Trends in

# Applied Sciences Research

ISSN 1819-3579

Academic Journals Inc.

www.academicjournals.com

Trends in Applied Sciences Research 6 (1): 73-80, 2011
ISSN 1819-3579 / DOI: 10.3923/tasr.2011.73.80


# Computational Method of Studying the Field Propagation through an Inhomogeneous Thin Film Medium Using Lippmann-Schwinger Equation

E.I. Ugwu
Deptartment of Industrial Physics, Ebonyi State University, Abakaliki, Nigeria

**ABSTRACT**

A computational technique was used to study the field propagation through an inhomogeneous thin film using Lippman-schwinger equation. The iterative formulation is constructed based on the principle of Born approximation method due to the difficulty in using direct numerical resolution which is as a result of implicit nature of the function. The computed field value, φ through the thin film with variation of the propagation distance was analyzed within the ultraviolet, visible and near-infrared of electromagnetic wave.

**Key words:** Lippman-schwinger equation, propagation, electromagnetic field, thin film, perturbation, dielectric constant, discrete

## INTRODUCTION

Various tools have been employed in studying and computing beam or field propagation in a medium with variation of small refractive index (Fleck *et al*., 1978; Feit and Fleck, 1979; Ugwu *et al*., 2007), some researchers had employed beam propagation method based on diagonalization of the Hermitian 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 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.

The parameters of the film that were paramount in this work are dielectric constant (Blatt, 1968) 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 to 0.7 μm [100 to 500 nm] based on the experimentally measured value, at the wavelength, 450 μm (Cox, 1978; Lee and Kong, 1983).

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 has ti be 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-t-point observation of the behavior 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.

## THEORETICAL METHOD

Lippman-schwinger equation is associated with the Hamiltonian H which goes with $H_0$+V where, $H_0$ is the Hamiltonian before the field penetrates the thin field and V is the interaction:

$$H_0\Phi_k\rangle = E_k\Phi_k\rangle \tag{1}$$

The eigenstate of $H_0$+V is the solution of:

$$(E_k - H_0)\Psi_k(z)\rangle = V \mid \Psi_k(z)\rangle \tag{2}$$

where, z is the propagation distance as defined in the problem:

$$\mid \Psi_k(z)\rangle = \left|\Phi_k + \frac{1}{E_k - H_0}\right|_n V \mid \Psi_k(z)\rangle \tag{3}$$

where, $\eta$ is the boundary condition placed on the Green's function $(E_k\text{-}H_0)^{-1}$. Since, energy is conserved, the propagation field component of the solutions will have energy $E_n$ with the boundary conditions that only handle the singularity when the eigenvalue of $H_0$ is equal to $E_k$. Thus, we write:

$$\mid \Psi_k(z)\rangle = \left|\Phi_n + \frac{1}{E_k - H_0 + i\eta}\right|_n V \mid \Psi_k^f(z)\rangle \tag{4}$$

as the Lippman-schwinger equation without singularity; where $\eta$ is a positively infinitesimal, $\left|\Psi_k^f(z)\right\rangle$ is the propagating field in the film while $\left|\Psi_k^f(z)\right.$ is the reflected. With the above Eq. 3 and 4 one can calculate the matrix elements with (z) and insert a complete set of z and $\mu$ states as shown in Eq. 5:

$$\langle z \mid \psi_k(z) = \langle z \mid \Phi_k\rangle + \int d^3z' \int \frac{d^3k'}{(2\pi)^3} \langle z \mid \frac{1}{E_k - H + in} \mid \Phi_{k'}\rangle\langle\Phi_{k'} \mid J' \mid z'\rangle\langle z' \mid \psi_z \tag{5}$$

$$\Psi_k(z)\rangle = e^{fk} + \int d^3z' \int \frac{d^3k'}{(2\pi)^3} \frac{e^{-fk(z-z')}}{E_k - E_k + i\eta} V(z')\Psi_k(z) \tag{6}$$

$$G(z) = \int \frac{d^3k'}{(2\pi)^3} \frac{e^{-fk(z-z!)}}{E_k - E_k + i\eta}$$

is the Green's function for the problem, which is simplified as:

$$G(z)=\int\frac{m}{2\pi^2h^2z}\int_{-\infty}^{\infty}dk^{\prime}\frac{\sin k^{\prime}z}{K^{\prime 2}-(k+i\eta)^2} \tag{7}$$

When $\eta\approx 0$ is substituted in Eq. 6, we have:

$$\Psi_k(z)=e^{ikz}-\frac{m}{2\pi^2h^2}\int_{-\infty}^{\infty}d^3z^{\prime}\frac{e^{ik(z-z^{\prime})}}{|z-z^{\prime}|}V(z^{\prime})\Psi_k(z^{\prime}) \tag{8}$$

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

$$\Psi_k(z)=-\frac{m}{2\pi^2h^2}\int_{-\infty}^{+\infty}d^3z^{\prime}\frac{e^{fk(z-z^{\prime})}}{|z-z^{\prime}|}V(z^{\prime})\Psi_k(z^{\prime}) \tag{8a}$$

$$\Psi_k(z)=-\frac{1}{4\pi}\frac{2}{h^2}\Delta_{k^{\prime}k} \tag{8b}$$

where, $\Delta_{kk}$ is determined by variation of thickness of the thin film medium and the variation of the refractive Eq. 3 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.

