Refraction at Media with Negative Refractive Index

S. Foteinopoulou$^1$, E. N. Economou$^2$, and C. M. Soukoulis$^{1,2,*}$

$^1$ Ames Laboratory-USDOE and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011
$^2$ Research Center of Crete, FORTH, Heraklion, Crete, Greece

* Author to whom correspondence should be addressed. Email: soukoulis@ameslab.gov

We show that an electromagnetic (EM) wave undergoes negative refraction at the interface between a positive and negative refractive index material. Finite difference time domain (FDTD) simulations are used to study the time evolution of an EM wave as it hits the interface. The wave is trapped temporarily at the interface and after a long time, the wave front moves eventually in the negative direction. This explains why causality and speed of light are not violated in spite of the negative refraction always present in a negative index material.

PACS numbers: 78.20.Ci, 41.20.Jb, 42.25.-p, 42.30.-d

Veselago$^1$ predicted that lossless materials, which possess simultaneously negative permittivity, $\epsilon$, and negative permeability, $\mu$, would exhibit unusual properties such as negative index of refraction, $n = -\sqrt{\epsilon/\mu}$, antiparallel wave vector, $\mathbf{k}$, and Poynting vector, $\mathbf{S}$, antiparallel phase, $\mathbf{v}_p$, and group, $\mathbf{v}_g$, velocities, and time-averaged energy flux, $\langle \mathbf{S} \rangle = \langle \mathbf{u} \rangle \mathbf{v}_g$, opposite to the time-averaged momentum density $\langle \mathbf{p} \rangle = \langle \mathbf{u} \rangle \mathbf{k}/\omega^2$, where $\langle \mathbf{u} \rangle$ is the time-averaged energy density. Furthermore if these materials are uniform, $\mathbf{k}, \mathbf{E}, \mathbf{H}$ form a left-handed set of vectors. Therefore, these materials are called left-handed materials (LHM) or negative index of refraction materials (NIM). The quantities, $\mathbf{S}, \mathbf{u}, \mathbf{p}$, refer to the composite system consisting of EM field and material. As a result of $\mathbf{k}$ and $\mathbf{S}$ being antiparallel, the refraction of an EM wave at the interface between a positive and a negative $n$ material would be at the “wrong” side relative to the normal (negative refraction). In addition, the optical length, $\int n dl$, is negative in a LHM.

Following Pendry’s suggestions$^{3,4}$ for specific structures which can have both $\epsilon_{\text{eff}}$ and $\mu_{\text{eff}}$ negative (over a range of frequencies), there have been numerous theoretical and experimental studies.$^{5-8}$ In particular, Markos and Soukoulis$^9$ have employed the transfer matrix technique to calculate the transmission and reflection properties of the structure suggested by Pendry$^3$ and realized experimentally by Smith et al.$^{6,7}$ Subsequently, Smith et al.$^{10}$ proved that the data of Ref. [9] can be fitted by length independent and frequency dependent, $\epsilon_{\text{eff}}$, and $\mu_{\text{eff}}$. They found that in a frequency region both $\epsilon_{\text{eff}}$ and $\mu_{\text{eff}}$ were negative with negligible imaginary parts. In this negative region, $n$ was found to be unambiguously negative. These unusual results$^{[3-10]}$ have raised objections both to the interpretation of the experimental data and to the realizability of negative refraction.$^{11,12}$

In this letter we report numerical simulation results, which clarify some of the controversial issues, especially the negative refraction considered as violating causality and the speed of light.$^{12}$ Our numerical calculations were performed on a well understood realistic system, which is essentially inherently lossless, namely a 2D photonic crystal (PC). The dielectric constant $\epsilon$ is modulated in space and both the permittivity $\epsilon$ and permeability $\mu$ are locally positive. Specifically, the photonic crystal consists of an hexagonal lattice of dielectric rods with dielectric constant, $\epsilon = 12.96$. The radius of the dielectric rods is $r = 0.35a$, where $a$ is the lattice constant of the system. A frequency range exists for which the EM wave dispersion is "almost" isotropic. For that range the group velocity, $\mathbf{v}_g$, is antiparallel to the crystal momentum $\mathbf{k}$.$^{13}$ In particular for the frequency of our simulations the angle between the group velocity and the phase velocity $\theta_{\text{pg}}$ varies between $176^0$ and $180^0$. We have studied systematically the equifrequency contours of the system$^{14}$ and have obtained the effective refractive index, $n$, as a function of frequency. The absolute value of $\alpha$, $n = c|\mathbf{k}|/\omega$, the phase velocity, $\mathbf{v}_p = (c/n)|\mathbf{k}_0|$, where $\mathbf{k}_0 = k/|\mathbf{k}|$, and the group velocity $\mathbf{v}_g = \partial \omega/\partial \mathbf{k}$ are defined the usual way. Then, it can be easily shown that $\mathbf{v}_g = \mathbf{v}_p/\alpha$, where $\alpha = 1 + (\omega/n)(dn/d\omega) = 1 + d \ln |n|/d \ln \omega$; given this last relation is natural to identify the sign of $n$ with the sign of $\alpha$ in order to associate negative $n$ with antiparallel $\mathbf{v}_p$ and $\mathbf{v}_g$.$^{15}$ Furthermore, it can be shown that $\langle \mathbf{S} \rangle = \langle \mathbf{u} \rangle \mathbf{v}_g$, where the symbol $\langle \mathbf{u} \rangle$ denotes averaged value over time and over the unit cell. Thus, $\mathbf{v}_p$ and $\mathbf{v}_g$ being antiparallel leads to almost all the peculiar and interesting properties associated with LHM.

