Behavior analysis of metamaterials with the FDTD method and the Lorentz model for dispersive media

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ABSTRACT

In electromagnetism, a material with a negative refractive index is a dispersive material called a metamaterial (MTM). In order to characterize the behavior of light in an MTM, this article uses the FDTD (Finite Difference Time Domain) method. To do this, the DB-FDTD formulation is used, and the dispersive medium is modeled by the Lorentz model. The frequencies of sources made up of sinusoids are defined so that the permittivity and permeability are equal and take negative values. This is so that the reflection coefficient of the MTM are $n_r \leq -1$. Studies of the effects of the variation of the refractive index are done in 1D space, with an FDTD grid terminated by loss layers. In order to demonstrate the effect of the negative refractive index, simulations in 2D space are performed.

Keyword: Metamaterial, negative refractive index, DB-FDTD, Lorentz Model, 1D, 2D

1. INTRODUCTION

Metamaterial (MTM) is a dispersive material that was first introduced in theory by Veselago in 1968. An interface between a vacuum and a medium made of MTM can produce negative refraction of light incident to it interface. Negative index materials do not exist in nature. However, artificially designed materials can play the role of MTM. However, it should be noted that obtaining an MTM requires both negative values of permittivity and permeability ($\epsilon < 0$ and $\mu < 0$) over the same frequency range [1].

The aim of this article is to characterize the behavior of light in an MTM with the FDTD method. To do this, the Lorentz model will be used for modeling the electrical and magnetic susceptibilities of a dispersive medium. The purpose being to be able to obtain negative values of the permittivity as well as of the permeability from the Lorentz model. The effects of negative refractive index on the propagation of light will be seen in the 1D and 2D domains.

2. MTM IMPLEMENTATION

For MTM, the refractive index is $n_r < 0$. In order to model this type of material, in this work, the desired refractive index is $n_r = -1$ (Eq.1). In special cases of incident wave frequency range, dispersive materials may exhibit negative refractive indices. In order to simulate a MTM, the ideal case is considered, that is to say that the susceptibility functions are equal (Eq.2). The susceptibility functions are modeled using the Lorentz model for frequency dependent materials [2].

$$n_r = \sqrt{\varepsilon_r \mu_r} = -1$$
; then $\varepsilon_r = \mu_r = -1 = j^2$ (1)

$$\hat{\chi}_{e,L}(\omega) = \hat{\chi}_{m,L}(\omega) = \frac{\omega_{pe}^2}{\omega_{0e}^2 - \omega^2 + j\gamma_e \omega} = \frac{\omega_{pm}^2}{\omega_{0m}^2 - \omega^2 + j\gamma_m \omega}$$
(2)

where ω_{pe} and ω_{pm} are the plasma frequencies, ω_{0e} and ω_{0m} are the resonance frequencies, and γ_e and γ_m are the damping coefficients.

2.1. FDTD formulation of Lorentz model

The Lorentz material equations for a dispersive material (Eq.3) can be in the discretized frequency domain (Eq.4) using the Z transformation. The Z transforms of the electrical and magnetic susceptibilities for a Lorentz material are given to Eq. 5. [2][3]

$$\widehat{D}(\omega) = \varepsilon_0 \varepsilon_\infty \widehat{E}(\omega) + \frac{\omega_{pe}^2}{\omega_{0e}^2 - \omega^2 + j\gamma_e \omega} \widehat{E}(\omega)$$
(3.a)

$$\hat{B}(\omega) = \mu_0 \mu_\infty \hat{H}(\omega) + \frac{\omega_{pm}^2}{\omega_{0m}^2 - \omega^2 + j\gamma_m \omega} \hat{H}(\omega)$$
(3.b)

$$\widehat{D}(z) = \varepsilon_0 \varepsilon_\infty \widehat{E}(z) + \varepsilon_0 \chi_e(z) \widehat{E}(z)$$
(4.a)

$$\hat{B}(z) = \mu_0 \mu_\infty \hat{H}(z) + \mu_0 \chi_m(z) \hat{H}(z)$$
(4.b)

