

Theoretical Study of Field Propagation Through a Nonhomogeneous Thin Film Medium Using Lippmann-Schwinger Equation

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ABSTRACT

A computational technique was used to study the field propagation through an inhomogeneous thin film using Lippmann-Schwinger equation.

The iterative formalism was used which was constructed based on the principle of Born approximation method due to the difficulty in using direct numerical resolution as a result of implicit nature of the function. The computed field value, Ψ through the thin film with variation of the propagation distance was analyzed within the ultraviolet, visible and near of electromagnetic wave and the absorption of the propagated wave by the thin film studied. The energy band gap was also estimated from the computed absorption coefficient obtained from our formalism.

Keyword: Lippmann-Schwinger equation, propagation, electromagnetic field, thin film, perturbation, dielectric constant, discrete

1. INTRODUCTION

Various tools have been employed in studying and computing beam or field propagation in a medium with variation of small refractive index Feit and (Fleck, et al, 1976) (Fleck, 1978) (Ugwu et al, 2007) some researchers had employed beam propagation method based on diagonalization of the Hermetician operator that generates the solution of the Helmholtz equation in media with real refractive indices (Thylen and Lee, 1992), while some had used 2×2 propagation matrix formalism for finding the obliquely propagated electromagnetic fields in layered inhomogeneous un-axial structure (Ong, 1993).

Recently, we have looked at the propagation of electromagnetic field through a conducting surface (Ugwu, 2005) and we observed the behaviour of such a material. The effect of variation of refractive index of F_eS_2 had also been carried out (Ugwu, 2005).

The parameters of the film that were paramount in this work are dielectric constants and the thickness of the thin film.

The dielectric constants were obtained from a computation using pseudo-dielectric function in conjunction with experimentally measured extinction co-efficient and the refractive indices of the film and the thickened of the film which was assumed to range from $0.1 \mu\text{m}$ to $0.7 \mu\text{m}$ [100 nm to 500 nm] based on the experimentally measured value, at the wavelength, $450 \mu\text{m}$ (Cox, 1978) (Lee and Brook, 1978).

This work is based on a method that involves propagating an input field over a small distance through the thin film medium and then iterating the computation over and over through the propagation distance using Lippmann-Schwinger equation and its counterpart, Dyson's equation (Economou, 1979) here, we first derived Lippmann-Schwinger equation

using a specific Hamiltonian from where the field function $\psi_k(z)$ was obtained. From this, it was observed that to ease out the solution of the Lippmann-Schwinger equation, it was discretized. After this, Born approximation was applied in order to obtain the solution. The formalism is logically built up step-by-step, which allowed point-to-point observation of the behaviour of the field propagating through the film. The advantage of this approach area, such as field in a medium with variation of dielectric constant, refractive index becomes apparent and above all our method requires no resolution of a system of equations and can accommodate multiple layers easily.

2. THEORETICAL PROCEDURE

We set out find the field, Ψ of a scalar wave equation

$$\nabla^2 \Psi(\mathbf{z}) + \omega^2 \epsilon_0 m_0 \epsilon_p(\mathbf{z}) \dots \quad (1)$$

Propagated through a thin film.

The assumption here is that the dielectric function is split into two parts comprising reference homogeneous medium, ϵ_{ref} and perturbed medium representing the deposited film medium.

Hence the dielectric function of the system is defined thus

$$\epsilon_p(\mathbf{z}) = \epsilon_{ref} + \Delta\epsilon(\mathbf{z}) \quad (2)$$

First Principle Green's function for the problem. The plane wave equation as defined by equation 3.1 depicts our model.

Where $\psi(z)$ represents scalar field which we intend to know its behavior as it propagating through the thin film μ_o and ϵ_o are permeability and permittivity of the free space respectively

$$\epsilon_p(z) = \epsilon_{ref} + i\Delta\epsilon_p(z) \quad (3)$$

Is the dielectric function which is arbitrarily complex in nature and comprises ϵ_{ref} representing the dielectric of the reference dielectric homogeneous medium ϵ_{ref} while $\Delta\epsilon_p(z)$ is the perturbed dielectric part which signifies the deposited thin film medium.

