Modelling and theory involving metamaterial photonic structures

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ABSTRACT

The literature is alive with papers devoted to the design of metamaterials and there appears to be a particular desire to create photonic applications that will operate at THz frequencies and above. At one level the modelling of suitable artificial molecules is straightforward but nevertheless the approximations involved need to be able to inspire confidence for optical frequency operation. This presentation will set out a modelling activity that is known to be satisfactory only over certain frequency ranges. Split-ring and omega particles will be specifically investigated and the possibilities discovered will be related to the current experimental expertise. The detailed manner in which the constitutive relations can be controlled and the novel way in which an envelope equation emerges for even the most complex structure is exposed. The transmission and reflection properties of nano-structured materials will be discussed within a magneto-optic environment. Simulations of sub-wavelength transmission through holes in metallic and magneto-optic screens will be discussed using finite-difference time-domain (FDTD) methods. Modelling the interaction of light beams with metamaterials is developed, again using FDTD techniques, and it is shown that special care needs to be taken with structures that have sharp external edges. Finally, a summary of the problems surrounding efficient computations will be shown and some discussion of the role of genetic algorithms in metamaterial design will be featured.

Keywords: LHM, left-handed, FDTD, split-ring, negative phase, metamaterials, modelling, end-fire

1. INTRODUCTION

Quite a lot of emphasis has been placed in the literature upon modeling metamterials in terms of equivalent circuits[1]. This is a very useful tool and leads to manageable forms for the relative permittivity and the relative permeability. Sometimes there is a desire to add only magnetic properties and hence rely upon a manipulation of the so-called magnetic resonance but usually the interest centres upon the double resonances associated with simultaneous negativity of the relative permittivity and permeability. The latter is often labelled as being a property of so-called left-handed materials[2, 3] but which could be more sensibly labelled as negative phase velocity media[4, 5](NPM), especially in isotropic cases. In this paper an examination of how an equivalent circuit can be modelled to give negative electric and magnetic properties within the constitutive relationships will be presented and some comments about homogenisation will also be given. It is interesting to note how powerful the equivalent circuit model is and the extent to which its predictions are borne out by detailed finite difference time domain (FDTD) calculations[6, 7]. It is also shown that it is possible to add active elements and still make progress towards outcomes that introduce gain and hence spearhead some kind of progress towards the elimination or at least substantial control of the losses that appear to be so troublesome when attempting to create even minor applications of this type of metamaterial.

It is important to extend the study of equivalent circuits, through the homogenisation stage and finally to reach a way of studying wave propagation in a number of scenarios[8, 9]. First of all, some fundamental manipulation of the homogenised

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equations can be used in a rather special way to achieve an important envelope equation. The method of attack demonstrated here has been given the name "Lorentz Lemma"[10]. It is a powerful approach that enables nonlinearity and other effects to be included but it will be restricted here to the important but limited layered structures that could form an application.

Naturally, many lessons can be learned from the microwave range of frequencies[11, 12] but the general global pressure is to push forward to the high THz and optical spectra[13]. As the optical range is embraced the use of equivalent circuit models becomes very limited or impossible because it is always important to bear in mind that the structures that constitute the artificial meta-particles need to be rather less in size than the wavelength. Hence an experiment involving split-rings could operate at a wavelength of 1.5 μm = 1500 nm then the rings should be the order of at most 200 nm. If the visible part of the optical range is to be accessible then some other form of nano-structure[14, 15] may well be needed and a plasmonic explanation of the dielectric behaviour is required[16, 17]. Nano-structures are going to be of increasing importance in magneto-optics with the main emphasis being on improving the optical Kerr effect[18-20]. The latter is the basis of data storage and a revolution in this area can be expected, especially if some use of metamaterials is made.

In this connection it may well be the case that sub-wavelength effects can be deployed. Some basic ideas of how to model sub-wavelength[21, 22] effects and relate them to useful nano-structures will be part of this presentation. It is an important area that utilises surface polaritons in a rather special way to increase transmissions in an unexpected direction. Finally, this discussion of modelling should mention a possibility of using genetic algorithms and a simple outline example will be given.

