Proceedings of the Second IASTED International Conference
ANTENNAS, RADAR, AND WAVE PROPAGATION
July 19-21, 2005, Banff, Alberta, Canada

MAGNETISM AND EFFECTIVE ELECTROMAGNETIC PARAMETERS FROM DIELECTRIC SPHERES

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ABSTRACT
The effective electric and magnetic properties are found for a material composed of non-magnetic spheres. These parameters are found in the long-wavelength limit as a function of the frequency, composition, size, and volume density of the spheres. A fundamental resonant magnetic response is found when polaritonic materials are used. The effective media parameters are verified by band structure calculations. Frequency ranges with negative permeability and negative group velocities are found. This simple composite extends magnetic materials into the infrared regime.

KEY WORDS
Metamaterials, magnetism, Mie scattering, polaritonic materials, negative permeability, negative group velocity.

1 Introduction

The recent interest in metamaterials has stimulated many studies on how to design particular electromagnetic responses of composite materials by altering the geometry of their constituent elements. The most notable and surprising metamaterials that have been discovered include those with negative permittivity [1] or negative permeability [2] in the GHz range, and negative index materials [3], which are a composite of the former two. However, such metamaterials are attractive in the GHz regime, where they are easy to fabricate and the material losses are minimal.

Another method of creating a negative effective index material is based on the use of photonic crystals [4, 5]. In these structure, the inherent Bragg scattering can be made to produce an effective negative angle of refraction which is governed by Snell's Law. These devices are more likely suitable for optical frequencies. Unfortunately, since the scattering effect requires a device geometry on the order of a wavelength, some possible applications, such as phase compensation, would not necessarily be more compact.

The magnetic response created by the split-ring resonators reported in Ref. [2] is not very practical for optical frequencies. Other reports of two-dimensional magnetic response in dielectric materials have been made, notably in the GHz range using ferroelectrics [6], and in the infrared range using polaritonic crystals [7].

This paper considers the electromagnetic scattering from three-dimensional arrays of non-magnetic spheres as a method for producing a magnetic and an electric response in the infrared regime. It is shown in Section 2 that a collection of non-magnetic spheres subject to an incident field can be considered equivalent to a collection of resonantly excited dipoles of electric and magnetic type. This equivalence, when in the long-wavelength limit, leads to a definition of an effective permittivity and permeability for the composite. Section 3 presents band structure calculations for a simple cubic lattice of the aforementioned (polaritonic) spheres which confirm the theory.

2 Effective material parameters

The effective permeability of a collection of spheres with an arbitrary material dispersion will now be derived. A dual derivation gives the effective permittivity. The interested reader will find the necessary background information on scattering by dielectric spheres in Ref. [8].

To begin, consider a plane wave with wavenumber $k = \omega/c$ incident on a single isolated sphere with relative dielectric permittivity $\epsilon_r = n_1^2$. The radius of the sphere is r_0. Let $m = n_1/n_0$, where n_0 is the index of the surrounding medium, which is assumed to be free space for the remainder of this work. Let the incident plane wave have a magnetic field

$$\mathbf{H}_i = H_0 e^{ikz}\hat{\mathbf{y}}, \qquad (1)$$

where a time dependence of $\exp(-i\omega t)$ is assumed. The 2^n-th multipole term of the scattered field is proportional to the Mie scattering coefficients [8]

$$a_n = \frac{m\psi_n(mx)\psi_n'(x) - \psi_n(x)\psi_n'(mx)}{m\psi_n(mx)\xi_n'(x) - \xi_n(x)\psi_n'(mx)}, \qquad (2)$$

$$b_n = \frac{\psi_n(mx)\psi_n'(x) - m\psi_n(x)\psi_n'(mx)}{\psi_n(mx)\xi_n'(x) - m\xi_n(x)\psi_n'(mx)}, \qquad (3)$$

where $x = kr_0$ and $\psi_n(x)$, $\xi_n(x)$ are the Riccati-Bessel functions. In particular, the a_1 term represents the strength of the electric dipole response, and b_1 represents the strength of the magnetic dipole response.

It is now assumed that the frequency and sphere permittivity are chosen such that the magnetic dipole response of the sphere is excited, and it is dominant over all other multipole terms. This condition is true when the denominator of the b_1 coefficient is close to zero. The far-field approximation of the scattered magnetic field [8] is then

$$\begin{aligned}\mathbf{H}_m^{\text{ff}} &= \frac{3i}{2}H_0 b_1 \frac{e^{ikr}}{kr}\left[\left(\hat{\mathbf{y}}\cdot\hat{\boldsymbol{\theta}}\right)\hat{\boldsymbol{\theta}}+\left(\hat{\mathbf{y}}\cdot\hat{\boldsymbol{\phi}}\right)\hat{\boldsymbol{\phi}}\right] \\ &= -\frac{3i}{2}H_0 b_1 \frac{e^{ikr}}{kr}\hat{\mathbf{r}}\times\left(\hat{\mathbf{r}}\times\hat{\mathbf{y}}\right). \qquad (4)\end{aligned}$$