$$\hat{\chi}_e(z) = \frac{\omega_{pe}^2 \Delta t}{\beta} \left(\frac{e^{-\alpha \Delta t} \sin(\beta \Delta t) z^{-1}}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}} \right)$$
(5.a)

$$\hat{\chi}_m(z) = \frac{\omega_{pm\Delta t}^2}{\beta} \left(\frac{e^{-\alpha\Delta t} \sin(\beta\Delta t) z^{-1}}{1 - 2e^{-\alpha\Delta t} \cos(\beta\Delta t) z^{-1} + e^{-2\alpha\Delta t} z^{-2}} \right)$$
(5.b)

$$\alpha = \frac{r_{e,m}}{2} \text{ et } \beta = \sqrt{\omega_{0e,0m}^2 - \frac{r_{e,m}}{4}}$$
(5.c)

By introducing Eq.5 into Eq.4, the flux densities in the Z domain are expressed in Eq.6. In these equations the flux densities are formulated with auxiliary terms (I_e and I_m) given in Eq.7 and Eq.8. Using Eq.4, the electric and magnetic fields, in the Z domain, are given in Eq. 9.

$$\widehat{D}(Z) = \varepsilon_0 \varepsilon_\infty \widehat{E}(z) + z^{-1} \widehat{I}_e(z)$$
(6.a)

$$\hat{B}(z) = \mu_0 \mu_\infty \hat{H}(z) + z^{-1} \hat{I}_m(z)$$
(6.b)

$$\hat{I}_{e}(z) = \varepsilon_{0} \frac{\omega_{pe}^{2} \Delta t}{\beta} \left(\frac{e^{-\alpha \Delta t} \sin(\beta \Delta t)}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}} \right) \hat{E}(z)$$
(7.a)

$$\hat{I}_e(z) = \varepsilon_0 \frac{\omega_{pe\Delta t}^2}{\beta} e^{-\alpha \Delta t} \sin(\beta \Delta t) \hat{E}(z) + 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} \hat{I}_e(z) - e^{-2\alpha \Delta t} z^{-2} \hat{I}_e(z)$$
(7.b)

$$\hat{I}_m(z) = \mu_0 \frac{\omega_{pm}^2 \Delta t}{\beta} \left(\frac{e^{-\alpha \Delta t} \sin(\beta \Delta t)}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}} \right) \hat{H}(z)$$
(8.a)

$$\hat{I}_m(z) = \mu_0 \frac{\omega_{pm\Delta t}^2}{\beta} e^{-\alpha \Delta t} \sin(\beta \Delta t) \hat{H}(z) + 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} \hat{I}_m(z) - e^{-2\alpha \Delta t} z^{-2} \hat{I}_m(z)$$
(8.b)

$$\hat{E}(z) = \frac{1}{\varepsilon_0 \varepsilon_\infty} \left[\hat{D}(z) - z^{-1} \hat{I}_e(z) \right]$$
(9.a)

$$\widehat{H}(z) = \frac{1}{\mu_0 \mu_\infty} \left[\widehat{B}(z) - z^{-1} \widehat{I}_m(z) \right]$$
(9.b)

The multiplications by z^{-1} and z^{-2} correspond respectively to one and two previous time step values. Thus the equations discretized in time of the fields and of the auxiliary terms are given respectively to Eq.10 and Eq.11.

$$E^n = \frac{1}{\varepsilon_0 \varepsilon_\infty} (D^n - I_e^{n-1}) \tag{10.a}$$

$$H^{n} = \frac{1}{\mu_{0}\mu_{\infty}} (B^{n} - I_{m}^{n-1})$$
(10.b)

$$I_e^n = \varepsilon_0 \frac{\omega_{p_e}^2 \Delta t}{\beta} e^{-\alpha \Delta t} \sin(\beta \Delta t) E^n + 2e^{-\alpha \Delta t} \cos(\beta \Delta t) I_e^{n-1} - e^{-2\alpha \Delta t} I_e^{n-2}$$
(11.a)

$$I_m^n = \mu_0 \frac{\omega_{pm\Delta t}^2}{\beta} e^{-\alpha \Delta t} \sin(\beta \Delta t) H^n + 2e^{-\alpha \Delta t} \cos(\beta \Delta t) I_m^{n-1} - e^{-2\alpha \Delta t} I_m^{n-2}$$
(11.b)

The FDTD procedure for dispersive materials using the Lorentz model is similar to the process of FDTD formulation using DB-FDTD formulation for an anisotropic medium, only the formulation of the auxiliary terms update coefficients differs.