2. SPLIT-RINGS, OMEGA PARTICLES AND "LORENTZ LEMMA"

Figures 1 and 2 illustrate nicely how meta-particles in the form of split-rings or omegas can be represented by an equivalent circuit. Indeed, in the case of the omega particle we have indicated how a diode can be included but of course this can also be done for the split-ring. It is now possible to analyse the circuits and to arrive at a form of homogenised constitutive equations. Because of its importance, this paper opts for an exposure of a derivation of nonlinear evolution equations in layered structures that include bi-anisotropic metamaterials. Generality is sustained by accounting for possible nonlinearities on the interfaces between the layers. The analysis leads to a familiar form of the homogenised constitutive equations[23]

$$\mathbf{D} = \boldsymbol{\varepsilon}_{eff} \bullet \mathbf{E} + \boldsymbol{\alpha}_{eff} \bullet \mathbf{H} + \mathbf{P}_{NL} \tag{1}$$

$$\mathbf{B} = \boldsymbol{\beta}_{eff} \bullet \mathbf{E} + \boldsymbol{\mu}_{eff} \bullet \mathbf{H} + \mathbf{M}_{NL} \tag{2}$$

in which the tensors $\boldsymbol{\varepsilon}_{eff}$, $\boldsymbol{\alpha}_{eff}$, $\boldsymbol{\beta}_{eff}$, $\boldsymbol{\mu}_{eff}$ are linear, and $\mathbf{P}_{NL}$, $\mathbf{M}_{NL}$ are nonlinear electric and magnetic polarisations.

To be specific, consider a bi-anisotropic plane layer, perpendicular to the z axis and of width d, where $-d/2 < z < d/2$ and the half-space $z < -d/2$ and $z > d/2$may be linear or nonlinear and also gyrotropic. Suppose that the nonlinear field is

$$\begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = A(t,\mathbf{r}) \begin{pmatrix} \mathbf{E}_L \\ \mathbf{H}_L \end{pmatrix} = A(t,\mathbf{r}) \begin{pmatrix} \mathbf{f}_E \\ \mathbf{f}_H \end{pmatrix} \exp\left(j\left[\omega t - \mathbf{k} \bullet \mathbf{r} \right] \right) \tag{3}$$

where A is a slowly varying amplitude, $\mathbf{k}$ is a wave vector and ω is an angular frequency. $\mathbf{f}_{E,\ H}$ could be called "polarisation functions" and describe the dependence of the linear fields in the z direction. They are obtained using the linear boundary conditions, taken into account the appropriate linear dispersion. In fact, $\mathbf{E}_L$ and $\mathbf{H}_L$ remain linear and unchanged in shape by the nonlinearity. The next step is to formulate the **linear** (dyadic) tensors as

$$\boldsymbol{\varepsilon}_{eff} = \boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}_{act}\,,\ \boldsymbol{\mu}_{eff} = \boldsymbol{\mu} + \boldsymbol{\mu}_{act}\,,\ |\,\boldsymbol{\varepsilon}\,|>>|\,\boldsymbol{\varepsilon}_{act}\,|\,,\ \ |\,\boldsymbol{\mu}\,|>>|\,\boldsymbol{\mu}_{act}\,| \tag{4}$$

$$\boldsymbol{\alpha}_{eff} = \boldsymbol{\alpha} + \boldsymbol{\alpha}_{act}\,,\ \boldsymbol{\beta}_{eff} = \boldsymbol{\beta} + \boldsymbol{\beta}_{act}\,,\ |\,\boldsymbol{\alpha}\,|>>\left|\boldsymbol{\alpha}_{act}\right|,\ \ \left|\boldsymbol{\beta}\right|>>\left|\boldsymbol{\beta}_{act}\right| \tag{5}$$

in which the values with the subscript “act” are created by the presence of active elements. In addition, the values $\boldsymbol{\varepsilon}$, $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\mu}$ have properties consistent with energy conservation. Suppose also that the nonlinear electric and magnetic polarisations $\mathbf{P}_{NL}$, $\mathbf{M}_{NL}$ have a form that is known. Given this starting point, one objective is to get a differential formulation for the nonlinear amplitude A, or a system of equations for parametric interactions. This is quite a complex algebraic business but another objective is to express the evolution in integral form. The method depends on taking the linear result and the nonlinear result and then combining in a Lorentz manner to give for a layered structure without spatial dispersion a general yet powerful integral form in which possible nonlinearities on the boundaries are taken into account. They can be caused by inclusions that could be special (real or imaginary) loads in the artificial molecules in the surface layers. The boundary conditions lead to