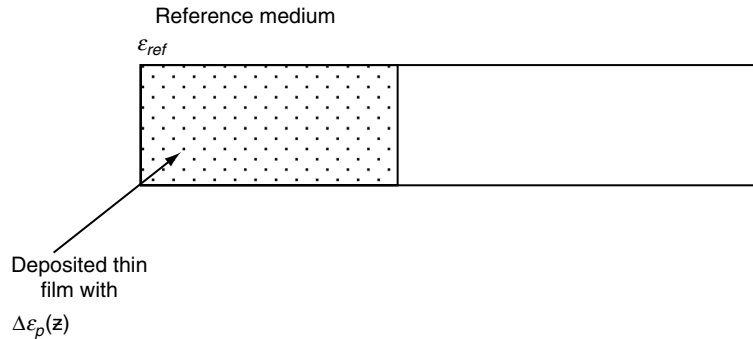


Figure 1 Deposited thin film in a glass substrate.

Substituting this into equation (1) we have

$$\nabla^2 \psi(z) + \mu_o \epsilon_o \omega^2 \epsilon_{ref} \psi(z) = \omega^2 \mu_o \epsilon_o \Delta \epsilon_p \psi(z) \quad (4)$$

Let $\Upsilon^2 = \omega^2 \mu_o \epsilon_o$ and $V(z) = -\Upsilon^2 \Delta \epsilon_p(z)$ being the function that describes the perturbation.

We now seek the Green's function satisfying

$$(\nabla^2 + \Upsilon^2)G(z, z') = \delta(z, z') \quad (5)$$

With the boundary condition that

$$G(o, z') = G(z_1, z') \quad V(z) = -\Upsilon^2 \Delta \epsilon_p(z) \quad (6)$$

Using the method of finite Fourier sine transform in which we multiply both side of equation (5) by $\sin \frac{n\pi z}{z_1}$ and integrate over $(0, z_1)$ to obtain

$$-\frac{n^2 \pi^2}{z_1^2} \frac{z_1}{2} \gamma_n(z') + \Upsilon^2 \frac{z_1}{2} \gamma_n(z') = \sin \frac{n\pi z'}{z_1} \quad (7)$$

With $\gamma_n(z)$ being the Fourier coefficient of $G(z, z')$, it follows that

$$\gamma_{n(z')} = \frac{2}{z_1} \frac{\sin n\pi \frac{z}{z_1}}{\Upsilon^2 - \frac{n^2 \pi^2}{z_1^2}} \quad (8a)$$

$$\text{where } \frac{z_1}{2} \gamma_n(z) = \int_0^{z_1} G(z, z') \sin \frac{n\pi z'}{z_1} dz' \quad (8b)$$

$$\text{and } G(z, z') = \frac{2}{z_1} \sum_{n=1}^{\infty} \frac{\sin n\pi \frac{z'}{z_1}}{\Upsilon^2 - \frac{n^2 \pi^2}{z_1^2}}$$

Here the symmetry property of Green's function is obvious while the formula fails if $\Upsilon^2 = \frac{n^2 \pi^2}{z_1^2}$ as Green's function has no solution or does not exist at that point.

If we now assume $\Upsilon^2 = \frac{n^2 \pi^2}{z_1^2}$ as a variable parameter of $G(z, z')$ on which it depends on

such that the solution is possible only within $-\ell \leq \lambda - \frac{n^2 \pi^2}{z_1^2} \leq \ell$

Green's function possesses simple pole at $\lambda = \frac{n^2 \pi^2}{z_1}$ where $n = 1, 2, 3 \dots$

This means that the solution of the Green's Function relies on analyticity of the denominator.

However, where $G(z, z')$ doesn't exist, there is resonance.

