air and Siactive medium/Mulilayer antireflection coating/Air [13-16].So, we have designed model related to QCLC model with some correction as shown in Fig. (3).

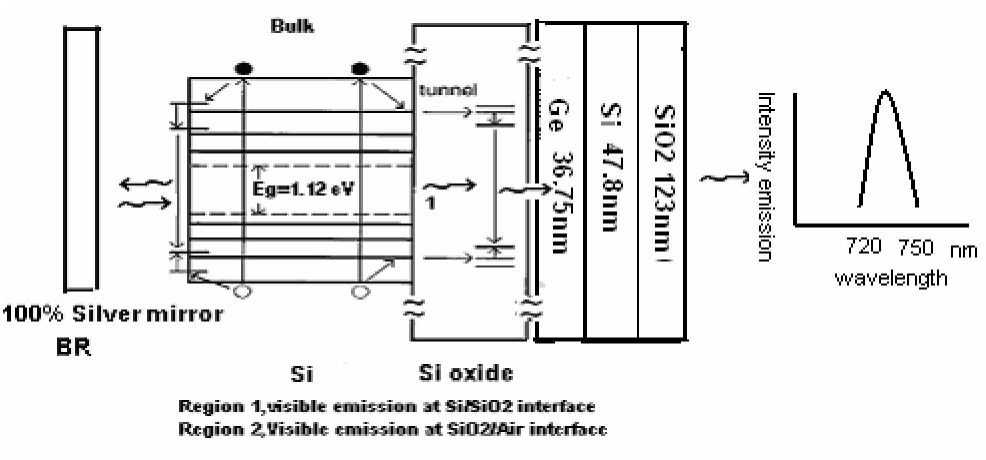

Fig. 3: Schematic illustration of the visible luminescence process as in our study.

The main point of this model is that the photo-excitation of the carriers does take place in the bulk (band to band transition) to cause the excitation in an energy range much bigger than the EgSi. The radiative recombination center of electron–hole pairs inside the bulk is smaller than that outside (region 1 and region 2 as shown in Fig.3), so that most carriers produced inside may tunnel into the surrounding SiO2 layer as example and then recombine to emit visible light through SiO2/ Air interface or Si/Air interface by energy much bigger than the energy of band to band transition .The visible emission of Si-based materials is the surface emission which depends on surface texture and surface temperature.

3. Result and Discussion

The transmissivity curves in the far red region (720-750) nm of electromagnetic spectrum for antireflection coatings of Si/Air, Si/Ge/Air, Si/SiO2/Air, Si/Ge/SiO2/air, Si/SiO2/Ge/Air, Si/Ge/Si/Air, Si/Ge/Si/Ge/Air,Si/Ge/Si/SiO2/Air and Si/SiO2/Si/SiO2/Air antireflection coating structures as single layer and multilayer thin film coatings have been simulated and plotted in Figs.(4-12).The maximum transmittance of these structures is shown in Fig. (12) of Si /Ge/Si/SiO2/Air structure.

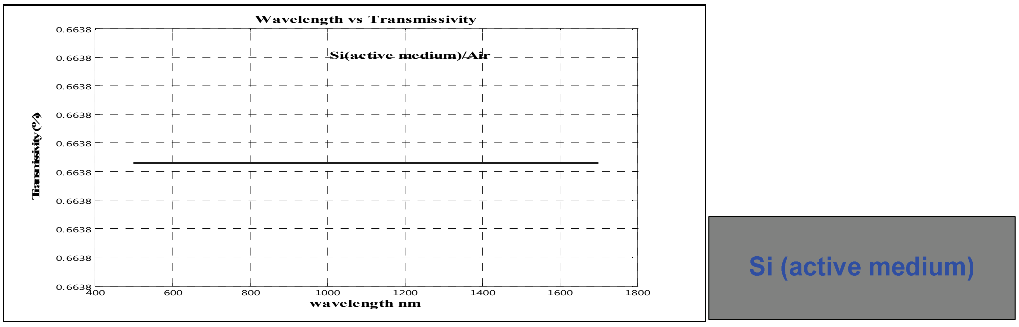

Fig. 4: Simulated transmissivity for $Si_{active\ medium}$/Air at λo=720nm: $n_{active\ medium,Si}$=3.76,n_{Air}=1.00.(Uncoated Si surface)

