Semiconductor Physics, Quantum Electronics & Optoelectronics. 2003. V. 6, N 4. P. 508-513.

PACS: 42.79.Wc, 78.20.–e

Modeling high performance multilayer antireflection coatings for visible and infrared (3–5μm) substrates

M.H. Asghar[1], M.B. Khan[1], and S. Naseem[2]
[1]Advanced Engineering Research Organization (AERO), Wah Cantt. Pakistan.
[2]Centre for Solid State Physics, Punjab University, Lahore. Pakistan.
[1]E-mail: mha_19@yahoo.com

Abstract. Multilayer antireflection coatings have been modeled in visible and IR (3–5μm) bands to reduce reflectance from glass, germanium (Ge), silicon (Si) and zinc selenide (ZnSe) substrates. The transmittance of bare glass substrate is around 95% whereas for Ge 64%, Si 70%, ZnSe 84%. Theses values are enhanced reasonably by the application of multilayers films. Starting from a single layer, the layers have been added systematically forming multilayer structures to reduce reflectance considerably with each increasing layer. The designed layers are optimized for their performance by varying their thickness and refractive indices. The analysis of these modals has shown that the proposed multilayer structures are very effective in reducing the reflectance for all the substrates in two spectra.

Keywords: antireflection coatings, multilayers.

Paper received 21.07.03; revised manuscript received 02.01.04; accepted for publication 11.12.03.

1. Introduction

Antireflection coatings have had the greatest impact on optics, and even today, in sheer volume of production, they still exceed all the other types of coatings. In some applications antireflection coatings are required for the reduction of surface reflections. In other not only reflection is reduced but also transmittance is increased considerably. As it is a known fact that radiations incident upon the surface of an optical material is separated into reflected, transmitted, absorbed and scattered fractions. The fraction of available energy that is distributed amongst these is determined by the indices of refraction. Antireflection coatings can range from a single layer having virtually zero reflectance at just one wavelength, to a multilayer system of many layers having virtually zero reflectance over a wide spectral range.

2. Theory of antireflection coatings

The simplest antireflection coating is a single layer deposited on a substrate [1]. To achieve antireflection properties, this layer depends on the cancellation of light at the upper and lower of the two surfaces. Assuming the refractive index of air as n_0, film as n_1 and that of substrate as n_s, then in order to cancel the two reflected beams the intensity of the radiation reflected at the upper and lower surfaces of the coating should be equal which means that the ratios of the refractive indices at each boundary should be equal, that is:

$$n_0 / n_1 = n_1 / n_s, \text{ with film thickness, } n_1 t_1 = \lambda/4$$

This configuration will give only one minimum in the reflectance profile. For more minima, more layers are required. The same theory is used to calculate the expressions for two- and three- layers antireflection coatings [2]. Similarly, multiple layers are used to achieve more minima in reflectance profile for broadband antireflection coatings [3, 4]. We have modeled multilayer antireflection coatings for glass and infrared substrates. These coatings are modeled at a design wavelength of $\lambda_0 = 0.55$ μm for visible and $\lambda_0 = 4$μm for infrared substrates, respectively. Moreover all the designs have been optimized by varying the individual layer refractive index and thickness.

2.1 Multilayer matrix calculations

Matrix calculations determine the spectral transmittance and reflectance profile for multilayer structures on a substrate. Consider a loss free multilayer design, normally incident radiations, and assume that films are optically homogenous. The electric field vector (E_{m-1}) and magnetic field and the magnetic field vector (H_{m-1}) at the incident boundary of a film are related to the electric field vector E_m and magnetic field vector H_m vectors at the boundary of the adjacent film by the product of the following matrices per layer. The matrix is calculated at each boundary throughout the multilayer as the magnitude of electric and magnetic field vectors alter with the properties of the layer [5]. Application of the appropriate boundary conditions between each layer requires that the tangential components of E and H vectors are continuous across each boundary to the equations of wave propagation.