$$\begin{aligned}&\frac{\partial A}{\partial t} + \left[V_g \frac{\partial}{\partial y} + \frac{j}{2}\frac{\partial^2 \omega}{\partial k_y^2}\frac{\partial^2}{\partial y^2}\right]A + j\omega\frac{Q}{W_0}A = \\ &\quad -\frac{1}{W_0}\int_{-\infty}^{\infty}\left(\mathbf{H}_L^{*}\bullet\frac{\partial \mathbf{P}_{NL}}{\partial t} + \mathbf{E}_L^{*}\bullet\frac{\partial \mathbf{M}_{NL}}{\partial t}\right)dz - \sum_{n=1,2}\left[E_{Lx}^{*} i_x^{(e)} + E_{Ly}^{*} i_y^{(e)} + H_{Ly}^{*} i_y^{(m)} + H_{Lx}^{*} i_x^{(m)}\right]_{z=z_{0n}}\end{aligned} \tag{6}$$

where $i_{x,y}^{(e,m)}$ are nonlinear electric and magnetic surface currents evaluated at $z = \pm\, d\,/\,2$, z_{0n} are defined as the locations of the interfaces, k_y is the y-component of the wave vector and V_g is the group velocity.

$$W_0 = \int_{-\infty}^{\infty}\left(\mathbf{f}_H^{*}\frac{\partial}{\partial\omega}(\omega\boldsymbol{\mu})\mathbf{f}_H + \mathbf{f}_E^{*}\frac{\partial}{\partial\omega}(\omega\boldsymbol{\varepsilon})\mathbf{f}_E + \mathbf{f}_H^{*}\frac{\partial}{\partial\omega}(\omega\boldsymbol{\alpha}^{+})\mathbf{f}_E + \mathbf{f}_E^{*}\frac{\partial}{\partial\omega}(\omega\boldsymbol{\alpha})\mathbf{f}_H\right)dz \tag{7}$$

$$Q = \int_{-\infty}^{\infty}\left\{\begin{aligned}&\left[\mathbf{f}_H^{*}\bullet\left(\boldsymbol{\mu}_{act}\bullet\mathbf{f}_H\right) - \mathbf{f}_H\bullet\left(\boldsymbol{\mu}_{act}^{*}\bullet\mathbf{f}_H^{*}\right)\right] + \left[\mathbf{f}_E^{*}\bullet\left(\boldsymbol{\varepsilon}_{act}\bullet\mathbf{f}_E\right) - \mathbf{f}_E\bullet\left(\boldsymbol{\varepsilon}_{act}^{*}\bullet\mathbf{f}_E^{*}\right)\right] \\ &\quad + \left[\mathbf{f}_E^{*}\bullet\left(\boldsymbol{\alpha}_{act}\bullet\mathbf{f}_H\right) - \mathbf{f}_H\bullet\left(\boldsymbol{\beta}_{act}^{*}\bullet\mathbf{f}_E^{*}\right)\right] + \left[\mathbf{f}_H^{*}\bullet\left(\boldsymbol{\beta}_{act}\bullet\mathbf{f}_E\right) - \mathbf{f}_E\bullet\left(\boldsymbol{\alpha}_{act}^{*}\bullet\mathbf{f}_H^{*}\right)\right]\end{aligned}\right\}dz \tag{8}$$

The physical senses of the terms on the left-hand side of (6) include self-evident terms and a final term describing possible losses or gains. The first and second terms in the right-hand side describe volume and surface nonlinearity respectively.

In (6), volume nonlinearity is included in a very general form. It is easy to show that in particular cases second-harmonic generation is possible. Surface nonlinearity is taken into account in a rather natural way as demonstrated by the second term in the right-hand side. Linear losses or a possibility of enhancement can be addressed with diodes having real negative impedances. Negative losses need the presence of a d.c. bias electric field and would be important in the case of a near-resonance regime with increased losses, to compensate them. The method is a part of more general approach dealing with wave propagation in layered structures.