The solution of equation 3.1 becomes

$$\psi(z) = \int_0^{z_1} G(z, z') V(z') \psi(z) dz' \quad (10)$$

With this equation, we can now spell out the total field propagating through the thin film as

$$\psi(z) = \psi^o(z) + \int_0^{z_1} G(z, z') V(z') \psi(z) dz' \quad (11)$$

Which is simplified as?

$$\psi(z) = e^{ikz} - e^{ikz} \int_0^{z_1} \Delta \epsilon_p(z) \psi(z) dz \quad (12)$$

Equation 3.8 is known as Lippmann-Schwinger equation which can better be handled in parallel with its counterpart Dyson's equation,

$$G(z, z') = G^o(z, z') + \int_0^{z_1} G^o(z, z') v(z') G(z, z') dz' \quad (13a)$$

$$\Psi_k(z) = e^{ikz} - \frac{m}{2\pi^2 h^2} \int_{-\infty}^{\infty} d^3 z' \frac{e^{ik(z-z')}}{|z-z'|} V(z') \Psi_k(z') \quad (13b)$$

The perturbed term of the propagated field due to the inhomogeneous nature of the film occasioned by the solid-state properties of the film is:

$$\begin{aligned} \Psi_k(z) &= -\frac{m}{2\pi^2 h^2} \int_{-\infty}^{+\infty} d^3 z' \frac{e^{ik(z-z')}}{|z-z'|} V(z') \Psi_k(z') \\ \Psi_k(z) &= -\frac{1}{4\pi} \frac{2}{h^2} \Delta_{kk'} \end{aligned} \quad (14)$$

Where $\Delta_{kk'}$ is determined by variation of thickness of the thin film medium and the variation of the refractive index (Ugwu, et al. 2007) at various boundary of propagation distance. As the field passes through the layers of the propagation distance, reflection and absorption of the field occurs thereby leading to the attenuation of the propagating field on the film medium. (Blatt, 1968)

3. ITERATIVE APPLICATION

Lippman-Schwinger equation can be written as

$$\Psi_k(z) = \Psi_k^o + \int dz' G^o \Delta \epsilon_p(z') \Psi(z') \quad (15)$$

Where $G^o(z, z')$ is associated with the homogeneous reference system, (Yaghjian 1980) (Hanson, 1996)(Gao et al, 2006) (Gao and Kong 1983)

The function

$$V(z) = -k_o^2 \Delta \epsilon_p(z) \quad (16)$$

define the perturbation

Where

$$k_o^2 = \frac{c^2}{\lambda^2} \epsilon_o \mu_o \quad (17)$$

The integration domain of equation (13) is limited to the perturbation. Thus we observe that equation (13) is implicit in nature for all points located inside the perturbation. Once the field inside the perturbation is computed, it can be generated explicitly for any point of the reference medium. This can be done by defining a grid over the propagation distance of the film that is the thickness. We assume that the discretized system contains Δ_{kk} , defined by T/N .

Where T is thickness and N is integer

($N = 1, 2, 3, N-1$). The discretized form of equation (13) leads to large system of linear equation for the field;

$$\Psi_i = \Psi_i^o + \sum_{k=1}^{\Delta} G_{i,k}^o V_k \Delta_k \Psi_k \quad (18)$$

$$\Psi_i = \Psi_i^o + \sum_{k=1}^{\Delta} G_{i,k}^o V_k \Delta_k \Psi_i \quad (19)$$

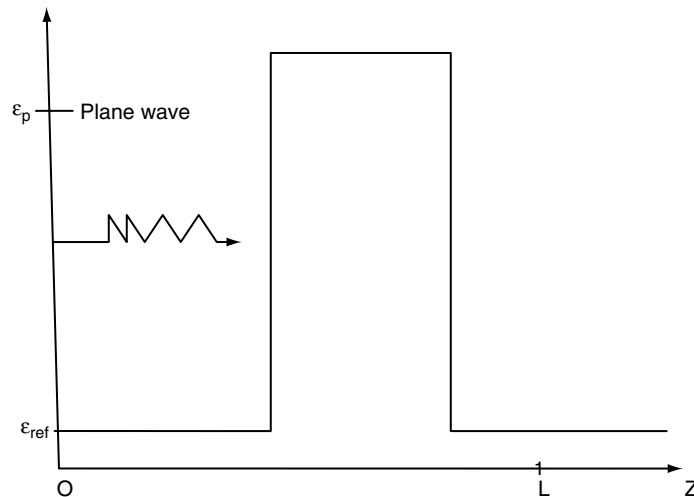


Figure 2 Plane wave impinging upon a dielectric barrier. The reference medium ϵ_{ref} corresponds to the fundamental level, where as perturbation ϵ_p , describes the barrier.