Let the electric and magnetic field vectors of the wave traveling in the direction of the incidence are denoted by symbol "+", and those waves traveling in the opposite direction by the symbol "–". At the interface of m^{th} layer, the tangential component of E and H are given as

$$E_m = E_m^+ + E_m^-$$

$$H_m/H_1 = E_m/E_1$$

$$H_m = E_m \times H_1/E_1 \tag{1}$$

Neglecting the common phase factors, and where E_m and H_m represent the resultants then:

$$E_m^+ = 1/2\left[\frac{H_m}{H_1/E_1} + E_m\right] \tag{2}$$

$$E_m^- = 1/2\left[-\frac{H_m}{H_1/E_1} + E_m\right] \tag{3}$$

$$H_m^+ = 1/2\left[H_m + \frac{E_m H_1}{E_1}\right] \tag{4}$$

$$H_m^- = 1/2\left[H_m - \frac{E_m H_1}{E_1}\right] \tag{5}$$

The fields at other interfaces m–1 are similar to equations 2–5 at the same instant of time and a position with identical x and y coordinates. These can be determined by multiplying by phase difference in z direction given by $e^{i\delta}$ or $e^{-i\delta}$ where:

$$\delta = \frac{2\pi N_1 d \cos\theta_1}{\lambda} \tag{6}$$

And θ_1 may be complex. The values of E and H at this interface are therefore:

$$E^+{}_{m-1} = E^+{}_m e^{i\delta} = 1/2\left[\frac{H_m}{\eta_1} + E_m\right]e^{i\delta} \tag{7}$$

$$E^-{}_{m-1} = E^-{}_m e^{-i\delta} = 1/2\left[-\frac{H_m}{\eta_1} + E_m\right]e^{i\delta} \tag{8}$$

$$H^+{}_{m-1} = H^+{}_m e^{i\delta} = 1/2\left[H_m + \eta_1 E_m\right]e^{i\delta} \tag{9}$$

$$H^-{}_{m-1} = H^-{}_m e^{-i\delta} = 1/2\left[H_m - \eta_1 E_m\right]e^{-i\delta} \tag{10}$$

Where η_1 is the tilted optical admittance given by $\eta_1 = H_1/E_1$

Now

$$E_{m-1} = E^+{}_{m-1} + E^-{}_{m-1}$$

$$E_{m-1} = E_m \cos\delta + H_m \frac{i\sin\delta}{\eta_1}$$

$$H_{m-1} = E_m \frac{i\sin\delta}{\eta_1} + H_m \cos\delta$$

This can be written in matrix form as:

$$\begin{bmatrix} E_{m-1} \\ H_{m-1} \end{bmatrix} = \begin{bmatrix} \cos\delta & (i\sin\delta)/\eta_1 \\ i\eta_1 \sin\delta & \cos\delta \end{bmatrix} \begin{bmatrix} E_m \\ H_m \end{bmatrix}$$

Solving the above given expression [6], the matrix expression for single layer is:

$$M_1 = \begin{bmatrix} A & iB \\ iC & D \end{bmatrix}$$

Where: $\cos\delta_m = A = D$, $i\sin\delta_m/\eta_m = B$, $i\sin\delta_m\eta_m = C$

For two successive layers:

$$\begin{array}{ccc} & \text{Layer 2} & \text{Layer 1} \\ M = & \begin{bmatrix} A_2 & iB_2 \\ iC_3 & D_2 \end{bmatrix} & \begin{bmatrix} A_1 & iB_1 \\ iC_1 & D_1 \end{bmatrix} \end{array} \tag{15}$$

After multiplication we have:

$$M = \begin{bmatrix} A_2A_1 - B_2C_1 \\ iC_2A_1 + D_2iC_1 \end{bmatrix} + \begin{bmatrix} A_2iB_1 + iB_2D_1 \\ -C_2B_1 + D_2D_1 \end{bmatrix} \tag{16}$$

Let $AA = A_2A_1 - B_2C_1$, $BB = A_2iB_1 + B_2iD_1$, $CC = iC_1A_1 + D_2iA_1$, $DD = C_2B_1 + D_2D_1$

Therefore matrix is written as:

$$M = \begin{bmatrix} AA & BB \\ CC & DD \end{bmatrix} \tag{17}$$

Therefore, for a multilayer containing q-layers:

$$\begin{bmatrix} E_0 \\ H_0 \end{bmatrix} = \prod_{m=1}^{q} M_m \begin{bmatrix} E_q \\ H_q \end{bmatrix} \tag{18}$$

The loss-free transmittance and reflectance for the multilayer assembly can be calculated from this product matrix by:

$$T_q = \frac{4 n_s n_0}{(n_0 AA + \_\, n_s DD)^2 + (n_0 n_s BB + CC)^2} \tag{19}$$

$$R_q = \frac{(n_0 AA - n_s DD)^2 + (n_0 n_s BB - CC)^2}{(n_0 AA + n_s DD)^2 + (n_0 n_s BB + CC)^2} \tag{20}$$

The reflectance, transmittance and absorptance are then related by $R + T + A = 1$. The solution of this matrix theory is a laborious job for multilayer coatings. Based on the matrix theory, we have developed a software program to design and simulate the performance of multilayer coatings [7].