2.2. MTM construction with Lorentz model

a. Definition of DNG (Double Negative) frequency

For an MTM made of dielectric material, the permittivity as well as the permeability are defined in Eq.12.a [4] [5]. The conductivity of a Lorentz material is defined by Eq.12.b, with $\varepsilon_{\infty} = 1$ and $\mu_{\infty} = 1$.

$$\hat{\varepsilon}_{r,L}(\omega) = \hat{\mu}_{r,L}(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + j\gamma\omega}$$
(12.a)

$$\hat{\sigma}_L(\omega) = \frac{\omega \varepsilon_0 \omega_p^2}{\gamma \omega + j(\omega^2 - \omega_0^2)}$$
(12.b)

The real part of the relative permittivity, for a Lorentz material, is given in Eq.13. For $\omega \in [\omega_{min}, \omega_{max}]$, the relative permittivity is negative. And for $\omega = \omega_{1,DNG}$, or $\omega = \omega_{2,DNG}$ the relative permittivity is $\varepsilon_r = -1$. The pulses ω_{min} , ω_{max} , $\omega_{1,MTM}$ and $\omega_{2,MTM}$ are defined in Eq.14.

$$\Re\{\hat{\varepsilon}_{r,L}(\omega)\} = 1 - \frac{\omega^2 \omega_p^2 - \omega_0^2 \omega_p^2}{\omega^4 + \omega^2 (\gamma^2 - 2\omega_0^2) + \omega_0^4}$$
(13)

$$\omega_{min} = \sqrt{2\left(2\omega_0^2 - \gamma^2 + \omega_p^2 - \sqrt{\gamma^4 - 4\gamma^2\omega_0^2 - 2\gamma^2\omega_p^2 + \omega_p^4}\right) \times \frac{1}{2}}$$
(14.a)

$$\omega_{max} = \sqrt{2\left(2\omega_0^2 - \gamma^2 + \omega_p^2 + \sqrt{\gamma^4 - 4\gamma^2\omega_0^2 - 2\gamma^2\omega_p^2 + \omega_p^4}\right) \times \frac{1}{2}}$$
(14.b)

$$\omega_{1,MTM} = \sqrt{4\omega_0^2 - 2\gamma^2 + \omega_p^2 - \sqrt{4\gamma^4 - 16\gamma^2\omega_0^2 - 4\gamma^2\omega_p^2 + \omega_p^4} \times \frac{1}{2}}$$
(14.c)

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$$\omega_{2,MTM} = \sqrt{4\omega_0^2 - 2\gamma^2 + \omega_p^2 + \sqrt{4\gamma^4 - 16\gamma^2\omega_0^2 - 4\gamma^2\omega_p^2 + \omega_p^4} \times \frac{1}{2}}$$
(14.d)

b. Frequency parameter for an MTM built with the Lorentz model

Considering $\gamma \ll \omega_p$, the negative permittivity is obtained for $\omega \in \left[\omega_0, \sqrt{\omega_0^2 + \omega_p^2}\right]$ and $\varepsilon_r = -1$ for $\omega_{1,MTM} = \omega_0$ and $\omega_{2,MTM} = \sqrt{\frac{2\omega_0^2 + \omega_p^2}{2}}$. Tab.1 presents the parameters of a dielectric modeled with the Lorentz model, with characteristics frequencies defined in Eq.15. The relative permittivities and conductivities of the MTM, at different DNG frequencies are illustrated in Fig.1. The conductivity of the MTM is proportional to the damping coefficient γ , so for an MTM with low absorbency γ is chosen with a relatively very small value.

$$f_0 = \frac{f_p}{10}$$
 ; $\gamma = \frac{f_p}{10^4}$ (15)