Essentially this means that for the PC system a frequency range exists for which the effective refractive index is negative, frequency dispersion is almost isotropic and $c < S > |k| < 0$, i.e. the PC behaves as a left-handed (LH) system. Consequently a wave hitting the PC interface for that frequency will undergo negative refraction for the same reason a wave undergoes negative refraction when it hits the interface of a homogeneous medium with negative index $n$ (the component of $\mathbf{k}$ along the normal to the interface reverses direction). In Fig.1 we plot our results for the effective refractive index $n$ for the PC system versus the dimensionless frequency $f$, where $f = \omega a/2\pi c = a/\lambda$ and $\lambda$ is the wavelength in air. Notice that the effective refractive index $n$ passes continuously from negative to positive values as $f$ increases. At this point we would like to alert the reader about other conditions under which negative refraction can occur in the...
air PC interface. For example, for some particular \( \mathbf{k} \), light bends “the wrong way” at the PC interface as a result of the curvature of the equifrequency surfaces\(^{16} \) in spite of \( \langle \mathbf{S} \rangle \cdot \mathbf{k} = 0 \) coupling to a higher order Bragg wave can lead to a negatively refracted beam. We would like to stress that in both the cases mentioned above, the PC is right-handed (RH). So the origin of the negative refraction in these cases is unrelated with that occurring on the interface between a RH and LH medium. Thus, these cases should not be confused with the case that we study in this paper where the PC is LH.

In our simulations a finite extent line source was placed outside a slab of PC at an angle of \( 30^\circ \) as shown in Fig. 2. The source starts gradually emitting at \( t = 0 \) a monochromatic TE wave (the \( \mathbf{E} \) field in the plane of incidence) of dimensionless frequency, \( f = 0.58 \), with a Gaussian amplitude parallel to the line source. Employing a FDTD\(^{17-19} \) technique, we follow the time and space evolution of the emitted EM waves as they reach the surface of the PC and they propagate eventually within the PC. The real space is discretized in a fine rectangular grid, (of \( a/31 \) and \( a/54 \) for the \( x \) and \( y \) axes, respectively), that stores the dielectric constant, and the electric and magnetic field values. By use of a finite time step, \( \delta t = 0.0128a/c \), the fields are recursively updated on every grid point. This algorithm numerically reproduces the propagation of the electromagnetic field in real space and time through the interface. In Fig. 2 we present the results for our FDTD simulation after 200 simulation steps. (The period, \( T = 2\pi/\omega \) corresponds to 135 time steps, \( T \sim 135\delta t \).

We found, as expected for a negative index \( n \), that the incident beam is eventually refracted in the negative direction (\( \sin \theta_{PC} \leq 0 \)). However, the most interesting finding is that each ray does not refract in the final direction immediately upon hitting the surface of the PC. Instead, the whole wavefront is trapped in the surface region for a relatively long time (of the order of a few tens of the wave period, \( T \), in our simulations); and then, gradually after this transient time, the wave reorients itself and starts propagating in the negative direction as expected from the steady state solution. Thus, the interface between the vacuum (positive \( n = 1 \)) and the PC (negative \( n \)) acts as a strong resonance scattering center which traps temporarily the wave before gradually re-emitting it. This time delay (which is much longer that the time difference, \( 2t_0 \approx 400\delta t \), between the arrival at the interface of the inner and outer rays) explains satisfactorily the apparent paradox of the outer ray propagating much faster than the velocity of light.\(^ {12} \)