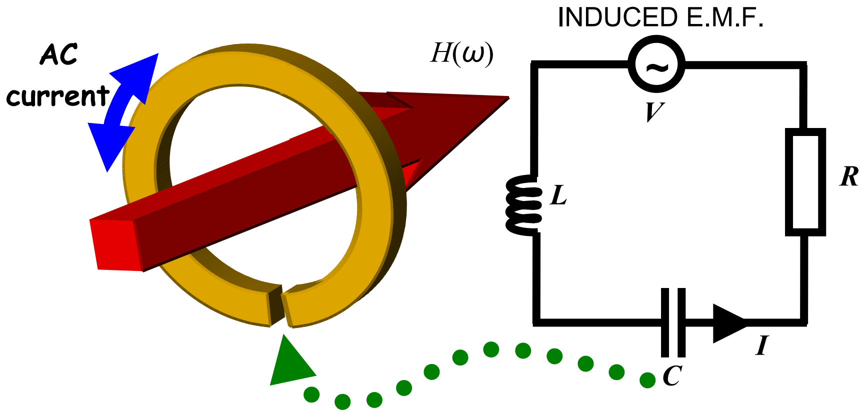

Figure 1: Split-ring equivalent circuit

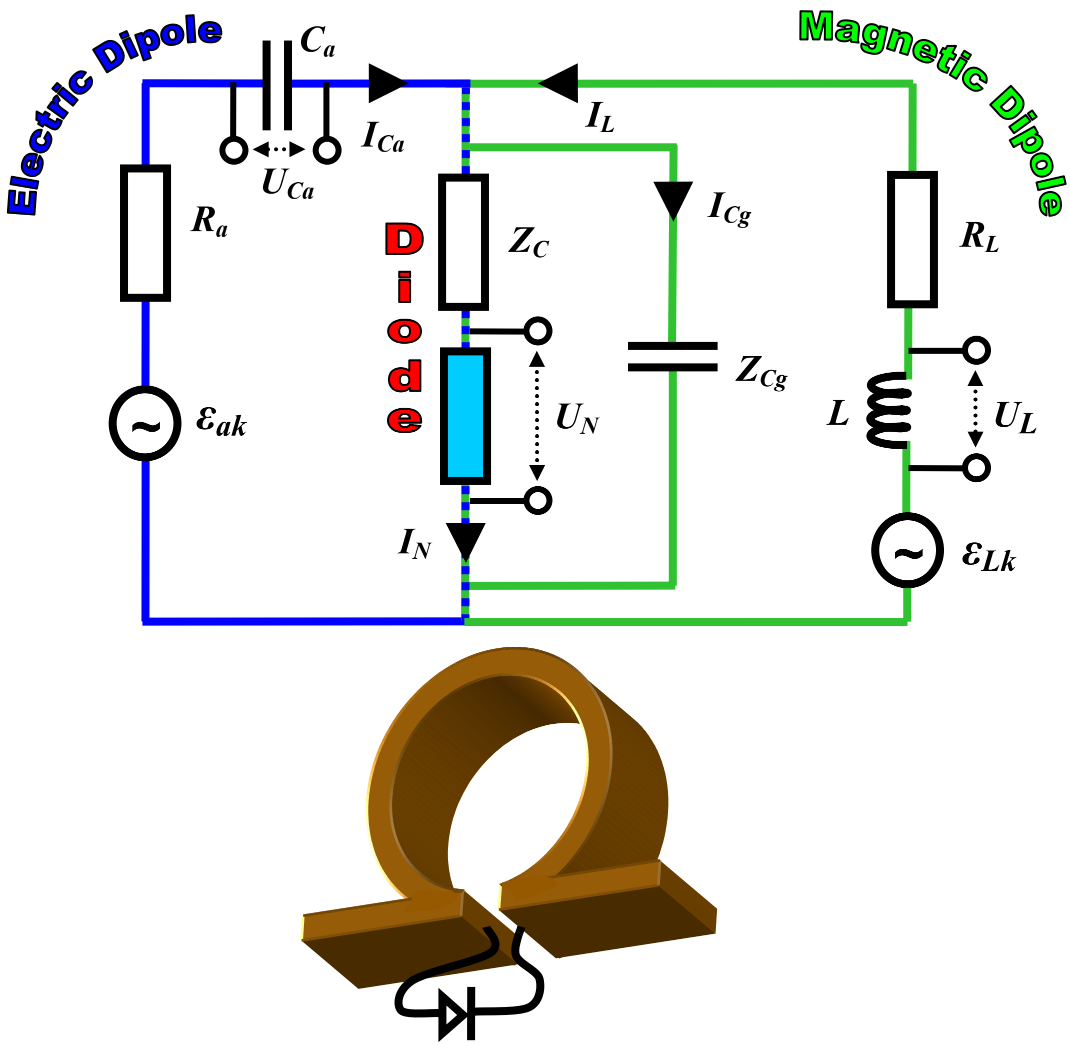

Figure 2: Omega particle equivalent circuit

3. INTERACTION WITH METALLIC AND MAGNETO-OPTIC NANO-STRUCTURES

The insight of Faraday in what is now known as magnetooptics is a wonderful example of how to anticipate new developments beyond anything that could be imagined in his time. In fact Disraeli, who was Prime Minister at the time, attended a famous exhibition and was introduced to Faraday. He asked Faraday what possible use could be made this thing called electricity. Faraday quickly responded by saying "One day, sir, you may be able to tax it." This exchange is a perfect example of how not to be too pessimistic when thinking of developments that can be built upon any current platform of research activity. It is true that pessimism has been displayed with respect to using magnetooptic effects and yet magnetooptic disks are widely used in computer technology and the advent of nano-structures seems set to create data storage capacity beyond our wildest dreams[24]. The Faraday effect is the name given to the nonreciprocal behaviour of light when propagating parallel, or antiparallel, to an applied magnetic field[25]. This effect puts us into intimate contact with the vectorial nature of light, which is manifested physically as a polarisation rotation. Another well-known magnetooptic effect that can be added to this is the Voigt or Cotton-Mouton effect[18]: also named after the co-discoverers. It occurs when the wave propagation is perpendicular to an applied field and in the bulk it is entirely reciprocal. It is the Kerr effect, however, that is the tool needed to create data storage devices. In its simple form, the Kerr effect is just the rotation of the polarisation plane of an incident light beam by a magnetised material that is in an orientation often called polar, as shown in figure 3.

