Analytical study of electromagnetic wave behaviour in fcc latice periodic material: Bloch theorem of Maxwell's equation

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ABSTRACT
In this work, we studied the behaviour of electromagnetic wave as it propagates through face centered cubic (fcc) lattice material with periodic structure using Bloch theorem which was analyzed by one dimensional wave equation solved by method of separation of variables. Bloch theorem was linearised and superposed on the wave function as a modulator to the free wave function constituting real part and imaginary part. The phonon dispersion relation within the long wave limit and the implication of the imposed Bloch function on the free electron model was analyzed for different wavelength such as, ultraviolent, visible and infrared wavelengths within the first Brilouin zone in conjunction with the real and imaginary part of the wave function respectively coupled with the behaviour of the dispersion relation.

Keywords: Electromagnetic wave, Bloch theorem, Dispersion Periodic material, Analysis, Brilouin zone, Wave propagation, Wavelength, Free electron

1. INTRODUCTION

The Bloch theory of the conduction properties of metals is based on the electrons assemblage of independent particles obeying Bose-Einstein statistics followed with the fact that an election is considered to be moving freely in the periodic lattice potential without being scattered while the potential modulates the free electron wave function. This appears to modify the relation between electron energy E and wave-vector K since the lattice vibrations could be resolved into lattice waves. According to Klemens, [1] it is clear that electrons are scattered by disturbances in the lattice of periodicity coupled with the emission or absorption of phonon which may result from such process. This particular case could be handled by perturbation as Bloch theory is not applicable to the concept. As a result of this shortcoming, electromagnetic wave propagation approach becomes the in thing the material scientists have resorted to understanding the response of material with periodic structure to under this situation one notices that electromagnetic field propagated through it.

The propagation of electromagnetic wave in a medium with a collection of scatterer is an old problem having to do with such diverse subjects as x-ray diffraction in crystals, the blue colour of the sky, the theory of rainbows, light scattering from interstellar dust rainfall measurement using radar, etc.

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Recently, there has been growing interest in EM wave propagation in natural and man-made structures with periodic array of particles with microscopic dimensions that have scattering characteristics. The stimulating ground was provided by experiments where for instance the existence of photon bands in thin crystal of dielectric sphere has been demonstrated and the possibility of the existence of band gap in the photonic band structure observed [1–3]. In the frequency range of the photonic gap, the EM wave would not propagate through the medium but rather suffers exponential decay which suggests the fact there is an inhibition of electron hole radioactive recombination as the corresponding photon frequency falls in the gap region.

So far, the photon band is periodic structure have been only examined theoretically only in the scalar wave approximation where the vector nature of the EM field is neglected. This has been studied by several researchers using the plane-wave (PW), the Kerringa-Kohn-Rostker (KKR) or Augmented Plane-Wave (APW) method [4] with the general result that for the material, the band gap appears in the entire Brillouin Zone. Also, the equation for the electric displacement vector, D in a periodic structure with space-dependent real dielectric constant $\varepsilon(r)$ and the magnetic permeability, μ being uniform throughout has been studied.

Other interesting study has been carried out [5] on analysis of wave propagation in a two-dimensional photonic crystal focused on the use of Bloch modes where the wave coupling at the interfaces is well explained using the reduced vector in the first Brillouin zone [5]. In the work of Veselago, the theoretically analyzed theoretically the electromagnetic properties of some media in which real part of the magnetic permeability, μ and electric permeability , were negative [6] it was found that this property gives rise to unexpected phenomena such as negative refraction at the interface between the air and observed that a composite structure consisting wire strips was demonstrated to refract negatively when electromagnetic wave impinge on it from free space [7–10]. Other material where electromagnetic wave has experienced negative refraction where it propagates is photonic crystals [11]. Van Roey in his work derived a general beam propagation relation in a number of specific cases along with the extensive simulation of wave propagation in variety of complex material. Scientists have looked at the propagation of electromagnetic field through a conducting surface [12] where the behaviour of wave propagated through such material coupled with the influence of the dielectric function of the medium such on such material was analyzed. The effect of variation of refractive index of FeS_2 had also been carried out [13] A close look on the concept made it clear to recognize the importance of the effect of the refractive index of the medium which in reality gives rise to the two velocity components that normally result to phase and group refractive indices as considered in the study of wave propagation [11].