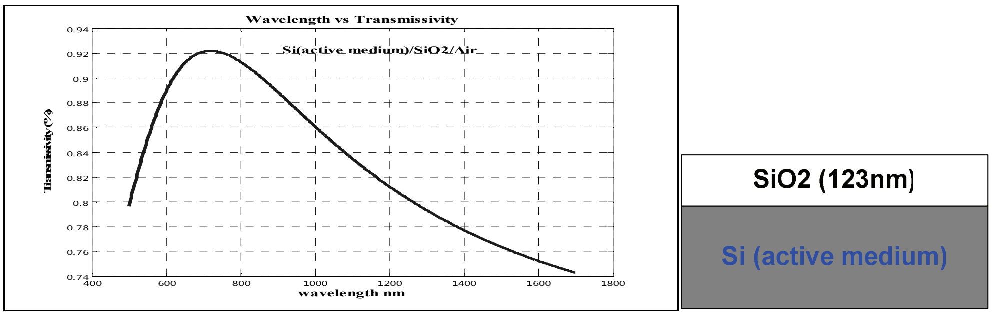

Fig. 5: Simulated transmissivity for Si/SiO_2/Air.Layer is λ/4 thick at λ0=720nm:Si | L | Air,n_{Si}=3.76, n_L=1.455.

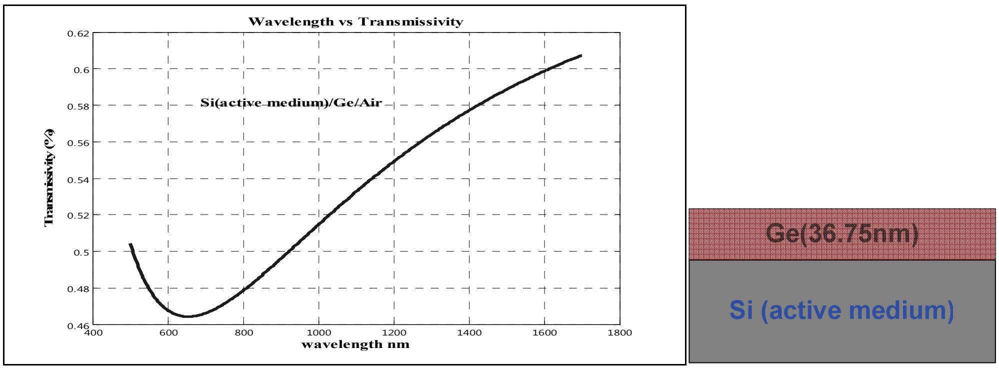

Fig. 6: Simulated transmissivity for Si /Ge/Air.Layer is λ/4 thick at λo=720nm:Si | H | Air,n_{Si}=3.76, n_H=4.897.

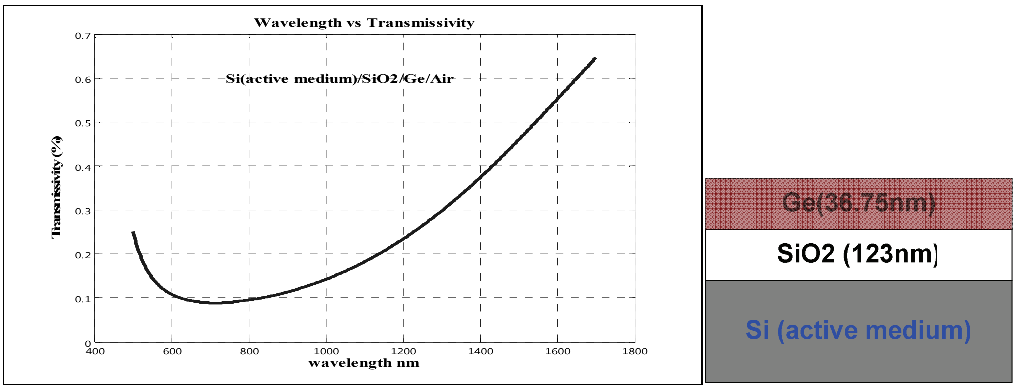

Fig. 7: Simulated transmissivity for Si /SiO_2/Ge/Air.Layers are λ/4 thick at λo=720nm:Si | LH | ,n_{Si}=3.76. n_L=1.455,n_H=4.897.