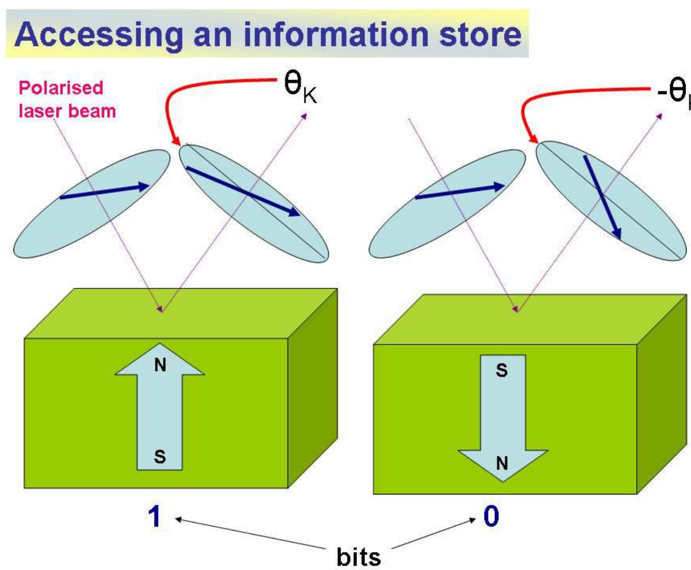

Figure 3: Elementary magnetooptic storage. θ_K is the Kerr rotation

Here, the basic idea of data storage is also shown in which the magnetisation is perpendicular to the reflecting surface and the N-S orientations can arbitrarily labelled as "1" or "0". Hence, a measurement of the Kerr effect captures very elegantly a digitised set of data if, for example, a magnetooptic computer disk can be constructed as a set of such domains. It is not appropriate here to consider the technical construction of a computer disk because the aim now is to comment upon the quality of the θ_K captured by a laser interrogation of a set of "1" or "0" domains. The bad news is that the quality of θ_K is low unless steps are taken to increase its value, enhance the associated reflectivity resonance and to increase the packing density of the domains. The enhancements take us into the nano-domain and one of the first things that can be done is to coat the reflecting surface with a Fabry-Perot cell of strategically selected nm layers. Figure 4 shows an experimental set-up known as attenuated total reflection (ATR) designed to investigate enhancement of the Kerr effect from a cobalt layer using specially selected nano-scale attached layers[21, 26]. The aim is to promote better resonant behaviour by exploiting surface polariton generation and to make a compromise between the advantages of extra resonance quality and possibility of extra loss that is certain to be associated with the reflectivity minimum.

