Accurate modeling of the optical properties of left-handed media using a finite-difference time-domain method

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This paper contains an important message regarding the numerical modeling of left-handed media (LHM) using the finite-difference time-domain (FDTD) method which remains at the moment one of the main techniques used in studies of these exotic materials. It is shown that conventional implementation of the dispersive FDTD method leads to an inaccurate description of evanescent waves in the LHM. This defect can be corrected using spatial averaging at the interfaces. However, a number of results obtained using the conventional FDTD method have to be reconsidered. For instance, accurate simulation of subwavelength imaging by the finite-sized slabs of left-handed media does not reveal the cavity effect reported by Chen *et al.* [Phys. Rev. Lett. **92**, 107404 (2004)]. Hence the finite transverse dimension of LHM slabs does not have significant effects on the subwavelength image quality, contrary to previous assertions.

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The finite-difference time-domain (FDTD) method is known as one of the most powerful numerical techniques in electrodynamics [1]. Being simple in implementation it has been proved to be very popular among researchers. This method is assumed to be extremely accurate since it involves direct numerical solution of Maxwell equations which are known as the basis of classical electrodynamics. However, the implicit belief in the FDTD method sometimes results in attributing certain physical properties to some electromagnetic structures based on simulation results. One typical example is a long row of works on FDTD modeling of left-handed media (LHM), materials with negative permittivity and permeability [2]. Such materials are not yet available experimentally, and thus numerical simulations still remain one of the most common ways to explore their properties and applications. However, as will be shown in this paper, the conventional implementation of the FDTD method for modeling of LHM in the same manner as for the usual dispersive dielectric materials leads to incorrect simulation results.

It may seem that the conventional FDTD method has been verified in the literature: the negative refraction effect which is inherent to the boundary between the free space and LHM was observed, and the planar superlens behavior has been successfully demonstrated [3–5]. Actually, this only means that LHM are correctly modeled for the case of propagating waves. As soon as the evanescent waves are considered the conventional implementation of the FDTD method fails. Usually, the evanescent waves decay exponentially over the distance, and thus they are concentrated in the close vicinity of sources, which is why conventional FDTD modeling of the usual materials does not suffer from this trouble. In the case of LHM, the evanescent waves play key roles and have to be modeled accurately because of the perfect lens effect [6]. A slab of LHM effectively amplifies evanescent waves which normally decay in the usual materials and allows transmission of subwavelength details of sources to significant distances. Ideally lossless LHM slabs provide unlimited subwavelength resolution. However, in realistic situations, the resolution is restricted by losses and the thickness of the slab [7], as well as the mismatch between the LHM and its surrounding medium [8].

In order to illustrate what we mean by an incorrect description of evanescent waves provided by conventional implementation of the FDTD method, we have simulated the propagation of plane electromagnetic waves (with TM polarization and various transverse wave vectors) through an infinite slab of LHM in free space. We choose this problem since an analytical expression for the transmission coefficient through the LHM slab is available [7], which allows us to check the validity of our numerical results. The LHM slabs with relative permittivity and permeability $\varepsilon=\mu=-1-0.001j$ and thickness $d=\lambda/5$, where λ is wavelength in free space, are tested. The frequency dispersion of the LHM has been modeled by the Drude model with plasma frequency $\omega_p=\sqrt{2}\omega$ and collision frequency $\gamma=0.0005\omega$, where ω is the operating frequency. It is implemented in the FDTD method using the auxiliary differential equation (ADE) method [1]. The two-dimensional (2D) simulation domain is bounded by perfectly matched layers (PMLs) and periodical boundary conditions (PBCs) as illustrated in Fig. 1(a). A soft current sheet source (which allows scattered waves to pass through) with phase delay corresponding to different transverse wave vectors k_x placed at distance $d/2$ from the slab is used as excitation. The PBCs are also specified by the particular wave vector k_x. The source is slowly and smoothly switched to its maximum value in order to avoid exciting other frequency components [3]. The computation continues until a steady state is reached. The simulation has been done for both propagating ($k_x<k$, where k is the wave vector in free space) and evanescent ($k_x>k$) waves. Berenger's original PMLs [9] are used for absorbing propagating waves, and the modified PMLs [10] are applied when the transmission coefficient for evanescent waves is calculated. The PMLs are placed at $\lambda/2$ distance away from the slab. We use Yee's square grid with periods $\Delta x=\Delta y=\lambda/100$ and time step $\Delta t=\Delta x/\sqrt{2}c$, where c is the speed of light in free space, chosen according to the Courant stability condition [1]. Since infi-