In Fig. 3, we present a time sequence of the amplitude of the magnetic field of the Gaussian beam undergoing reflection and refraction at the interface between vacuum (\( n = 1 \)) and a negative index (\( n = -0.7 \)) material. We would like to stress that despite the fact that the fronts are obscured by the Bloch modulation the refraction of the wave (after a transient time) is clearly in the negative direction. We have also calculated the Poynting vector (Fig. 4) which shows that (in the steady state) the energy flows in the same negative direction as shown in Fig. 3e. Since one can prove in general that \( \langle \mathbf{S} \rangle = (u)\mathbf{v}_g \), it is clear that the group velocity in the PC is along the direction indicated in Fig. 3e. We present the results in terms of the time difference, \( 2t_0 \), between the arrival of the outer and the inner rays at the interface. Figure 3a shows the results for \( t = 2.5t_0 \approx 3.7T \approx 500\delta t \). Notice that no refracted front has developed yet. Fig. 3b shows the results for \( t = 4.5t_0 \). Notice that the wave front has crossed the interface and seems to move along positive angles. Figure 3c shows the results for \( t = 10.5t_0 \), where both the reflected and refracted wave fronts are shown. Notice there seem to appear two fronts for the refracted beam, one moving towards positive angles and one towards negative angles. Figure 3d clearly shows that the wavefront at \( t = 15t_0 \) along positive angles has diminished and the wavefront along the negative angles is more pronounced. Also, notice the clear reflected wavefront. Finally, Fig. 3e for \( t = 31t_0 \) clearly shows that the wavefront moves along negative angles, a behavior that continues for \( t \gtrsim 31t_0 \). This is an unambiguous proof that negative refraction exists in media with a negative refraction index. This time sequence of the wavefronts shows that once the one end of the Gaussian wavefront hits the interface, it does not mean that the other side of the wavefront must move in “zero time” or “at infinite speed” to refract negatively (see Fig. 1b of Ref. 12). There is a transient time of the order of \( 30t_0 \approx 45T \) needed for the refracted wave to reorganize and move eventually along the negative directions. Notice that the wavefronts move finally along negative angles. The same is true for the directions perpendicular to the wavefronts, which can be considered parallel to the group velocity.

We would like to note that Ziolkowski and Heyman\(^ {20} \) have observed a similar transient time effect numerically in a 1D model system with homogeneous negative permittivity \( \varepsilon \) and permeability \( \mu \). In [20] it was shown that there exists a time-lag between the wave hitting the interface and the medium responding with negative effective index \( n \) indicating that causality is maintained. In the present paper we have shown that in a realistic structure transient effect precedes the establishment of steady state propagation in the negative refracted direction.\(^ {21} \)

We note in passing that our time-dependent results are unrelated with the steady state solution obtained by Valanju et al.\(^ {12} \). In Ref. 12, a modulated plane wave, composed of two plane waves with different frequencies, is incident on the interface with a certain angle. Indeed, this steady state solution of propagation of a modulated plane wave, shows the interference fronts refracting in the positive direction, while the phase fronts refract in the negative direction. However Smith and Pendry\(^ {22} \) have demonstrated that when two frequencies are superimposed in the NIM with wavevectors that are not par-
allel - which is the case in [12]- propagation is *crabwise* meaning that the interference fronts are not the group fronts and should not be associated with the direction of propagation. In addition, Smith\textsuperscript{23} has considered an incident modulated beam with a finite Gaussian profile. The steady state solution shows that the group velocity moves along negative angles, despite the distortion in the modulated fronts. Negative refraction is also obtained by Lu et. al.\textsuperscript{24} where they consider more than two frequency components for the incident wave.

In conclusion, we have shown by a FDTD simulation that an EM wave coming from a positive $n$ region and hitting a plane interface of a negative $n$ material refracts eventually in the negative angle direction. Our detailed time-dependent sequence shows that the wave is trapped initially at the interface, gradually reorganizes itself, and finally propagates along the negative angle direction. This transient time explains why negative refraction does not violate causality or light speed.

We would like to thank P. Markoš for useful discussions. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82. This work was supported by the director for Energy Research, Office of Basic Energy Sciences. This work was also supported by DARPA, EU, and NATO grants.

\begin{figure}[h]
    
    \centering
    \includegraphics[width=\textwidth]{fig1.png}
    
    \caption{The effective index of refraction, $n$, versus dimensionless frequency $a/\lambda$ for a 2d photonic crystal.}
\end{figure}