Recently more complicated work had been embarked upon on the study of wave propagation through a modeled thin film with dielectric perturbation in which W.K.B approximation technique in conjunction with numerical approach were used [14, 15] in order to analyze beam propagating through the film material.

In this work our interest is to study the electromagnetic wave propagation through a metal using the concept of Bloch theorem in which we consider the first Brillion zone of the Fermi surface. This is because of Bloch theory of the conduction properties of the metal is based on the electron assemblage of independent particles obeying Bose-Einstein statistics coupled with their unimpeded motion in the periodic lattice potential. Structure of crystal using one dimensional Bloch theorem is assumed in order to analyze the behavior of the wave function.

2. FORMULATION WAVE EQUATION PROPAGATING THROUGH FCC PERIODIC LATTICE WITH A GIVEN DIELECTRIC CONSTANT

We begin with Maxwell's equations that relate electromagnetic wave propagation through material medium and the solid property of the material.

$$Curl\,H = \frac{4\pi j}{c} + \frac{1}{c}\frac{\partial D}{\partial t} \qquad [1]$$

$$div\,D = 4\pi j \qquad [2]$$

$$Curl\,E = -\frac{1}{c}\frac{\partial B}{\partial t} \qquad [3]$$

where $D = \varepsilon E$ and $B = \mu H$

ε and μ are the dielectric constant and permeability while j is the current due to the conduction electrons. The permeability is assumed to be unity in the lattice medium.

Conversely, since $D = E + 4\pi\rho$, ρ now is considered to result from charge density ρ' given by

$$\text{Div}\rho = \rho' \qquad [4]$$

Associated with j' the current density that exists in parallel with the current density due to conduction electrons j given by

$$\text{div}\, j' = \frac{\partial \rho'}{\partial t} \qquad [5]$$

From equations 4 and 5, we can write

$$j' = \frac{\partial \rho}{\partial t} \qquad [6]$$

Equation [6] represents the additional current [known as bound current] in conjunction to the current associated with the conduction electrons.

Conversely, we consider j to be absorbed into $\frac{\partial D}{\partial t}$, as we regard the entire solid as the medium through which electromagnetic wave propagates. For consistency, we take $j = 0$ in equation [1and 2] obtaining

$$Curl\,H = \frac{\varepsilon}{c}\frac{\partial E}{\partial t} \text{ and } Curl\,E = \frac{1}{c}\frac{\partial H}{\partial t} \qquad [7]$$

For wave with time variation $e^{i\omega t}$ travelling in the z-direction with E and H parallel to x-and y-directions respectively, we have

$$\frac{\partial H_y}{\partial z} = \frac{i\omega\varepsilon E_x}{c} \qquad [8]$$

$$\frac{\partial E_x}{\partial z} = \frac{i\omega}{c} H_y \qquad [9]$$

Equations [8 and 9] enable us to obtain

$$\frac{\partial^2 E_x}{\partial z^2} = \frac{\omega^2\varepsilon}{c^2} E_x \qquad [10]$$

whose solution is given as

$$E = E_o \exp i\omega\left[t - \frac{\mu z}{c}\right] \qquad [11]$$

where $\mu = \sqrt{\varepsilon}$ one can write equation [11] thus

$$E = E_o \exp i\omega\left(t - \frac{nz}{c}\right)\exp\left(\frac{-\omega kz}{c}\right) \qquad [12]$$