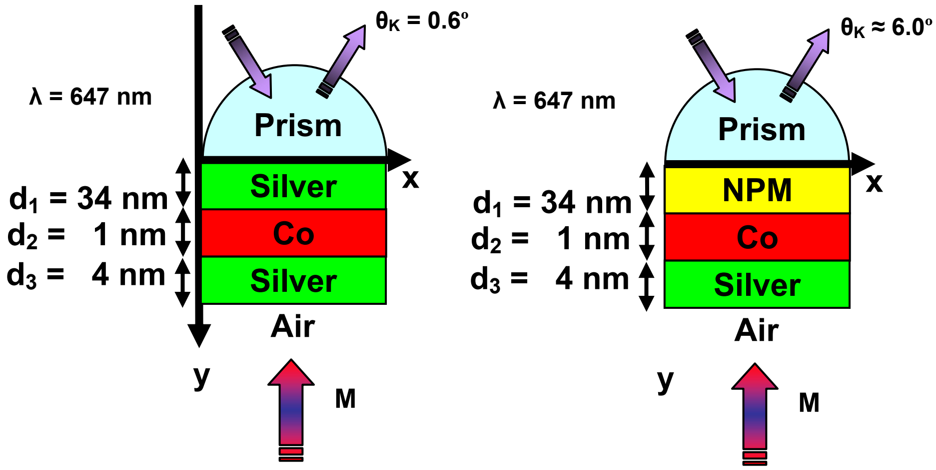

Figure 4: Enhancing the Kerr effect

Figure 4 shows an example of how to enhance the Kerr effect. In fact, it shows that a disposition of silver layers does lead to an enhancement but replacing one of the silver layers with a metamaterial exhibiting negative phase behaviour leads to a dramatic improvement. Naturally using negative phase media in the optical range would require the use of an interesting nano-structure and the physical explanation of negative relative permittivity and permeability requires a plasmonic model and would not be described in terms of split-rings or omega particles. The whole question of data storage of this kind is developing however and nano-structures are being examined for their capacity to store a massive amount of data. As figure 5 shows, it is possible to create a set of nano-wires that can be magnetised and packed together and the state of magnetisation of each column can be read in terms of the Kerr effect by scanning a laser beam over it[27]. As is always the case the quality of the Kerr rotation needs to be enhanced and some work is going on to add a Fabry-Perot set of layers to each column to achieve this enhancement. Clearly, the same principle that was applied above can be invoked and that the nano-columns can be coated with metamaterials to achieve even higher Kerr rotations. This topic is still very much under review.

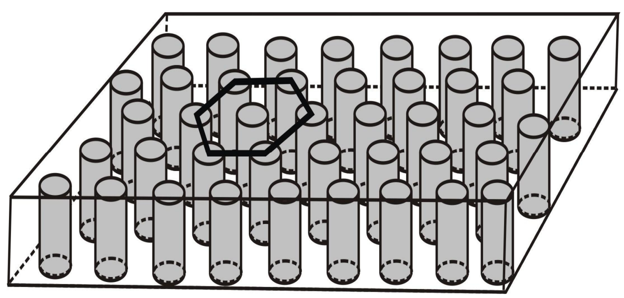

Figure 5: A nano-structure in which the columns are magnetised parallel or antiparallel to the cylinder axes. In this way the data packing density is high. Figure after ref [27].

Increasing the efficiency of the read out process means a suitable manipulation of the interrogating laser beam. It is quite possible that using sub-wavelength behaviour can lead to a substantially improved read out. One possibility is to use nano-structure screens punctuated with sub-wavelength holes to guarantee distortion free illumination and to reduce the overall laser intensity needed in the scanning beam. The whole area of sub-wavelength behaviour is still developing and the use of specialised holes to give the laser beam access is a fascinating possibility. In general, the connection between sub-wavelength behaviour and complex nano-structured materials is a very important one and is likely to lead to many applications.