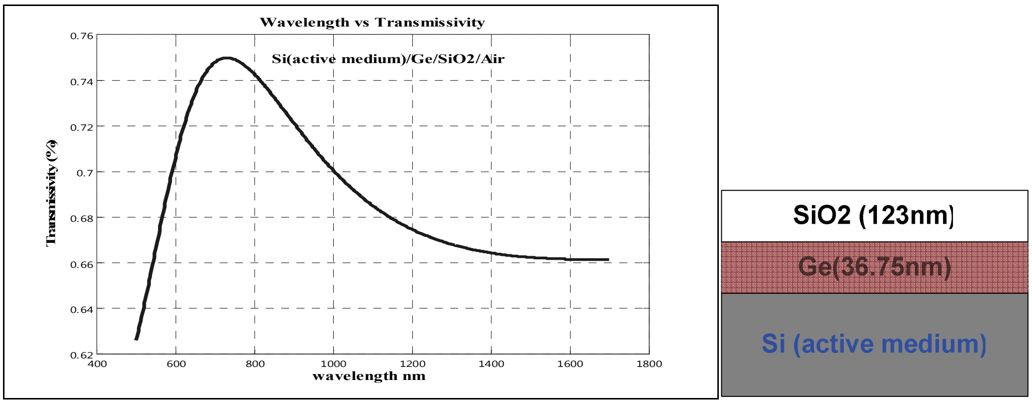

Fig. 8: Simulated transmissivity for Si /Ge/SiO2/Air.Layers are λ/4 thick at λo=720nm:Si | HL | ,n_{Si}=3.76, n_H=4.897,n_L=1.455

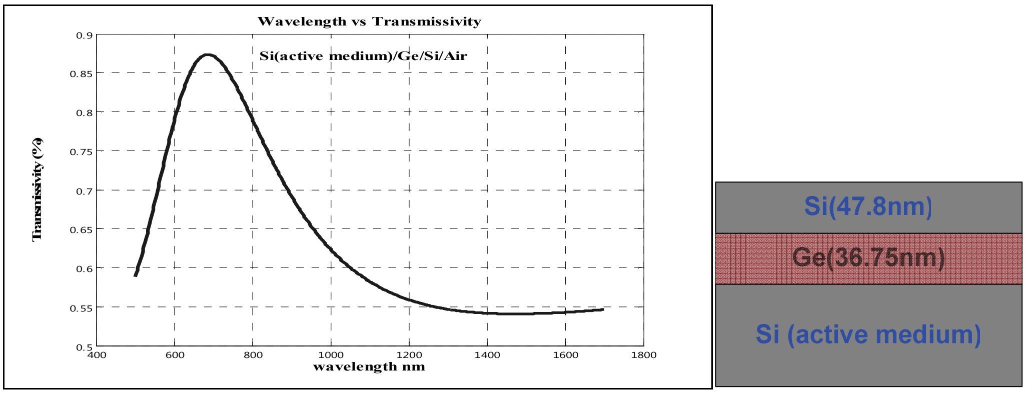

Fig. 9: Simulated transmissivity for Si /Ge/Si/Air.Layers are λ/4 thick at λo=720nm:Si | H | Si,$_n$, Si=3.76,n_H=4.897,n_{Si}=3.76.