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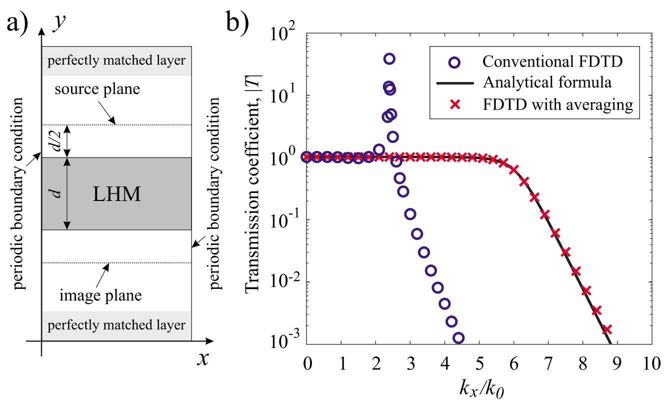

FIG. 1. (Color online) (a) The simulation domain for calculation of the transmission coefficient. (b) The comparison of transmission coefficients as functions of transverse wave vector k_x for the LHM slab with $\varepsilon=\mu=-1-0.001j$ and thickness $d=\lambda/5$, calculated using the conventional FDTD method (circles) with analytical result (solid line). The result provided by the scheme with averaging at the boundaries is given by crosses.

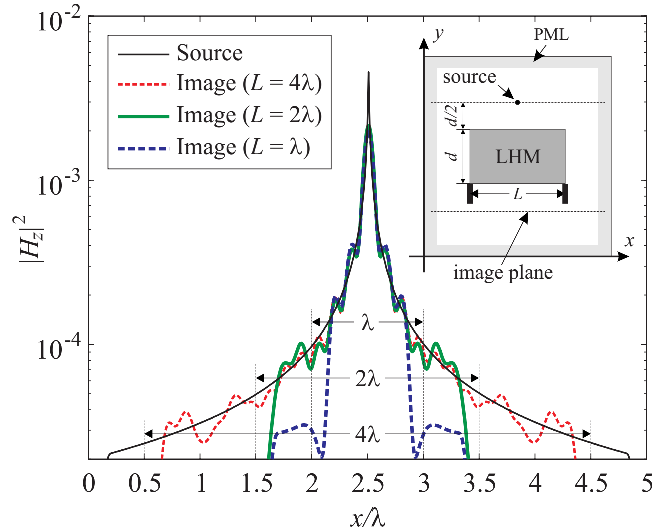

FIG. 2. (Color online) The magnetic field intensities at the image planes of the planar LHM lenses ($\varepsilon=\mu=-1-0.001j$, $d=\lambda/5$) with various transverse dimensions $L=\lambda$, 2λ, and 4λ.

nite structures can be truncated with any period, in order to save computation time, we use only four FDTD cells along the x direction.