4. LIGHT INTERACTING WITH METAMATERIALS: LAUNCHING SURFACE WAVES USING AN END-FIRE CONFIGURATION

An end-fire configuration is a special name that is given to a situation of the kind that is displayed in figure 6. This is an interesting possibility because the incoming beam encounters an interface between two half-spaces. In principle this interface can sustain surface waves but the question that arises is whether configuring the excitation beam in this way can actually create the surface wave that is desired. The terminology "end-fire" has been used in the past and it is clearly important for integrated optical applications. Upon examination of figure 6 it is apparent that there are two interfaces one being perpendicular to the excitation beam direction and another being parallel. The question that immediately arises is whether the parallel interface will carry surface polaritons and to what extent is this possibility influenced by the presence of a metamaterial. If operation is required in the high THz optical range the metamaterial will appear to the exciting beam as an homogenised nano-structure.

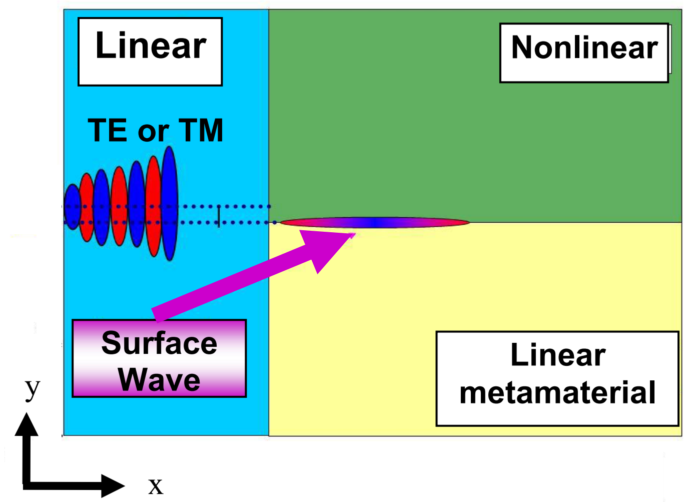

Figure 6: An end-fire configuration.

An end-fire configuration does not need a phase-matched condition, as is the case in ATR configurations. Instead, the end-fire system matches the incident beam intensity to the intensity of the surface polariton[28]. Consequently, it could be important to have a transmission coefficient of approximately unity across the vertical interface. Enough energy must be launched to form the surface wave and also the possible scattered waves from the corner must be a lot smaller than the transmitted ones. This will minimise the impact of encountering a sharp corner and hold out some promise for applications.

In this paper the treatment of the end-fire problem is purely numerical using the FDTD method. The computational area is divided into the kind of cells that are the heartbeat of the FDTD method. There is however a problem associated with the corner that is located where the horizontal interface intersects the vertical. Figure 7 shows a blown up picture of the corner area in which one of the cells intimately associated with the corner is shown in a grey shaded format. Clearly there is another cell associated with the corner as well. A discussion of what effect the corner can have on the modelling outcomes can proceed as shown in figure 7 by considering the permittivities associated with the cells surrounding the selected grey cell. The other selection of corner cell would change the environment.

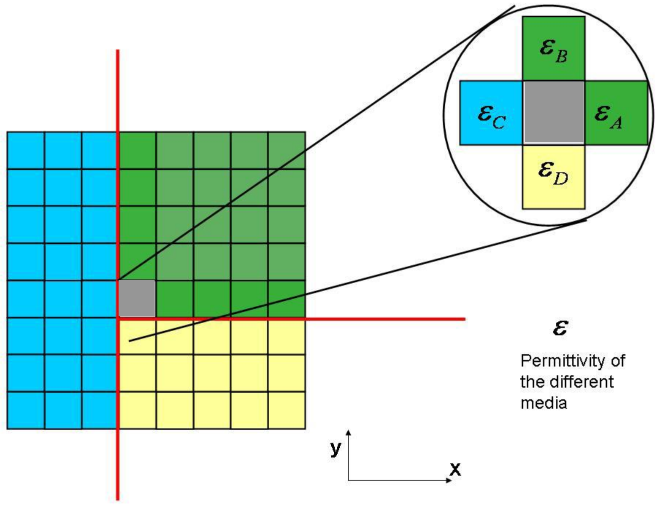

Figure 7: Enhanced view of the neighbourhood of the corner in the end-fire configuration. The different colours signify the different permittivities.