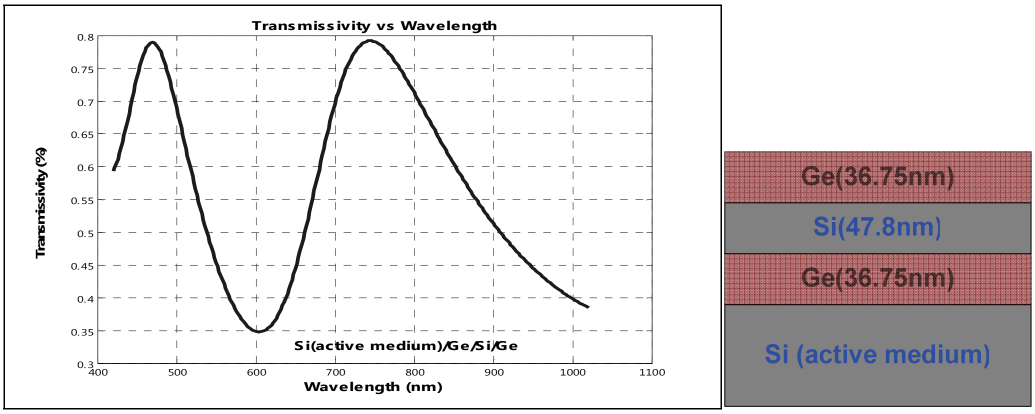

Fig. 10: Simulated transmissivity for Si /Ge/Si/Ge/Air.Layers are λ/4 thick at λo=720nm:Si | H | Si | H | Air, n_{Si}=3.76,n_H=4.897,n_{Si}=3.76.

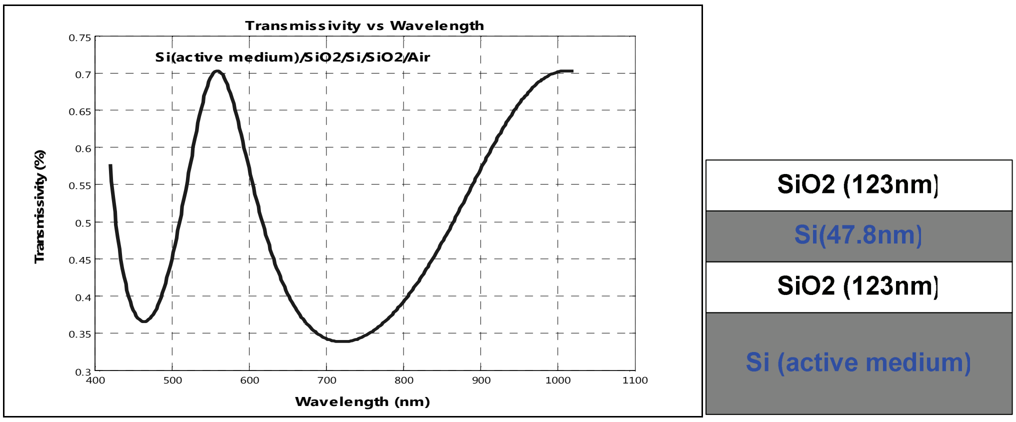

Fig. (11): Simulated transmissivity for Si /SiO$_2$/Si/SiO$_2$/Air.
Layers are λ/4 thick at λo=720nm:Si | L | Si | L | Air.
nsi=3.76,n$_L$=1.455,n$_{Si}$=3.76