4. RESULTS AND DISCUSSION

In this case the field behaviour was obtained using born approximation technique both equations in parallel considering the variation of field with the film thickness and mesh size which is given as z/N (N_{max}) for wavelength in electromagnetic spectrum of regions in ultraviolet, visible/optical and near infrared.

FORTTRAN program was used in facilitating the computation with $N_{max} = 10, 50$ and 100. As observed from the graphs of the filed profiles, the field in the ultraviolet region has a higher absorbance for all the mesh sizes. It is also seen that for a longer wavelength within the near infrared region, the profile of the field exhibited negative trend within the film medium as shown in fig. 3 to fig. 6. Close observation shows that at about 0.05 m just as the field penetrates the film medium, the absorbance appears to be very small, but tends to rise sharply with a slight variation from that point to the maximum specified propagation distance which is just the thickness of the thin film. At just about the end of the size of the specified film thickness, the filed fall sharply again. This peculiar case of sharp/sudden rise in the field profile tends to suggest the influence of scattering and reflection on the propagating field which is as a result of the particles of thin film medium in accordance with Brillouin and Agarwal [Brillouin, 1963 and Agarwal, 1977]. From the graph of absorbance plotted as a function of wavelength, as shown in fig. 6 it is seen that the absorbance is generally low within the optical region to near infrared in our computation this goes on to confirm the profile behaviour in computed relative amplitude in fig. 3 to fig. 6

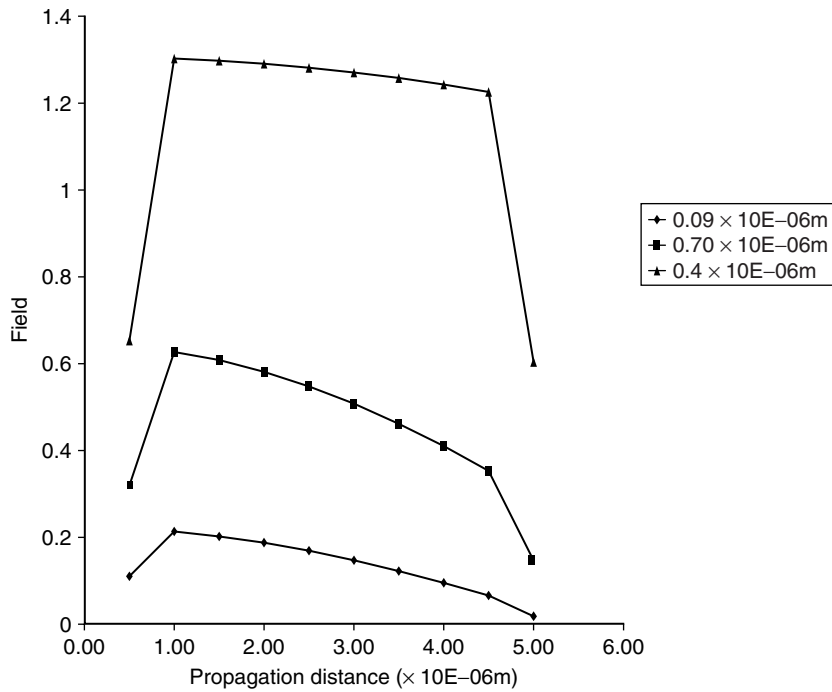


Figure 3 The field behaviour as it propagates through the film thickness $z\text{ }\mu\text{m}$ for mesh size = 10 when the input wavelength, $\lambda = 0.4\text{ }\mu\text{m}$, $0.7\text{ }\mu\text{m}$ and $0.9\text{ }\mu\text{m}$.