The calculated transmission coefficient from the source plane to the image plane (located at distance $d/2$ from the other side of the slab) as a function of k_x is presented in Fig. 1(b) by circles. The reference curve calculated using the analytical expression [7] is also shown for comparison. It is clearly visible that the numerical results from the conventional FDTD method are correct only for $k_x<2k_0$. This range of k_x covers all propagating waves ($k_x<k_0$) and a small part of weakly decaying evanescent waves ($k_0<k_x<2k_0$). For the evanescent waves with $k_x>2k_0$ the numerical results dramatically differ from the analytical results and the former show resonant behavior with a strong peak at $k_x=2.4k_0$. This effect can be explained as resonant excitation of a "numerical surface plasmon" at the back interface of the LHM slab. Similar phenomena can be observed in the case of metallic slabs [6] or for unmatched LHM [8], but in this particular case it is purely numerical artifact. The incorrect behavior of numerical solutions remains similar if the FDTD grid period is reduced to $\lambda/200$ and $\lambda/400$, but the resonance shifts to $k_x=2.8k_0$ and $k_x=3.2k_0$, respectively.

The presence of numerical surface plasmons provides evidence that the boundaries between the LHM and free space have not been modeled accurately. If at the boundaries the mean value of permittivity of LHM and free space is used for updating the tangential component of electric field (which is equivalent to the spatial averaging suggested in [11]), then the spurious numerical surface plasmons disappear and the modeling happens to be extremely accurate. The transmission coefficients calculated using the proposed spatial averaging at the boundaries are presented in Fig. 1(b) by crosses. It is clear that the result repeats the estimated analytical values with very good accuracy for the whole spatial spectrum of waves. The calculation has been performed for $\Delta x=\Delta y=\lambda/100$, and it remains accurate even for larger grid periods. The above simple test allows us to conclude that the conventional FDTD method fails to describe the propagation of high-order evanescent waves in the LHM if no corrections at the boundaries of the LHM are made. As a result, a number of previously obtained results using the conventional FDTD method have to be reconsidered. This especially concerns the modeling of subwavelength imaging by LHM slabs [6] which involves operation with evanescent waves. Note that simulations where only propagating waves are involved (e.g., demonstration of negative refraction for an obliquely incident plane wave) are not affected by this problem.

The numerical transmission coefficient for LHM slabs reported in [12] is a typical example of using the FDTD method without averaging. The study can actually be treated as an investigation of the numerical surface plasmons, their sensitivity to losses, and efficiency of their excitation for various thicknesses of the slab. Unfortunately, these results have no relations with the properties of actual LHM slabs. The performance of the LHM slab as a subwavelength imaging device indeed depends on the losses and the thickness of the slab as is shown in [7], but it has a completely different dependence as compared to results reported in [12].

One of the recent most puzzling results related to the quality of imaging provided by LHM slabs is reported in [13]. It is claimed that the operation of finite-sized structures is significantly affected by their transverse dimensions. Having the FDTD code with spatial averaging at the interfaces which has been proven to be accurate, we decide to check this statement. The finite-sized slabs of LHM excited by magnetic current sources are modeled for three different transverse dimensions $L=\lambda$, 2λ, and 4λ, as illustrated by the sketch in Fig. 2. The parameters of the LHM slab ($\varepsilon=\mu=-1-0.001j$, $d=\lambda/5$) and distance between the source and the front interface equal to $d/2$ are kept the same for all simulations. The simulation domain is truncated by PMLs located at $\lambda/2$ distance away from the LHM slab and both source and image planes. The same grid periods $\Delta x=\Delta y=\lambda/100$ and time step $\Delta t=\Delta x/\sqrt{2}c$ are used as for previous plane-wave simulations. The source is switched slowly and smoothly in order to avoid contributions from undesired frequency components [3], and the simulations last until a steady state is reached. The intensity distributions in the image planes for all three cases of different transverse dimensions are plotted in Fig. 2. It is clear that the image quality is practically unaffected by the transverse size of the slab. The distributions repeat the source distribution, which is plotted in the same figure, with good subwavelength resolution. We do not observe any distortion of images caused by the finiteness of the transmission device, in contrast to the conclusions made in [13]. The slight disagreement between the image and the source is due to the finite resolution of lenses caused by the losses in LHM. We suppose that the resonant effects and image distortions related to transverse dimensions reported in [13] can be interpreted as excitation of "numerical surface plasmons" at the interfaces of the slab and can be observed only in inaccurate FDTD simulations without spatial averaging at the boundaries. Thus, these effects are purely numerical and have no relation to the properties of actual LHM slabs. In reality, the imaging performance of finite-sized LHM slabs is unaffected by their transverse dimensions. This statement also has been confirmed by full-wave electromagnetic simulation using the Ansoft HFSS package.