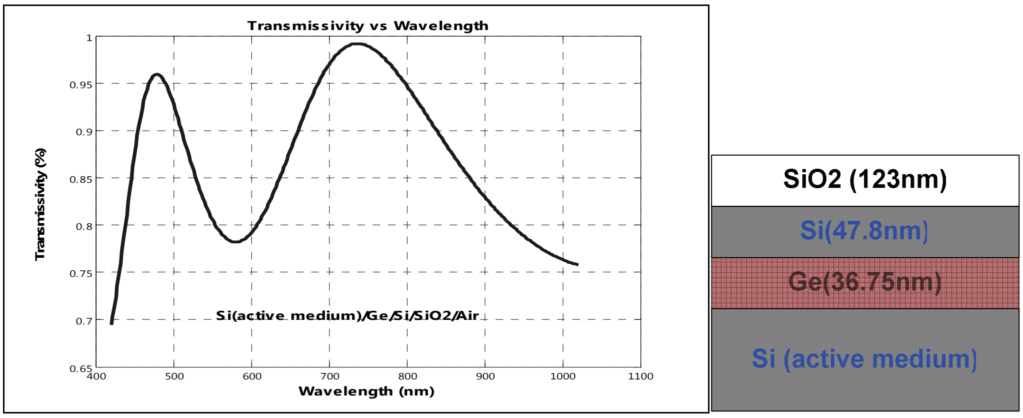

Fig. (12): Simulated transmissivity for Si /Ge/Si/SiO$_2$/Air:
Layers are λ/4 thick at λo=720nm:Si | H | Si | L | Air.
n$_{\text{active medium}}$=3.76,n$_H$=4.897,n$_L$=1.455,n$_{Si}$=3.76.

In curves of figures (5,8,9), the width of the high-transmissivity region decreases while its height increases, due to the refractive index difference (□n) between antireflection coatings materials .The difference between curves of Fig. (12) and Fig.(5) is caused by the refractive index difference at interfaces as illustrated in regions(1c ,1d) and region (2b) of Fig.(13,see Fig.(1)) .These curves show good transmissivity due to the refractive index difference at interfaces (Fig. (13)), SiO2-Air interfaces (1d, 2b, Fig. (13) as well as insertion an extra Si layer between the periodic structures.

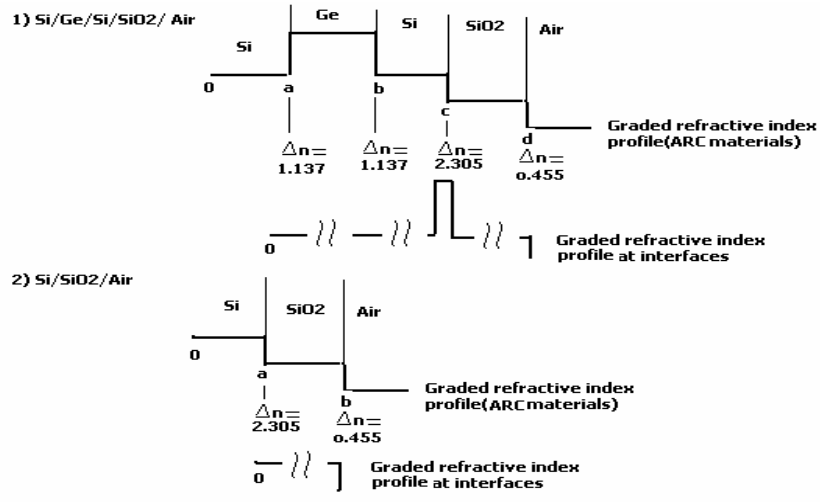

Fig. (13): A schematic illustrating the graded refractive index Profile of $Si_{active\ medium}$/Ge/Si/SiO_2/Air and $S_{active\ medium}i$/SiO_2/Air antireflection coating structure.

Figs.(10-12) show blue transmissivity at ~ (440-490) nm and Fig. (12) shows high blue transmissivity (~96%) at ~480nm because the rejection zone is solely a function of the indexes of the two materials used to construct the multilayer in the case of a quarter wave stack with layers of refractive index nL and nH .So, we can expressed our results as shown in figures in term of the width of the rejection zone (2□g) [17]:

$$\triangle g = 2/\Pi \sin^{-1} (n_H - n_L) / (n_H + n_L), \quad (12)$$

4. Conclusion

In this paper, we present the simulated transmissivity of Si as emitter using transfer matrix method .This method directly calculates the theoretical optical transmissivity values of far red emission of Si using only refractive indexes and thickness of coating materials (Si, SiO2 and Ge).

The maximum transmissivity of Si in (720-750) nm region of electromagnetic spectrum can be obtained with insertion of an extra Si layer between the periodic structures of alternately high and low index of Ge and SiO2 as shown in Fig. (12). The red emission of (720-750) nm has been investigated related to QCLC Model.

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