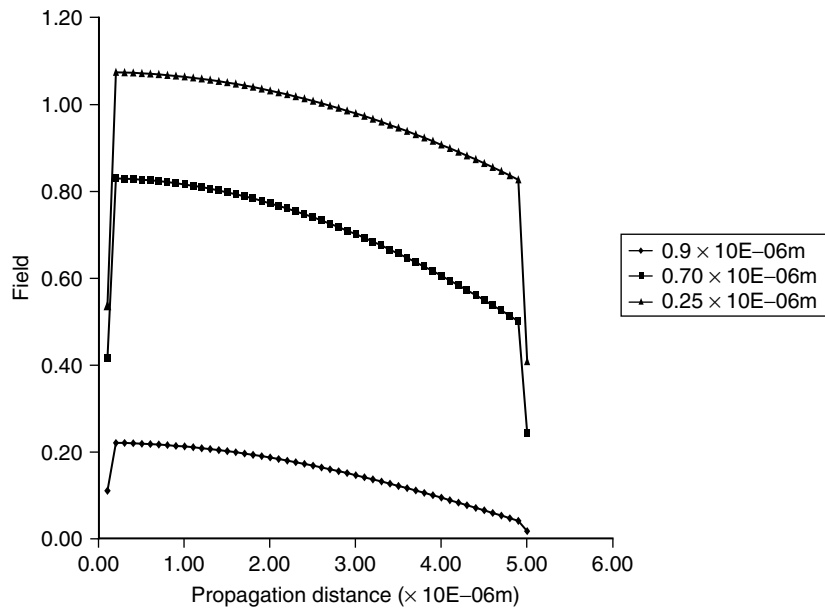


Figure 4 The field behaviour as it propagates through the film thickness z μm for mesh size = 50 when the input wavelength, $\lambda = 0.25$ μm , 0.70 μm and 0.90 μm .

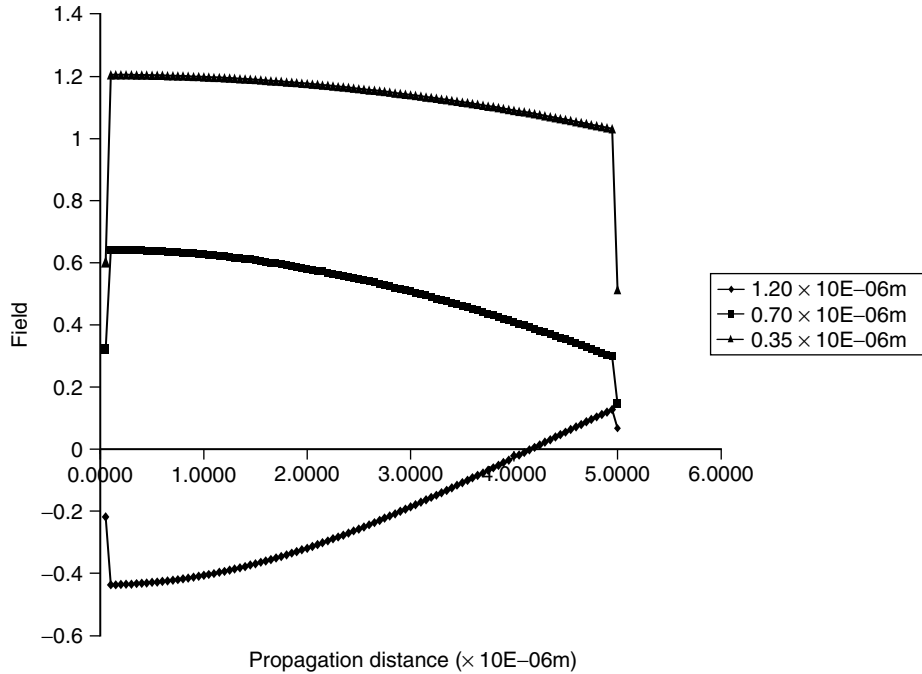


Figure 5 The field behaviour as it propagate through the film thickness z μm for mesh size = 100 when the input wavelength $\lambda = .35$ μm , 0.70 μm and 1.20 μm .