However, base on the complexity of Hamiltonian involved in on the use of unconserved momentum associated with the lattice we consider

$$\frac{-h}{2m}\frac{d^2}{dz^2}E_{(z,t)} = ih\frac{d}{dt}E_{(z,t)} \qquad (13)$$

In conjunction with free electron model

$$E_{(z,t)} = Z_{(z)}, T_{(t)} \qquad (14)$$

We obtain

$$\frac{d^2}{dz^2}E_{(z,t)} = \frac{Zd^2T}{dt} \qquad (15)$$

and

$$\frac{d^2E}{dt^2} = \frac{Td^2Z}{dz} \qquad (16)$$

With solutions given as

$$E_{(z,t)} = ab\cos(nz-\alpha)e^{-n^2h^2/2m^t}$$

From Bloch theorem,

$$E_{(z)} = U_{(z)}e^{ikz} \qquad (17)$$

where $E_{(z)}$ is the Bloch function in one dimension since in a Bravais lattice, a plane wave function multiplies a function with periodicity of the Bravais lattice to give equation (5) which is the Bloch theorem where e^{ikx} is wave function for free electron model.

The linearized periodic function $U(x)$ modifies the wave function as given below

$$E_R = z.\cos(\cos(kz - \omega t)) \tag{18}$$

and

$$E_{im} = z.\sin(kz - \omega t) \tag{19}$$

With normal incident wave to the metal, we considered three regions of electromagnetic wave spectra such as ultraviolet, visible and infrared regions, λ_u, λ_v and λ_i for real and imaginary part of the wave function. Similarly, by complete solution of the wave equation, we obtain

$$\nabla^2 E(r) - k^2 a(r) \exp ik.r \qquad [20]$$

This expression satisfies the scalar wave equation with $a(r)$ signifying the amplitude of the wave propagating through the system. Noting that $k = \frac{\omega}{c}, k^2 = \frac{\omega^2}{c^2} = \omega^2 \varepsilon_o \mu_o$.

When the value of k^2 as obtained above is substituted in equation [20], it gives the expression as used in this work as below

$$\nabla^2 E(r) + \omega^2 \varepsilon_o \mu_o E(r) = 0 \tag{21}$$

3. ANALYSIS OF BLOCH WAVE SOLUTION

It has been noted that the scattering vector of a EM waves from a single particle which is considered spherical has been studied (Ugwu and Okeke 2006) as such, we assume that the wave equation for the electric displacement vector, D in a periodic structure with a space-dependent real dielectric constant, $\varepsilon(x)$ having a uniform magnetic permeability, μ.

From Maxwell equations, the wave equation for D is

$$-\nabla^2 D = \left(\omega^2 / c^2\right) D + \nabla x \nabla x \left[V(x)\right] \tag{22}$$

where $V(x)$ is the potential given as

$$V(x) = 1 - \frac{1}{\varepsilon(x)} \tag{23}$$

Given that the electric displacement D satisfying Bloch theorem can be expanded in terms of the plane wave is

$$D = \sum_G d_G e^{i(k+G)x} \tag{24}$$

Where k is the Bloch momentum

Due to the orthogonality condition of the wave corresponding to the plane wave.

This enables us to write the expansion co-efficient d_G. Thus

$$H_G d_G + \sum_G V(G-G^{/})\left\{(k+G)\,d_G(k+G) - |k+G|^2\right\} = 0 \tag{25}$$

Where

$$H_G = |k-G|^2 - \omega^2/c^2 \tag{26}$$

This equation reflects the dynamical theory of X-ray diffraction in a crystal.

We carried out the numerical computations for FCC lattice with a given dielectric constant within first Brillouin zone for a number of sphere packing fraction.

4. RESULTS/DISCUSSION

The solution of equation [20] enables to spell out the total field propagating through the material.

Figure 1 represents the graph of wave function as a function $E(x)$ of position(x) in one dimension when $\lambda_1 = 250 \times 10^{-9}$ in the real part. Figure 2 depicts the graph of wave function $E(x)$ as a function of position(x) in one dimension when $\lambda_1 = 250 \times 10^{-9}$ imaginary part. This particular graph maintain a damped periodic oscillation and the frequency decreases as it tends to the origin and increases as it moves away from the origin.