The launching of beams into corners is a difficult problem that has been treated elsewhere[29, 30]. A corner is defined, with reference to figure 7, as a cell that does not satisfy, the conditions

$$\varepsilon_A + \varepsilon_D - \varepsilon_B - \varepsilon_C = 0 \tag{9}$$

$$\varepsilon_A \varepsilon_B - \varepsilon_D \varepsilon_C = 0 \tag{10}$$

where $\varepsilon_A, \varepsilon_B, \varepsilon_D, \varepsilon_C$ are the permittivity values in each material. Obviously if a metamaterial is used there must be similar conditions for the relative permeability. Basically, (9) and (10) do not meet this requirement. Hadley[29], has pointed out that, when a corner arises, the finite difference formulation has to be altered to include the errors caused by the corner; the potential errors here are related to the possibility of having unphysical harmonic radiation "sources" at the corner. Consequently, the convergence will be achieved very slowly, or not achieved at all. However, numerical errors produced by corners are generally of second-order on the grid size. Hence, it seems that, by having a much finer mesh, the errors could be diluted. This is a reasonable strategy when no highly accurate solutions are sought. Perhaps, a sub-gridding technique[31] could also be implemented into the code, forcing the resolution near the corner to be extremely high. This would make the area of trouble (the corner), almost an infinitesimal point. The sub-gridding technique will also make the FDTD code more efficient.

Figure 8 shows a full FDTD simulation in which surface waves are launched by end-fire coupling onto the interface between a nonlinear medium and a metamaterial. Technically, these can be called surface solitons.

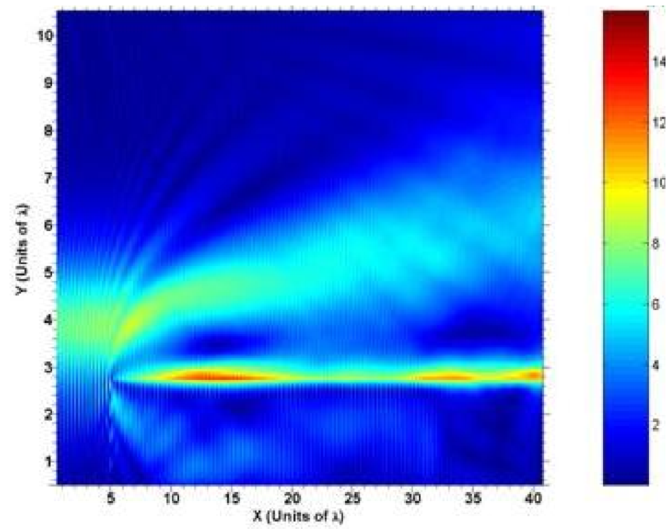

Figure 8: Formation of a surface wave at the interface of a nonlinear material and a LHM. Number of sample points per wavelength is 100.

5. CONCLUSIONS

This paper covers a number of modelling possibilities associated with the presence of metamaterials in reflection and guiding systems. The implication of the discussion is always to point towards the high THz or optical ranges and hence an implied scaling is assumed. The discussions begin with equivalent circuits with the objective of creating a formalism to deal with envelope propagation. This formalism is given the technical name “Lorentz Lemma” because of the similarities built into the derivation and the often quoted Lorentz Lemma in electromagnetic theory. A lot of effort has been put in to make sure that the formulism can be generalised to include active devices although the numerical examples have been left for another occasion. As progress towards the optical proceeds there is always going to be a meeting between the properties of metamaterials and the deployment of nano-structures. This is nevermore evident than in the data storage area that relies on magnetooptics. The latter deploys the Kerr effect and this has been discussed quite thoroughly with some dramatic examples of how nano-structures and metamaterials can combine to enhance the observed Kerr rotations that are so important for data storage. The paper has a final section on what has been called “end-fire” coupling and some discussion of how the FDTD method can be deployed to create special kinds of surface waves is presented. It is realised that in a paper of this kind it is not possible to cover all the areas but we hope that the selection is interesting and that the promise held out by sub-wavelength applications will become apparent in the near future.

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