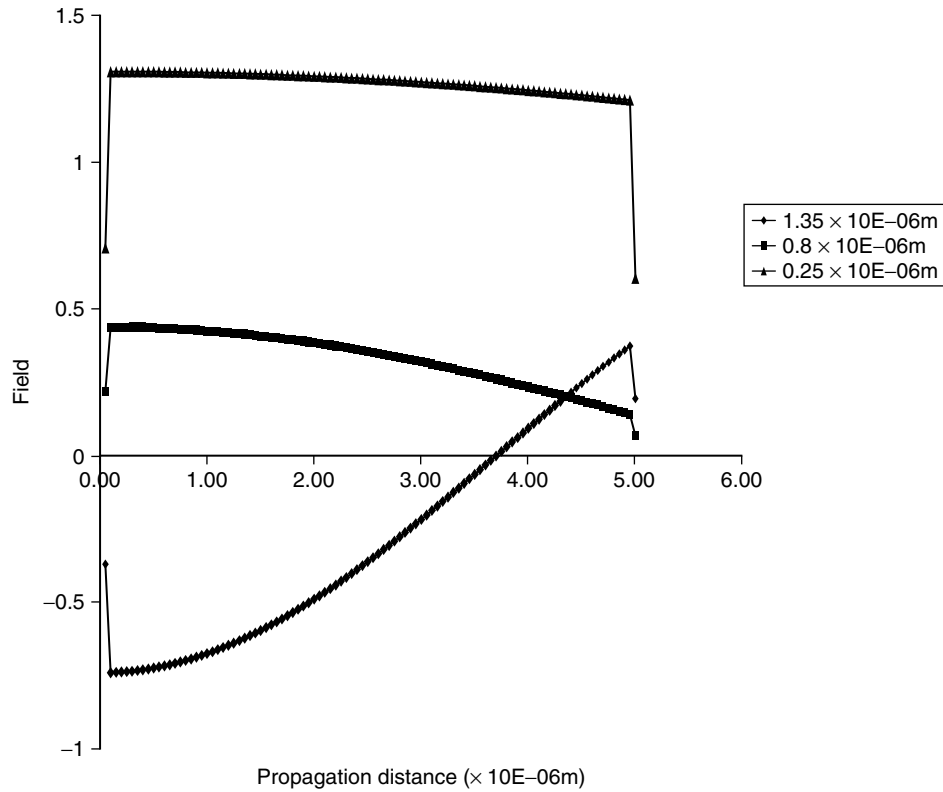


Figure 6 The field behaviour as it propagate through the film thickness z μm for mesh size = 100 when the input wavelength $\lambda = .25 \mu\text{m}$, $0.70 \mu\text{m}$ and $1.35 \mu\text{m}$.

where the cases of nonabsorbing. Limited absorption and strong absorbing thin film were considered.

The values of the band gap were obtained by extrapolating the graphs of $(\alpha h\nu)^2$ against $(h\nu)$ to meet at $h\nu$ axis. The points on the graphs as in fig. 7 fig. 8 and fig.9 where the extrapolated lines met the photon energy axis is where $(\alpha h\nu)^2$ is zero signify the band gaps. They are 2.35eV, 3.25eV and 15.25eV for the three cases we considered. From these energy band value, it is seen that the third one that represents that of the strongly absorbing case has the highest energy band gap, (15.25eV) indicating that it offers the largest impedance to photon energy transmission follows by that of the limited absorbing case with 3.25eV band gap. Non-absorbing case has the last band gap of 2.35eV. This therefore confirms high optical impedance of strongly absorbing case.