## ITERATIVE APPLICATION

Lippman-Schwinger equation can be written as:

$$\Psi_k(z)=\Psi_k^o+\int dz^{\prime}G^o\Delta\varepsilon_p(z^{\prime})\Psi(z^{\prime}) \tag{9}$$

where, $G^o(z, z')$ is associated with the homogeneous reference system (Yaghjian, 1980; Hanson, 1996; Gao *et al.*, 2005; Lee and Kong, 1983).

The function $V(z)=-k_o^2\Delta\varepsilon_p(z)$ define the perturbation.
Where:

$$k_o^2=\frac{c^2}{\lambda^2}\varepsilon_o\mu_o \tag{10}$$

The integration domain of Eq. 9 is limited to the perturbation. Thus, we observe that Eq. 9 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, which is the thickness. We assumed that the discretized system contains $\Delta_{kk}$ defined by T/N.

where, T is thickness and N is integer.

(N = 1, 2, 3, N-1). The discretized form of Eq. 9 leads to large system of linear equation for the field:

$$\Psi_i = \Psi_i^o + \sum_{k=1}^{\Delta} G_{i,k}^o V_k \Delta_k \Psi_k \tag{11a}$$

$$\Psi_i = \Psi_i^o + \sum_{k=1}^{\Delta} G_{i,k}^o V_k \Delta_k \Psi_i \tag{11b}$$

However, the direct numerical resolution of Eq. 10 is time consuming and difficult due to singular behaviour of $G_{i,k}^o$. As a result, we use iterative scheme of Dayson's equation, which is the counter part of Lippman-schwinger equation to obtain $G_{i,k}^o$. Equation 10 is easily solved by using Born approximation, which consists of taking the incident field in place of the total field as the driving field at each point of the propagation distance. With this, the propagated field through the film thickness was computed and analyzed.

## RESULTS AND DISCUSSION

From the result obtained using this formalism, the field behaviour over a finite distance was contained and analyzed by applying Born approximation method in Lippman-Schwinger equation involving step by step process. The result yielded reasonable values in relation to the experimental result of the absorption behavior of the thin film (Ugwu *et al.*, 2001).

The splitting of the thickness into more finite size had not much affected on the behavior of the field as regarded the absorption trends.

The trend of the graph obtained from the result indicated that the field behavior have the same pattern for all mesh size used in the computation. Though, there is slight fall in absorption within the optical region, the trend of the graph look alike when the thickness is 1.0 μm with minimum absorption occurring when the thickness is 0.5 μm. within the near infrared range and ultraviolet range, (0.25 μm) the absorption rose sharply, reaching a maximum of 1.48 and 1.42, respectively when thickness is 1.0 μm having value greater than unity.

From the behaviour of the propagated field for the specified region, UV, visible and near infrared (Cody *et al.*, 1982) the propagation characteristic within the optical and near infrared regions is lower when compared to UV region counter part irrespective of the mesh size and the number of points the thickness is divided. The field behaviour is unique within the thin film as observed in Fig. 3 and 4 for wavelength 1.2 and 1.35 μm and Fig. 1 and depict the field trend when the mesh size is 10 for wave length = 0.40, 0.70 and 0.90 μm while Fig. 2 shows the propagated field 50 mesh size for wavelength = 0.25, 0.70 and 0.90 μm. Figure 5 shows the picture of the absorbance characteristics of the film.

We also observed in each case that the initial value of the propagation distance Z μm, initial valve of the propagating field is low, but increase sharply as the propagation distance increases within the medium suggesting the influence of scattering and reflection of propagating field produced by the particles of the thin film as it propagates.

Again, as high absorption is observed within the ultraviolet (UV) range, the thin film can be used as UV filter on any system the film is coated with on the other hand, it has low absorption within the optical (VIS) and near infrared (NIR) regions of solar radiation.