3. Modeling and analysis

Thin film materials are required to have certain characteristics to become a potential candidate for multilayer structures. This includes high transparency, homogeneity, high packing density, good adhesion, low stress, hardness and ability to survive in different environmental and deposition conditions [8, 9]. These materials are then used to reduce reflection from the surfaces, which are basically caused by the sharp variation of the refractive index at the incident medium-substrate interface. Multilayer coating structures based on those materials have wide band of applications in electronics, optoelectronics, optics and optoelectronics equipments.

(A) visible region: The reflectance from the surface of bare glass substrate is 4.2%. Starting from single layer reflectance is reduced by application of five layers. The design data and reflectance values for all these designs are given in table 1. Initially single layer of MgF_2 has been employed to reduce the magnitude of this reflectance. The maximum reflectance from the substrate has reduced from 4.2% to 2.2%, with reduction in average reflectance to 1.65%. For a single layer coating only one minimum is achievable. Two layer coating comprising MgF_2 and Al_2O_3 (Air/MgF_2/Al_2O_3/Glass) has been designed to further reduce the reflectance obtained by single layer configuration. In this configuration we have two distinct minima of reflection as compared to one for single layer. Earlier we had a maximum reflectance of 2.26%, which has reduced to 1.77% by the addition of second layer. Further the average reflectance has gone down to 1.02%. The reflectance profile of three-layer coating comprising of SiO_2, HfO_2, and MgO (Air/SiO_2/HfO_2/MgO/Glass) is more effective than the previous two designs. SiO_2 is very low index material with a value of 1.46 in the visible spectrum, and HfO_2 has a moderately high index of nearly 2.0 with a good environmental durability [9]. The maximum reflectance from the substrate has further reduced to 1.37% with average reflectance to 0.91%. Therefore, the performance of the coating is further improved by the addition of third layer. The reflectance is further reduced by four-layer design comprising MgF_2, ZrO_2, Al_2O_3 and MgF_2 (Air/MgF_2/ZrO_2/Al_2O_3/MgF_2/Glass). A slight increase in reflectance at the edges of the band can be seen, but the important feature of this design is the zero reflectance at two spectral points. In this case maximum and average reflectance has appreciably reduced to 1.28% and 0.45%, respectively. On the application of the fifth layer in the model (Air/MgF_2/ZrO_2/Al_2O_3/Cryolite/MgF_2/Glass) maximum and average reflectance further reduced to 1.11% and 0.42% respectively. The combined reflectance plot of the five configurations is shown in Fig. 1. This application of multiple layers encourages the use of multi-layers to achieve wide transmission bands. By increasing number of lay-

Table 1. Design data and reflectance values for all configurations on glass.

Configurations	Material	Refractive Index (n)	Thickness (μm)	R_p(%)	R_{ave}(%)
Single Layer	MgF_2	1.38	0.099	2.26	1.65
Two-Layers	MgF_2	1.38	0.099	1.77	1.02
	Al_2O_3	1.62	0.169		
Three-Layers	SiO_2	1.46	0.087	1.37	0.91
	HfO_2	1.98	0.128		
	MgO	1.73	0.073		
Four-Layers	MgF_2	1.38	0.090	1.28	0.45
	ZrO_2	2.05	0.121		
	Al_2O_3	1.62	0.077		
	MgF_2	1.38	0.181		
Five Layers	MgF_2	1.38	0.094	1.11	0.42
	ZrO_2	2.05	0.126		
	Al_2O_3	1.62	0.080		
	Cryolite	1.35	0.096		
	MgF_2	1.38	0.094		