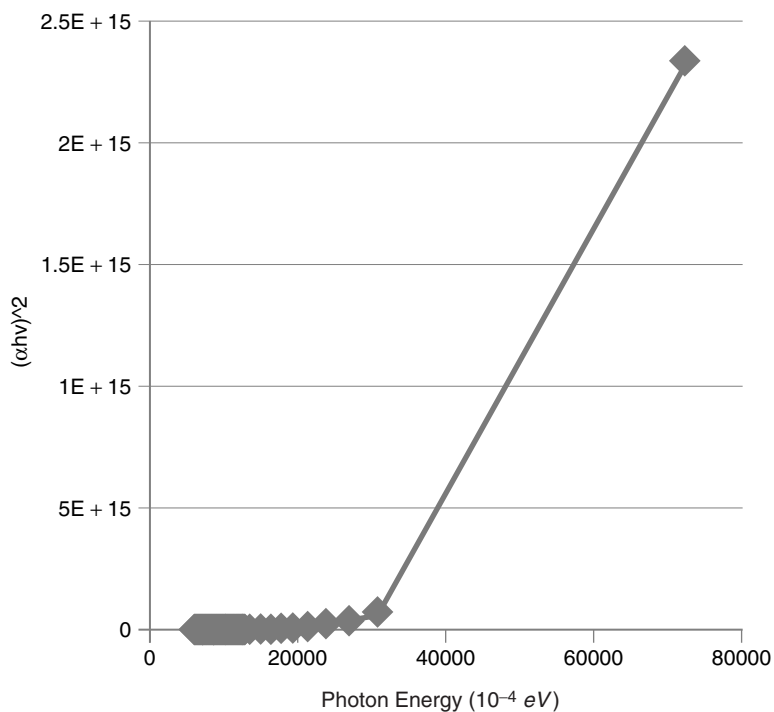


Figure 7 Graph of $(\alpha h\nu)^2$ against photon Energy for limited absorbing case.

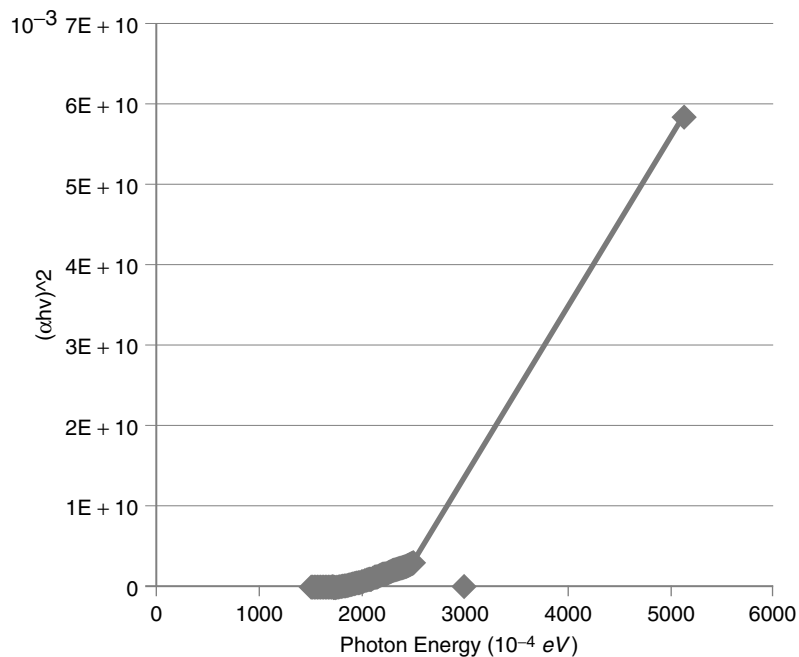


Figure 8 Graph of $(\alpha h\nu)^2$ against photon Energy for non-absorbing case.