In order to illustrate this statement we have performed the simulation for a LHM slab with transverse size $L=\lambda$ excited by two magnetic line sources placed at $\lambda/8$ distance between each other using the FDTD method with spatial averaging at the boundaries. The rest of the parameters are the same as before. The distance between the sources is larger than the resolution of the lens which should be better than $\lambda/12$ based on the fact that the transfer function plotted in Fig. 1 is close to unity for $k_x/k<6$. This allows us to expect two well-resolved maxima in the image plane. The distribution of magnetic field intensity in a subdomain near the LHM slab (the actual FDTD domain is larger) in the steady state is presented in Fig. 3(a). The distribution in the image plane is shown in Fig. 3(c) together with the source. Two maxima at a distance of $\lambda/8$ are clearly visible in the image plane. This confirms the subwavelength imaging capability of the LHM lens with only one wavelength width. Thus, we do not observe any limitations on the functionality of the LHM slabs as subwavelength imaging devices due to their finite transverse dimensions. However, if the same system is modeled by the FDTD method without corrections at the boundaries, then a completely different distribution of the field around the slab is observed; see Fig. 3(b). The distribution of the field along the slab interface is smooth which once again confirms that high-order evanescent waves are not correctly modeled. As a result, the subwavelength details of the source are not resolved in the image plane. Instead of the expected two closely located maxima, the intensity distribution in the image plane has only one wide maximum; see Fig. 3(c).

We suppose that the comparison presented between FDTD models with and without spatial averaging at the boundaries clearly demonstrates the limitation of the conventional FDTD method for modeling LHM lenses. The significant discrepancies appear only in the cases when evanescent waves are involved. However, we encourage the use of the

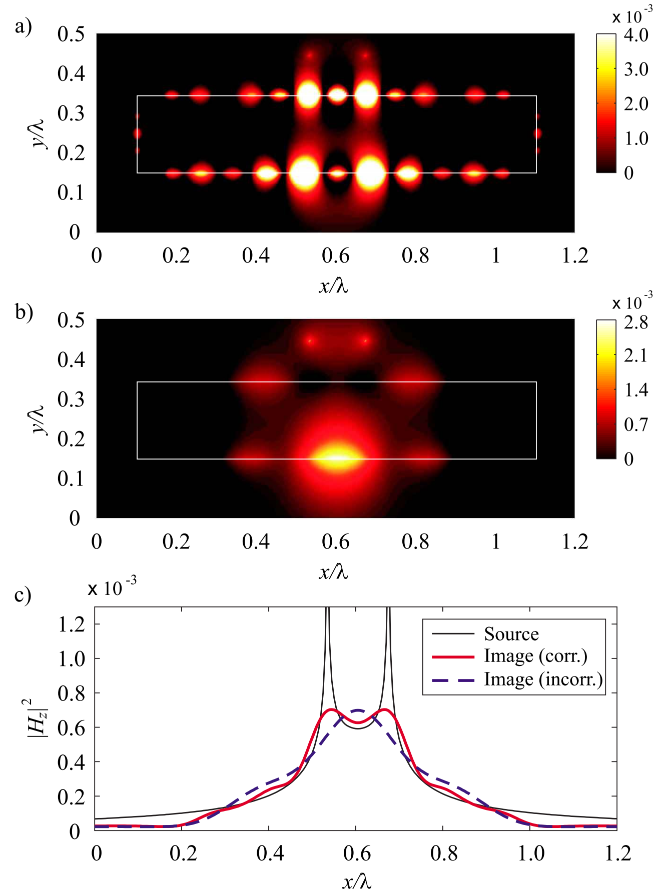

FIG. 3. (Color online) The magnetic field intensity distributions around the LHM slab with transverse size $L=\lambda$ excited by two magnetic line sources placed at $\lambda/8$ distance between each other obtained using the FDTD method (a) with and (b) without spatial averaging. (c) The image and source plane cuts.

model with corrected updating equations at the boundaries (with spatial averaging of permittivity as we propose or with averaging of the current as proposed in [11] which are equivalent) in all cases in order to avoid numerical artifacts. The spatial averaging is known as a second-order correction in the case of boundaries between dielectrics with positive permittivity [14], but in the case of evanescent waves in LHM it transforms into an essential and mandatory correction.