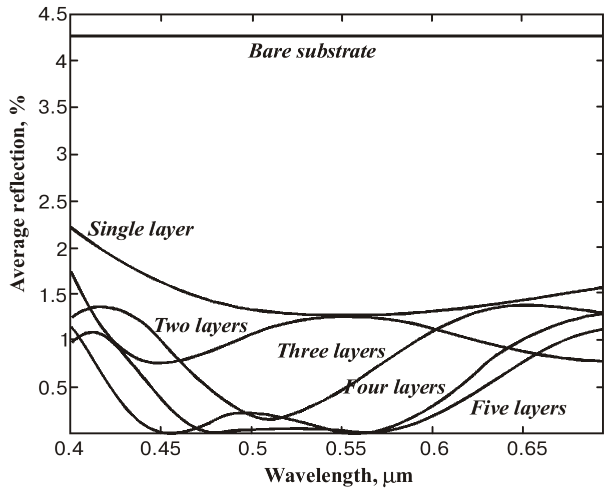

Fig. 1. Combined reflectance profiles for all configurations on glass.

ers and optimizing their index and thickness [11], the reflectance from the substrate can be reduced to a reasonably low value. In other words the transmittance through the substrate can be increased substantially. It should be noted from Fig. 1 that decrease is pretty sharp up to the addition of fourth layer. How ever, the magnitude of reduction in reflectance with the addition of fifth layer is very small. This may suggest the threshold limit for multilayer configuration in which performance requirements are not very stringent.

(B) infrared region: Ge, Si and ZnSe have been used as substrates material as they are commonly used in 3–5μm band for many optical and electro-optical applications [12–17]. All these substrates exhibit a very high reflectance value in the said spectrum. In most of the applications, this high value of reflectance is not acceptable as it reduces the total energy reaching the detector surface with every increasing optical component in the system or device. Therefore, it is necessary to reduce their surface reflectance by appling ARC's. The materials used as film layers are ZrO_2, Si, SiO, CdTe, BaF_2, ZnSe, Y_2O_3 and SiO_2, LaF_3 and YF_2. All these materials are suitable for antireflection films in the desired region of wavelength [18].

The reflectance of bare germanium substrate in 3–5μm is 36%. Multilayer coatings can be used to reduce this value to an appreciably low level [19]. We have modeled such coatings on germanium substrate at a design wavelength of 4μm. The process starts from a single layer model, and the layers are increased to reduce the value of maximum and average reflectance over the desired band. Table 2 shows the model data and calculated values of maximum and average reflectance over the entire band for a single layer modal. The data shows that the maximum and average value of reflectance has decreased form 36% to 12.36% and 2.97% respectively. The combined reflectance plot of all the four designs is shown in Fig. 2. We have adopted an approach of smooth transition of layer indices with every increasing layer in all models, starting from incidence medium right up to the substrate. This approach helps in avoiding sharp interfaces between the layers, helping in smooth reduction of reflectance from the surface of the substrate. The Fig. 2 clearly shows the reduction of peak and average values with increasing number of layers.

The reflectance from bare silicon substrate surface is 30%. This value is lower as compared to the germanium, as it has got a lower refractive index in the given spectrum. Similar procedure of layer addition has been employed to model and analyze multilayer structures for reducing reflectance from the substrate. Table 3 shows the model data with maximum and average values of reflectance for all configurations. Fig. 3 shows the combined plots for one, two, three and four layer configura-

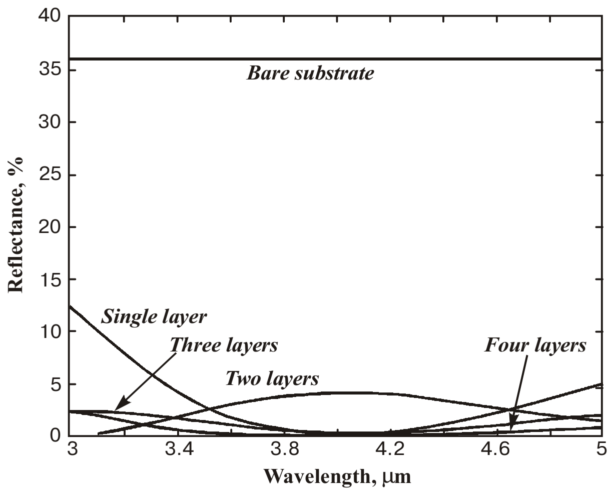

Fig. 2. Combined reflectance profiles for all configurations on germanium.