Figure 3 represents the graph of wave function $\varphi(x)$ as a function of position(x). Figure 4 also represent the graph of wave function $E(x)$ as a function of position(x) in one dimension when $\lambda_2 = 650 \times 10^{-9}$ in real and imaginary part respectively. These graphs experience a damped oscillation tending to a fractal meaning that it has the same statistical function as a whole with increase in frequency.

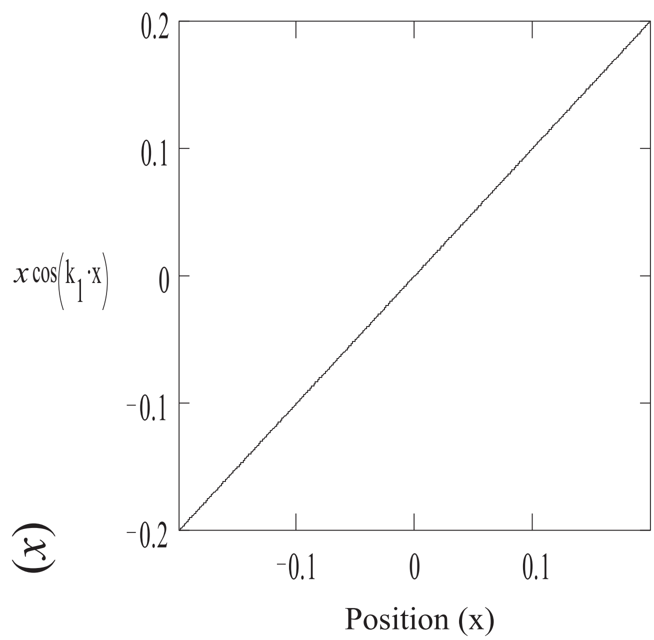

Figure 1: Wave function ψ (x) abs a function of position (x) for real part when $\lambda_1 = 250 \times 10^{9}$

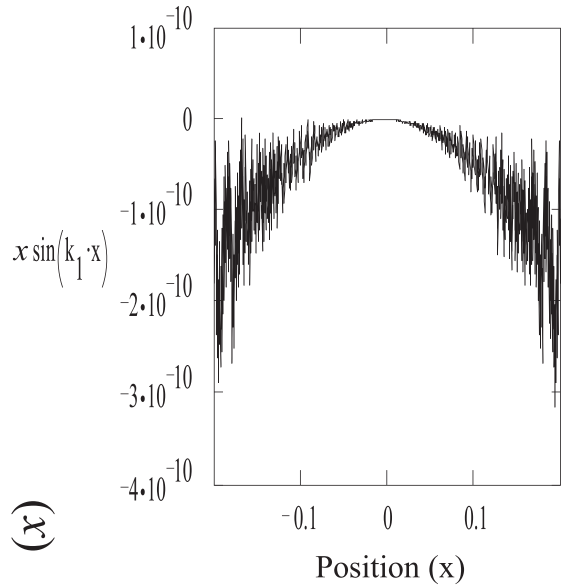

Figure 2: Wave function $\psi\,(x)$ as a function of position (x) for imaginary part when λ_2 = 250 × 10^{-9}