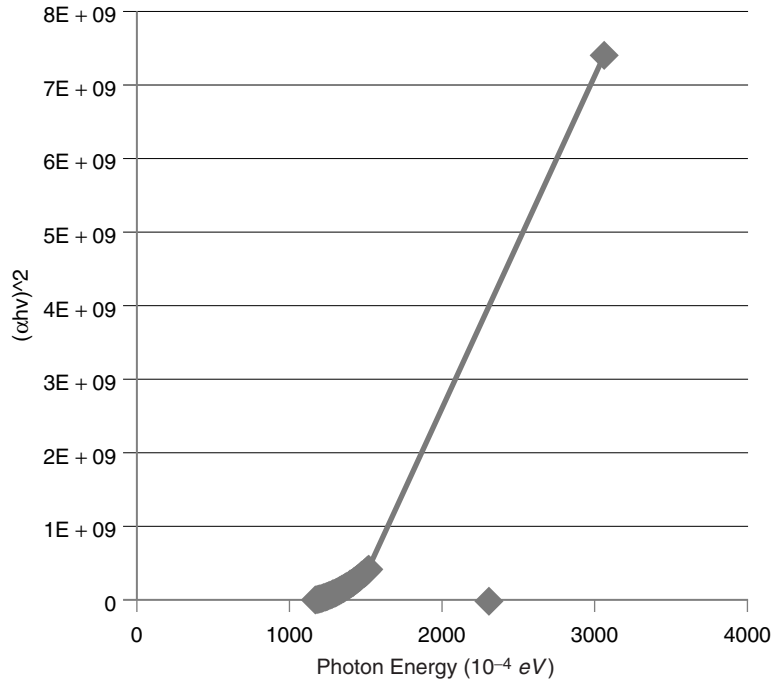


Figure 9 Graph of $(\alpha h\nu)^2$ against photon Energy for strongly absorbing case.

5. CONCLUSION

- Lippmann-Schwinger equation in conjunction with Born Approximation had been used in analyzing the propagation of field through thin film. An iterative scheme was applied to the formalism by building up step-by-step solution and observation that enabled us to determine the behaviour of the propagated field. The results obtained showed that variation of the field with thickness depended on the wavelength of the photon energy. The mesh size had no significant contribution in the behaviour of the propagated wave pattern through the thin film. This study helped in determining the absorption behavior. The energy band gap and the probable applications of the thin film.

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REFERENCES

- [1] J.A Fleck, J.R Morris and M.D. Feit 1976 "Time – dependent propagation of high energy laser beams through the atmosphere" *Applied phys* 10, 129–160.
- [2] M.D Feit and J.A Fleck 1978 "Light propagation in graded – index optical fibers" *Applied optical* 17, 3990–3998.
- [3] E.I. Ugwu, P.C Uduh and G.A Agbo 2007 "The effect of change in refractive index on wave propagation through (FeS₂) thin film". *Journal of Applied Sc.7* (4). 570–574.

- [4] L. Thylen and C.M Lee 1992 “Beam propagation method based on matrix digitalization” *J. optical science A*/9 (1). 142–146.
- [5] H.L Ong 1993 “ 2×2 propagation matrix for electromagnetic waves propagating obliquely in layered inhomogeneous unaxial media” *J. Optical Science A*/10(2). 283–393.
- [6] E.I. Ugwu 2005 “Effects of the electrical conductivity of thin film on electromagnetic wave propagation. JICCOTECH Maiden Edition. 121–127.
- [7] E.N Economou 1979 “Green’s functions in Quantum physics”, 1st. Ed. Springer. Verlag, Berlin.
- [8] A.D Yaghjian 1980 “Electric dynamic green’s functions in the source region’s Proc IEEE 68, 248–263.
- [9] G.W. Hanson 1996 “A Numerical formation of Dyadic Green’s functions for planar Bianisotropic Media with Application to printed Transmission line” IEEE Transaction on Microwave theory and techniques, **44**(1).
- [10] G. Gao, C Tores – Verdin and T.M Hat 2005 “Analytical Techniques toe valuate the integration of 3D and 2D spatial Dyadic Green’s function” *progress in Electromagnetic Research PIER* 52, 47–80.
- [11] E.I. Ugwu, C.E Okeke and S.I Okeke 2001. “Study of the UV/optical properties of FeS₂ thin film Deposited by solution Growth techniques JEAS Vol. 1 No. 13–20.
- [12] P.A. Cox 1978 “The electronic structure and Chemistry of solids” Oxford University Press Ch. 1–3.
- [13] F.J Blatt 1968 “Physics of Electronic conduction in solid”. Mc Graw – Hill Book Co Ltd New York, 335–350.
- [14] A.B Cody, G. Brook and Abele 1982 “Optical Absorption above the Optical Gap of Amorphous Silicon Hydride”. Solar Energy material, 231–240.
- [15] Lee, J.K and Kong J.A 1983 Dyadic Green’s Functions for layered an isotropic medium. Electromagn. Vol. 3 pp. 111–130.
- [16] Agarwal, G.S, 1977, Interaction of Electromagnetic waves at rough dielectric surface “Phy Rev. B, condens matter vol. 15 pp. 2371–2383.
- [17] Brillouin, L, 1963, Wave propagation and group velocity Acamemic press, New York.