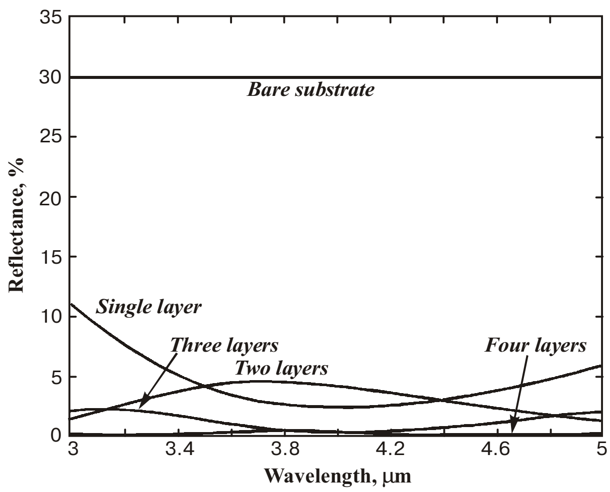

Fig. 3. Combined reflectance profiles for all configurations on silicon.

Table 2. Design data and reflectance values for all configurations on germanium.

Configurations	Material	Refractive Index (n)	Thickness (μm)	R_p(%)	R_{ave}(%)
Single Layer	ZrO_2	2.05	0.487	12.36	2.97
Two-Layers	SiO	1.6	0.625	4.19	2.67
	CdTe	2.6	0.384		
Three-Layers	SiO	1.6	0.625	2.37	1.15
	CdTe	2.6	0.384		
	Si	3.42	0.292		
Four-Layers	BaF_2	1.3	0.769	2.37	0.487
	ZrO_2	2.05	0.487		
	CdTe	2.6	0.375		
	Si	3.42	0.292		

Table 3. Design data and reflectance values for all configurations on silicon.

Configurations	Material	Refractive Index (n)	Thickness (μm)	R_p(%)	R_{ave}(%)
Single Layer	LaF_3	1.6	0.632	11.17	4.46
Two-Layers	MgF_2	1.38	0.679	4.64	3.26
	ZrO_2	2.05	0.457		
Three-Layers	MgF_2	1.38	0.724	2.35	1.17
	ZrO_2	2.05	0.487		
	CdTe	2.64	0.378		
Four-Layers	MgF_2	1.38	0.679	0.419	0.150
	ZnSe	2.39	0.784		
	MgF_2	1.38	1.3587		
	ZnSe	2.39	0.392		

tions. The trend in the reduction of reflectance for all the configurations is similar to that for germanium. However, in this case the performance for three and four layer configurations is even better and the curves are more flat and comparatively closer to the horizontal axis. Only two materials are used in four layers configuration. This shows that proper optimization not only helps in getting good performances but also tend to reduce unnecessary variety of materials which is very critical in manufacturing process.

The reflectance of bare ZnSe substrate is 16.81%. Multilayer antireflection coatings are employed on the substrate to drastically lower this value. Table 4 shows the model data and calculated values of maximum and average reflectance for single, two, three and four layer structures to reduce the reflectance from the substrate. Fig. 4 shows the combined plots of all the configurations. The sharp fall in the reflectance values is observed, even with single layer coating configuration due to low index under lying surface.

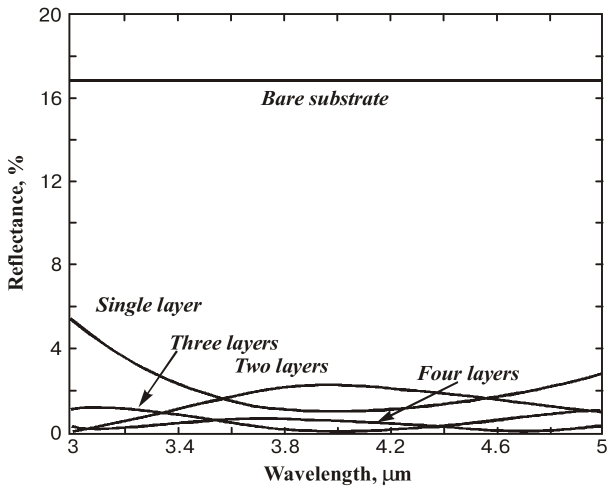

Fig. 4. Combined reflectance profiles for all configurations on ZnSe.