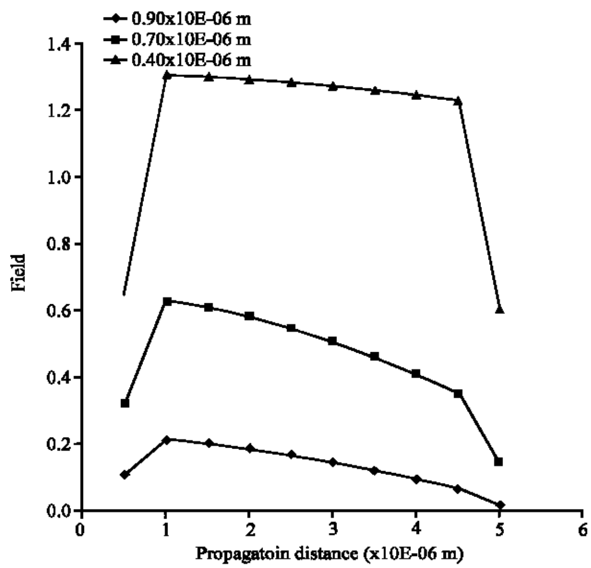


Fig. 1: The field behaviour as it propagates through the film thickness Z μm for mesh size = 10 when $\lambda = 0.4$, 0.7 and 0.9 μm

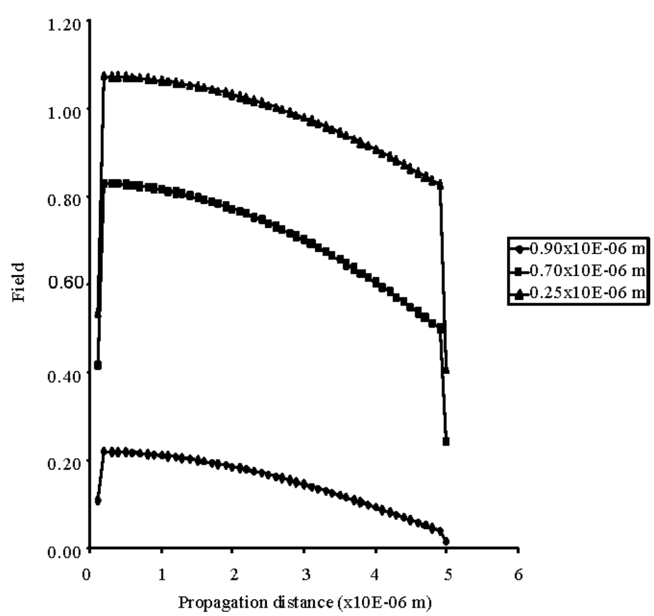


Fig. 2: The field behaviour as it propagates through the film thickness Z μm for mesh size = 50 when $\lambda = 0.25$, 0.7 and 0.9 μm

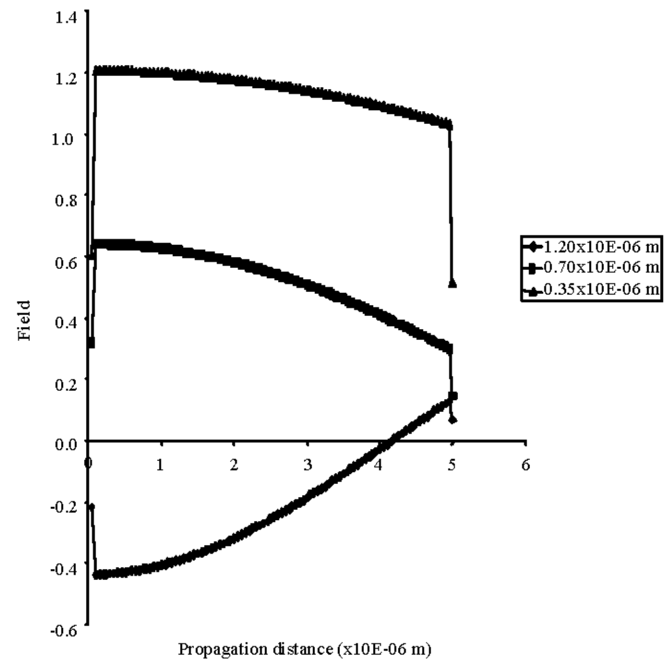


Fig. 3: The field behaviour as it propagates through the film thickness Z μm for mesh size = 50 when λ = 0.25, 0.7 and 0.9 μm