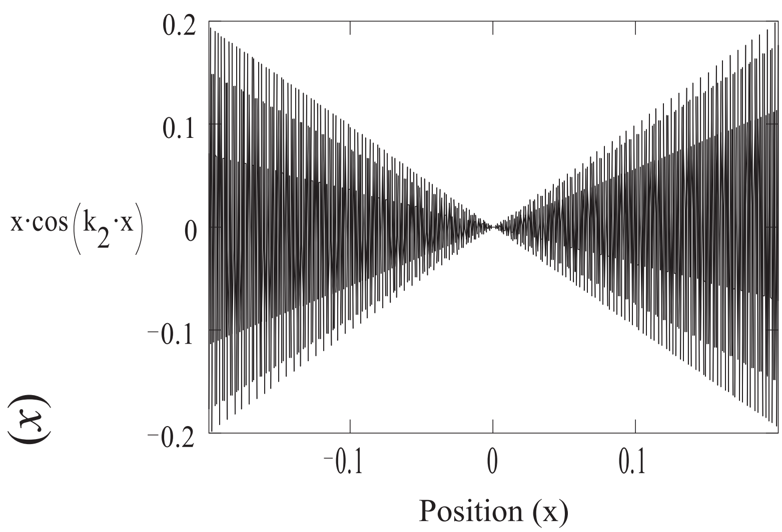

Figure 3: Wave function $\psi\,(x)$ as a function position (x) for Real part when λ_1 = 650 × 10^{-9}

Figure 5 shows the graph of wave function $E(x)$ as a function of position(x) and Figure 6 also represent the graph of wave function when $\lambda_3 = 950 \times 10^{-9}$ in real and imaginary part. These graphs have very high oscillatory frequency which is comparable as seen in Fig 4.3 and Fig 4.4. They maintained the same damped oscillation characteristic leading to a fractal display in their profiles with the same statistical distribution pattern as a whole.

The photon band in this material as computed here was considered as a dielectric perturbation, Figure 7 which ranged from 1.0 to 13.25 experienced by the free photo bands

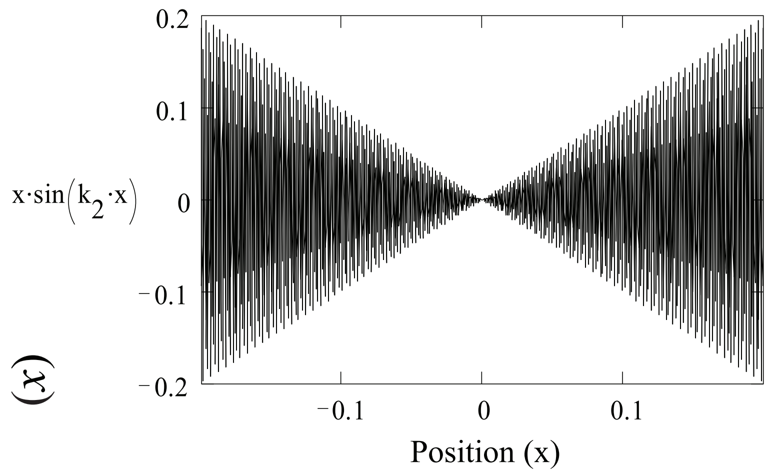

Figure 4: Wave function ψ (*x*) as a function position (x) for imaginary part when $\lambda_1 = 650 \times 10^{-9}$

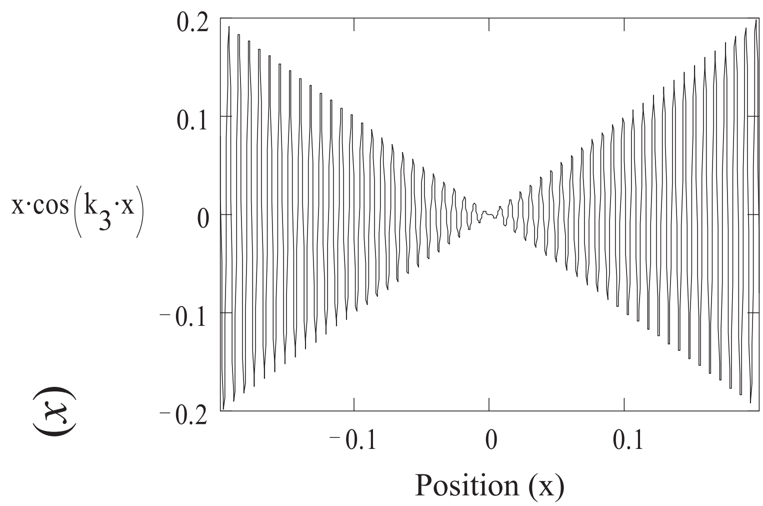

Figure 5: Wave function ψ (*x*) (x) a function of position (x) for real part, when λ_3 = 950 × 10-9

constrained within the first Brillouin zone, BZ of fcc without varying the packing fraction β of the fcc sphere. (Ze and Sash, 1990) as large or small sphere affects the scattering strength.