Table 4. Design data and reflectance values for all configurations on zinc selenide.

Configurations	Material	Refractive Index (n)	Thickness (μm)	R_p(%)	R_{ave}(%)
Single Layer	YF_2	1.4	0.714	5.47	1.99
Two-Layers	BaF2	1.3	0.769	2.21	1.49
	Y_2O_3	1.73	0.578		
Three-Layers	BaF_2	1.3	0.769	1.23	0.54
	$Y2O_3$	1.73	0.578		
	ZrO_2	2.05	0.487		
Four-Layers	SiO_2	1.4	0.664	0.60	0.34
	ZrO_2	2.05	0.914		
	Y_2O_3	1.73	0.541		
	ZrO_2	2.05	0.457		

4. Conclusions

Multilayer antireflection coatings in visible and IR (3–5μm) have been modeled, starting from single layer up to five layer configuration. The performance of each successive configuration has been optimized in order to demonstrate efficient use of multiple layers for antireflection applications. The analysis of these designs reveal that by increasing number of layers in a judicious manner with suitable refractive indices and thickness, the maximum and average reflectance from the surface of the substrate can be decreased to very low magnitudes .

References

1. J. D. Rancourt, *Optical thin films: User's handbook*, SPIE Optical Engineering Press, p.8, (1996).
2. A. Thelen, *Design of optical interference coatings*, McGraw-Hill, p 91, (1989).
3. R. Willey, Optical thin films and applications // *Proc. SPIE* **1270**, p. 36-38, (1990).
4. R. Willey, Realization of a very broad band AR coating // *Proc. Soc. Vac. Coaters Techon.*, **33**, p. 232, (1990).
5. H.M. Liddell, *Computer aided techniques for the design of multilayer filters*, Adam Hilger Ltd, ISBN 0-85274-233-9, p.2, (1981).
6. G.J. Hawkins, *Spectral Characteristics of Infrared Optical Materials*, Ph.D. Theses, University of Reading, UK. p.89, (1998)
7. M.H. Asghar, M.B. Khan and S. Naseem, Proc. 2nd International Bhurban Conference on Applied Sciences and Technology, Pakistan, (2003) In press.
8. H. Selhofer, E. Ritter and R. Linsbod // *App. Opt.*, **41**, p.756 (2002).
9. J.M. Bennett, E. Pelletier, G. Albrand, J.P. Borgogno, B. Lazarides, C.K. Carniglia, R.A. Schmell, T.A. Allen, T.T. Hart, K.H. Guenther and A. Saxer // *App. Opt.*, **28**, p.3303, (1989).
10. R. Willey, Comparison of two broad beam/ion plasma sources for optical coatings, // *Vacuum Coating and Technology*, **3**, p.30, (2002).
11. H A. Macleod, *Thin Film Optical Filters*, IOP, Institute of Physics Publishing, Bristol and Philadelphia, p.126, (2001).
12. G. J. Hawkins, *Spectral Characteristics of Infrared Optical Materials*, Ph.D. Theses, University of Reading, UK, p.89, (1998).
13. R.R. Willey, infrared System and Components III, SPIE **1050**, (1989).
14. A. Ghosh, P. Kant, P. K. Bandyopadhyay, P. Chandra, O.P. Nijihawan, // *Infrared Physics & Technology*, **40**, p. 49, (1999).
15. J.A. Dobrowlski and F. Ho // *App. Opt.*, **21**, p.288 (1982).
16. C. Cole, "Broadband Antireflection Coatings for Spaceflight Optics, Ph.D. Theses, University of Readig, UK, p.21, (1995).
17. Y.A. Zagoruiko, O.A. Fedorenko, N.O. Kovalenko and P.V. Mateychenko, // *Semiconductor Physics, Quantum Electronics & Optoelectronics*, **3**, p.247, (2000).
18. G. Hawkins, R. Hunneman, R. Sherwood and B. M. Barrett, *SPIE Proceeding "Specialized Optical Developments in Astronomy"*, 4842, p.43, (2002).
19. H.A. Macleod, *Thin Film Optical Filters*, IOP, Institute of Physics Publishing, Bristol and Philadelphia (2001).