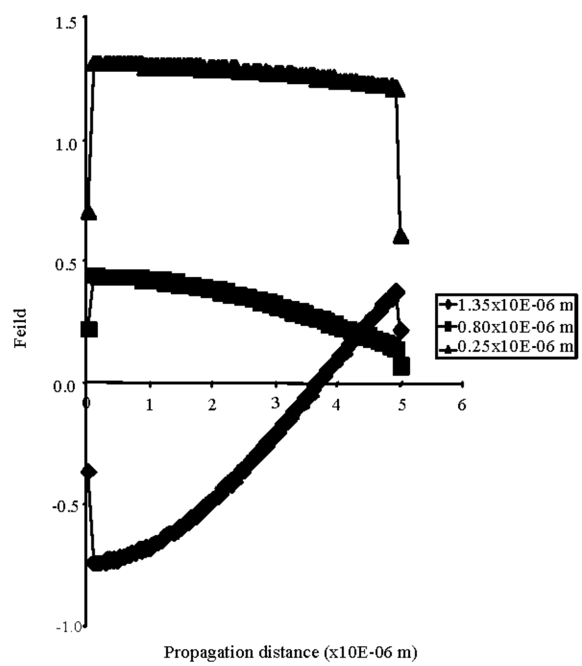


Fig. 4: The field behaviour as it propagates through the film thickness Z μm for mesh size = 100 when λ = 0.25, 0.8 and 1.35

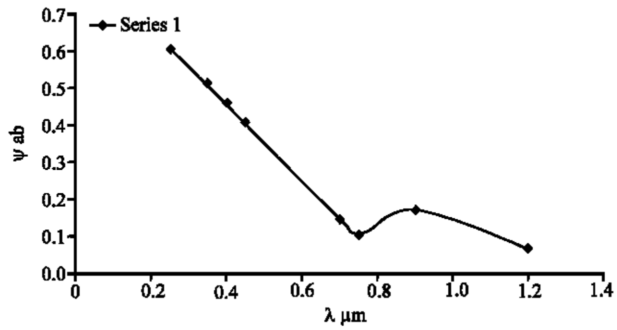


Fig. 5: The filed absorbance as a function wavelength

## CONCLUSION

Lippmann-schwinger equation in conjunction with Born Approximation had been used in analyzing the propagation of field through $F_eS_2$ thin film. 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 filed. The results showed that variation of the field with thickness depended on the wavelength of the photon energy not on the T/N, even the mesh size did not have any significant change in the behaviour. This study helped in determining the absorption behaviour and the probable applications of the thin film.

## ACKNOWLEDGMENTS

Authors humbly acknowledge the contribution of Dr M.I Echi of Department of Physics, University of Agric. Makurdi, Benue State for his effort in developing the program used for this work. Also Engr Onu of Department of Computer Sciences, Ebony State University and Abakaliki is left out for his help in facilitating the running of the program.

## REFERENCES

Blatt, F.J., 1968. Physics of Electronic Conduct in Solid. McGraw – Hill Book Co Ltd., New York, pp: 335-350.

Cody, A.B., G. Brook and F. Abelle, 1982. Optical absorption above the optical gap of amorphous silicon hydride. Solar Energy Mater., 8: 231-240.

Cox, P.A., 1978. The Electronic Structure and Chemistry of Solids. Oxford University Press, London, pp: 1-3.

Economou, E.N., 1979. Greens Functions in Quantum Physics. 1st Edn., Springer, Verlag, Berlin.

Feit, M.D. and J.A. Fleck, 1979. Light propagation in graded–index optical fibers. Applied Optical, 17: 3990-3998.

Fleck, J.A., J.R. Morris and V. Feit, 1978. Time–dependent propagation of high energy laser beans through the atmosphere. Applied Phys., 10: 129-160.

Gao, G., C. Tores-Verdin and T.M. Habashy, 2005. Analytical techniques to evaluate the integration of 3D and 2D spatial dyadic greens function. Prog. Electromagn. Res., 52: 47-80.

Hanson, G.W., 1996. A numerical formation of dyadic greens functions for planar bianisotropic media with application to printed transmission line. IEEE Trans. Microwave Theory Tech., 44: 144-151.

Lee, J.K. and J.A. Kong, 1983. Dyadic greens functions for layered an isotropic medium. Electromagnetics, 3: 111-130.

Ong, H.L., 1993. 2x2 propagation matrix for electromagnetic waves propagating obliquely in layered inhomogeneous unaxial media. J. Optical Soc. Am. A., 10: 283-294.

Thylen, L. and C.M. Lee, 1992. Beam propagation method based on matrix digitalization. J. Optical Soc. Am. A., 9: 142-146.

Ugwu, E.I., C.E. Okeke and S.I. Okeke, 2001. Study of the UV/optical properties of FeS2 thin film deposited by solution growth techniques. JEAS., 1: 13-20.

Ugwu, E.I., P.C. Uduh and G.A. Agbo, 2007. The effect of change in refractive index on wave propagation through (FeS2) thin film. J. Applied Sci., 7: 570-574.

Yaghjian, A.D., 1980. Electric dyadic greens functions in the source regions. Proc. IEEE., 68: 248-263.