In addition to the corrections at the boundaries we would like to stress a few other aspects which are important to accurate FDTD modeling of LHM. The numerical dispersion is usually assumed to have very little influence on the quality of FDTD simulations. However, the properties of LHM are known to be extremely sensitive to minor changes of material parameters. A typical example is the degradation of resolution due to small variations of material parameters from $\varepsilon=\mu=-1$ [7,8]. This means that even a tiny amount of numerical dispersion may cause a crucial discrepancy between simulated and theoretical results. Fortunately, the numerical dispersion can be easily analyzed analytically and an estimation for the difference between effective numerical material parameters and the "real" ones is known [11]. This allows one to adjust the parameters of the FDTD simulation to ensure that the effective numerical material parameters correspond to the required values. We suggest using this adjustment in the cases of large time steps and small losses.

It is well known that the switching time considerably influences the oscillation of images created by LHM lenses. The switching time equal to 30 periods was used in [5,12]. However, perhaps this is the reason why no stable images could be obtained in [3,12]. Recently, it was reported in [15] that a switching time equal to 100 periods is required to obtain stable images. We have used such a switching time in all our simulations, and we recommend that attention be paid to the issue of switching time in all FDTD simulations of LHMs. The high-order evanescent waves travel very slowly in the LHM slabs, and the procedure of the amplification of evanescent waves requires a very long time to reach a steady state. That is why, in addition to smooth and slow switching of the source, we recommend to add losses into the simulations in order to limit the spatial spectrum of evanescent waves which are involved in operation. Otherwise, in the lossless case the transient processes may last extremely long.

The diffraction on the wedges and corners also may provide certain problems because of the singularity effects reported in [16]. However, in the case of LHM with $\varepsilon=\mu \approx -1$ the singular behavior disappears and the wedges operate mainly as retroreflectors [17]. That is why, in the simulations presented in this paper, we have not observed any singularities at the wedges.

In conclusion, we have demonstrated that the conventional FDTD method for modeling of LHM leads to an inaccurate description of high-order evanescent waves and does not simulate subwavelength imaging correctly. The simulations suffer from the artifact of "numerical surface plasmons" which appear at the interfaces of LHM. In order to solve this problem and ensure accurate FDTD modeling, a spatial averaging scheme at the boundaries has been proposed in the same manner as in [11]. This technique has been tested on the analytically solvable example of a plane-wave propagation through an infinite LHM slab, and extremely good accuracy of the simulation has been revealed for all angles of incidence including high-order evanescent waves. The finite-sized slabs of LHM excited by a single line source have been modeled using the proposed technique for various transverse dimensions of the slab, and the subwavelength imaging capability of the structures has been confirmed. No distortions of the image due to the finite transverse dimensions of the structure have been revealed, in contrast to the results reported in [13]. We suspect that resonant effects due to the finite transverse dimensions of the LHM slab reported in [13] are caused by excitation of the numerical surface plasmons and are completely numerical. These effects are absent in real structures, and there are no restrictions on the functionality of LHM subwavelength lenses due to their transverse dimensions. Our FDTD simulations with spatial averaging at the boundaries demonstrate the imaging of two line sources located at subwavelength distance between each other by a LHM slab with only a one-wavelength width. Keeping in mind that simulations using the FDTD method remain one of the most popular approaches in the studies of LHM, general recommendations as to how to accurately model LHM using the FDTD method are also provided.

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