1. V. G. Veselago, Usp. Fiz. Nauk 92, 517 (1968) [Sov. Phys. Usp. 10, 509 (1968)].
2. The momentum density, $\mathbf{p}$, of the composite system consisting of the EM field and the material is given by the following expression $\mathbf{p} = \frac{\partial}{\partial \mathbf{r}} (\mathbf{S}) + \frac{1}{c} \left( \frac{\partial}{\partial \omega} (\mathbf{E}^2) + \frac{\partial}{\partial \omega} (\mathbf{H}^2) \right)$. The energy density, $\langle u \rangle$, is given by $\langle u \rangle = \frac{1}{8\pi} \left[ \frac{\partial}{\partial \omega} (\mathbf{E}^2) + \frac{\partial}{\partial \omega} (\mathbf{H}^2) \right]$.
3. J. B. Pendry et al., Phys. Rev. Lett. 76, 4773 (1996); J.B. Pendry et al, J. Phys: Condens. Matt. 10, 4785 (1998); J. B. Pendry et al, IEEE Trans. Microwave Theory Tech. 47, 2075 (1999).
4. J. B. Pendry, Phys. Rev. Lett. 85, 3966 (2000).
5. For a recent review, see the articles of D. R. Smith and J. B. Pendry in *Photonic Crystals and Light Localization in the 21st Century*, ed. by C. M. Soukoulis, NATO Science Series C, vol. 563 (Kluwer, Dordrecht, 2002), p 329 and 351.
6. Dr. R. Smith, W. J. Padilla, S. Schultz, D. C. Vien and S. C. Nemat-Nasser, Phys. Rev. Lett. 84, 4184 (2000).
7. R. A. Shelby, E. R. Smith, S. C. Nemet-Nasser and S. Schultz, Appl. Phys. Lett. 78, 489 (2001).
8. R. A. Shelby, D. R. Smith and S. Schultz, Science 77, 292 (2001).
9. P. Markoš and C. M. Soukoulis, Phys Rev. B 65, 033401 (2001); ibid Phys. Rev. E 65, 03622 (2002).
10. D. R. Smith, S. Schultz, P. Markoš and C. M. Soukoulis, Phys. Rev. B 65, 195104 (2002).
11. N. García and M. Nieto-Vesperinas, Phys. Rev. Lett. 88, 207403 (2002).
12. P. M. Valanju et al., Phys. Rev. Lett. 88, 187401 (2002).
13. M. Notomi, Phys. Rev. B 62, 10696 (2000).
14. S. Foteinopoulou and C. M. Soukoulis, unpublished.
15. The choice of the sign of $n$ we have adopted here, i.e., to have $n_\alpha \geq 0$, is what one would obtain in a uniform lossless system where the definition of $n$ is $n = \frac{\sqrt{\epsilon \mu}}{c}$ if $\epsilon$ and $\mu \geq 0$ and $n = -\frac{\sqrt{\epsilon \mu}}{c}$ if $\epsilon$ and $\mu \leq 0$. Using this definition and the definition of $\alpha$ and $\mu$, one can see that $\alpha = 1 + d \ln |n|/d \ln \omega = (1/2)[1 + d \ln |\epsilon|/d \ln \omega] + (1/2)[1 + d \ln |\mu|/d \ln \omega]$ has the same sign as $n$. Notice that the $n$ is usually called phase index of refraction and is denoted by $n_p$. If we introduce the group index of refraction $|n_g| = n_\alpha$ we can write that $|\nu_g| = c/|n_g|$.
16. C. Luo, S. G. Johnson, J. D. Joannopoulos, J. B. Pendry, Phys. Rev. B 65, 201104(R) (2002).
17. K. S. Yee, IEEE Trans. Antennas Propag. AP-14, 302 (1966).
18. A. Taflove, *Computational Electrodynamics - The Finite-Difference Time-Domain Method* (Artech House, Norwood, MA 1995).
19. J. Berenger, Journal of Computational Physics 114, 185 (1994); IEEE Trans. Antenna Prop. 44, 110 (1996).
20. R. W. Ziolkowski and E. Heyman Phys. Rev. E, 64, 056625 (2001).
21. After this manuscript submitted for publication, C. Parazoli et. al. performed a time dependent calculation in a wedge geometry with a frequency dependent homogeneous negative $\epsilon$ and $\mu$. They also found a long lasting transient effect preceding the negative refraction.
22. J. B. Pendry and D. R. Smith, cond-matt/0205653.
23. D. R. Smith, unpublished.
24. W. T. Lu, J. B. Sokoloff and S. Sridhar, cond-matt/0207689.
FIG. 2. An incident em wave is propagating along a 30° direction. The time is 200 simulation steps.

FIG. 3. The magnetic field of the Gaussian beam undergoing reflection and refraction for (a) $t = 2.5t_0$, (b) $t = 4.5t_0$, (c) $t = 10.5t_0$, (d) $t = 15t_0$, and (e) $t = 31t_0$. $2t_0$ is the time difference between the outer and the inner rays to reach the interface; $t_0 \simeq 1.5T$, where $T$ is the period $2\pi/\omega$. 
FIG. 4. The magnitude of the Poynting vector for an EM wave propagating along a $30^\circ$ direction. The time is 6200 simulation steps, and is the same as the one shown in Fig. 3e.