6. CONCLUSION

From this work, we have been able to obtain from Maxwell equation a relation that depicts a links between electromagnetic wave with unconserved momentum of the free electron in the periodic lattice as in equation (17) in conjunction with the explicit deduction of the expression for scalar wave equation for the free electron model. In the analysis as regards the propagated wave profile depicted unique characteristic in accordance with the spectral wavelength ranging from uv,visible and near-infrared within the considered first Brillouin zone(BZ) [15–17]. As a matter of fact, it was observed in this work, there was no true band gap extending throughout the said BZ for the studied structure as the scalar wave equation was used instead of vector wave equation.

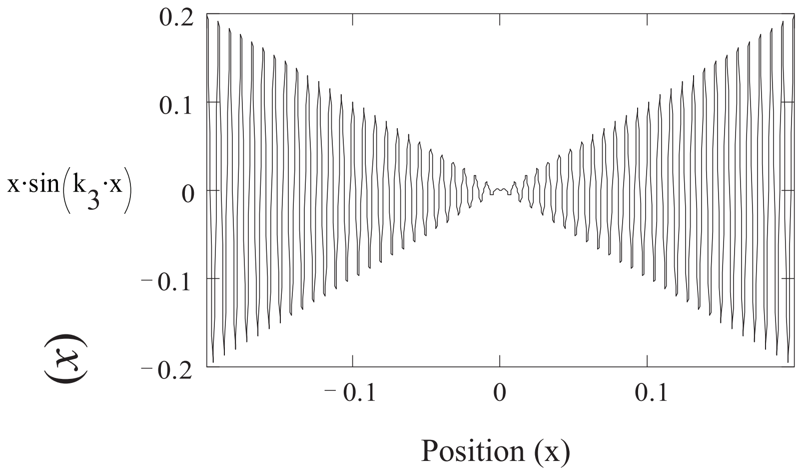

Figure 6: Wave function ψ (x) as a function of position (x) for imaginary part when λ_1 = 950 × 10^{-9}

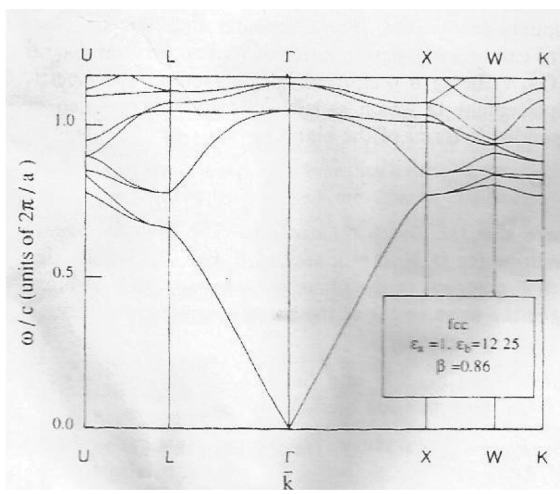

Figure 7: Photon bands in the fcc lattice structural material within the first BZ

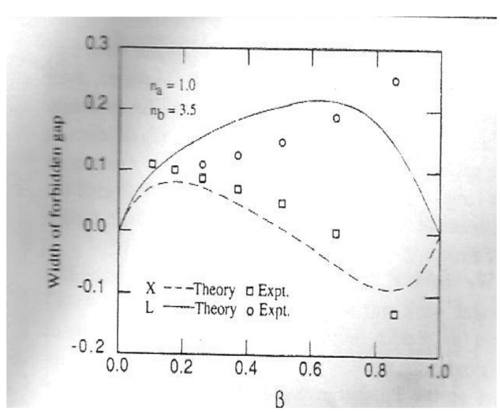

Figure 8: Estimated forbidden band gap width in the long wave length range within the BZ point of fcc

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