Tab.1: Characteristics of an MTM using the Lorentz model

Refractive index	Plasma frequency	Resonant frequency	Damping coefficients	DNG frequencies	Conductivity
	f _p en THz	f ₀ en THz	γ en THz	f _{DNG} en THz	σ en S/m
$n_r = -1$	2 127.83	212.78	0.21	1519.6	24.17
$n_r = -2$	2 127.83	212.78	0.21	1246.0	36.63
$n_r = -6$	2 127.83	212.78	0.21	830.94	88.89



<u>Fig.1</u>: Permittivity and conductivity of an MTM using the Lorentz model

3. FDTD SIMULATIONS OF AN MTM USING THE LORENTZ MODEL

3.1. 1D simulation

Fig. 1, Fig. 2 and Fig. 3 show the snapshots of a sine wave traveling in vacuum and crossing an MTM (i = [160,240]) of refractive index $n_r = -1, -2$ and -6 respectively. The source is introduced by TFSF limit at node $i_{src} = 30$ [6]. The grid is terminated by 15-node loss layers [7]. As shown in Tab. 1, the more the refractive index decreases, the more the frequency at double negativity decreases but the more the conductivity increases. This can be seen with the amplitudes of the reflected waves absorbed at the left edge of the FDTD grid at time step n = 1500.

In Fig. 1, the backward propagation of light within the MTM is seen. The celerity of light in the MTM is the same as that of light propagating in a vacuum.



<u>Fig.2</u>: Snapshots of electric field for an LHM (n = -1) using the Lorentz model

In Fig.3 and Fig.4, the propagation in the reverse direction is also observed within the MTM. For Fig.3, $n_r = -2$, the speed of light in the LHM is multiplied by 2. In Fig.4, $n_r = -6$, the speed of light is multiplied by 6.

Considering the propagation of light in the MTM, the celerity within the MTM is given by Eq.16. This considering that the light propagates from the MTM towards the vacuum. The speed of light in the MTM is obtained from observations during simulations.

$$c = \sqrt{\mu_r \varepsilon_r} c_0 \tag{16}$$



<u>Fig.4</u>: Snapshots of electric field for an LHM (n = -6) using the Lorentz model

3.2. 2D simulation

The simulation consists on modeling of the propagation of a beam traveling in a vacuum then hitting a rectangle of MTM ($n_r = -1$). The simulation parameters are given in Tab. 2.

f _{src} (THz)	N _{src}	Angle _{src} (°)	Rectangle _{LHM}
1 519	(50,200)	30	[(150,15); (230,385)]
Dimension _{Grid}	N _λ	$\Delta \boldsymbol{x} = \Delta \boldsymbol{y} \left(\boldsymbol{n} \boldsymbol{m} \right)$	$\Delta t (fs)$
400 × 400	40	4.93	1.10×10^{-2}

Tab.2: 2D simulation parameters

Fig. 5 illustrate the propagation of a beam hitting a rectangle of LHM. The wave propagation in the reverse direction is observed in the MTM. In addition, the inverse Snell effect is present and is characterized by a negative refraction angle.



Fig.5: Snapshot of a wave passing through an MTM with $\varepsilon_r = -1$ and $\mu_r = -1$

4. CONCLUSION

This paper concerns the modeling of MTM with the FDTD method and the Lorentz model for dispersive materials. By judiciously choosing the frequency of the source, various negative refractive indices were seen during the simulations. Therefore, it has been seen that within an MTM light propagates in the opposite direction of propagation. In addition, the speed of light within the MTM is proportional to the refractive index of the MTM. Smaller the refractive index is, then faster the speed of light in the MTM is. The simulation in two-dimensional space, showed the inverse Snell effect. Upon encountering an MTM, light is refracted with a negative refractive angle.

In this work, the FDTD method was used to characterize the behavior of light in an MTM. The results show the effectiveness of the method for a simple medium composed of vacuum and MTM. In order to implement simulations for a complex environment including devices, the attenuation or even the elimination of reflections at the interfaces should be carried out.

5. REFERENCES

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