If the magnetic dipole resonance occurs at a frequency such that wavelength outside the sphere is much larger than the diameter of the sphere, the sphere may be replaced by an equivalent effective magnetic dipole. This equivalent dipole has a moment $\mathbf{m}$ which radiates

$$\mathbf{H}_e^{\text{ff}} = -\frac{k^3}{4\pi}\frac{e^{ikr}}{kr}\hat{\mathbf{r}}\times\left(\hat{\mathbf{r}}\times\mathbf{m}\right) \qquad (5)$$

in the far-field [9]. Equating (4) and (5) provides a link between the equivalent magnetic dipole moment and the Mie scattering coefficient b_1 of a single sphere [10].

Proceeding with the above analysis, one can obtain the response of a large collection of such dipoles, and in the process obtain an effective relative permeability, μ_r^{eff}. The induced magnetic dipole moment is related to the incident wave by $\mathbf{m} = \alpha_m\mathbf{H}_0$, where the magnetic polarizability α_m is found from the Clausius-Mossotti equation [9]

$$\alpha_m = \frac{3}{N}\left(\frac{\mu_r^{\text{eff}}-1}{\mu_r^{\text{eff}}+2}\right). \qquad (6)$$

Here $N = 1/a^3$ is the number of dipoles per unit volume, and a^3 is the volume of a unit cell. The density N can be found from the filling fraction f of the composite,

$$f = \frac{4\pi r_0^3}{3a^3} = \frac{4\pi}{3}Nr_0^3. \qquad (7)$$

Finally, the resulting magnetic polarizability is

$$\alpha_m = \frac{6\pi i}{k^3}b_1, \qquad (8)$$

and the effective permeability is

$$\mu_r^{\text{eff}} = \frac{k^3+4\pi iNb_1}{k^3-2\pi iNb_1}. \qquad (9)$$

A similar derivation gives the effective permittivity ϵ_r^{eff}. In this case it is assumed that the dominant contribution to the scattered electric field is proportional to a_1, which also behaves in a resonant manner. Again assuming that the wavelength outside the sphere is much larger than the sphere at resonance, an equivalent electric dipole moment $\mathbf{p} = \epsilon_0\alpha_e\mathbf{E}_0$ may be defined. The resulting effective relative permittivity is then given by

$$\epsilon_r^{\text{eff}} = \frac{k^3+4\pi iNa_1}{k^3-2\pi iNa_1}. \qquad (10)$$

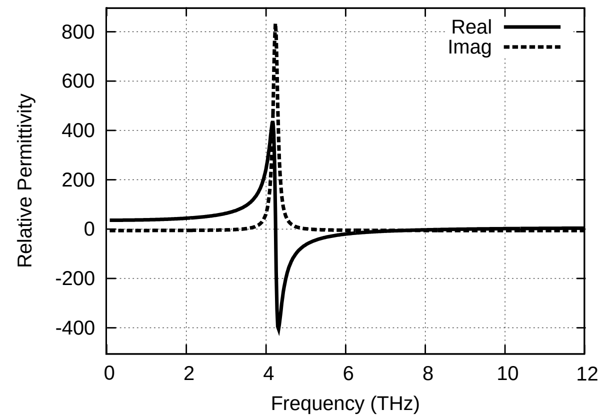

Figure 1. Relative permittivity for bulk $LiTaO_3$ where $\epsilon_0 = 41.4$, $\epsilon_\infty = 13.4$, $\omega_T = 2.67\times10^{13}$ rad/s, and $\gamma = \omega_T/30$.

3 Numerical results

3.1 Effective material parameters

Now that the effective permittivity and permeability of a collection of spheres have been derived, it remains to be seen how to excite these resonances, particularly the magnetic dipole.

A few years ago it was shown that a two-dimensional array of dielectric cylindrical rods could excite a magnetic response [6]. This initial work considered using ferroelectric rods at GHz frequencies and was followed by a study of polaritonic materials to push the response to infrared frequencies [7]. The main requirement satisfied by both of these reports is that the dielectric constant had to be large to drive the magnetic response into resonance. This is the reason why the magnetic resonance is actually the fundamental resonance. In contrast, a traditional derivation of scattering by small spheres [8], which would only consider low-valued dielectrics or metals, ignores the magnetic dipole term since its amplitude is very small. In such cases the fundamental resonance is the electric dipole term, which occurs when $\epsilon_r = -2$.

Here we follow the work in Ref. [7], in that we also consider polaritonic materials. Let the sphere have a relative permittivity [11]

$$\epsilon_r(\omega) = \epsilon_\infty\left(1+\frac{\omega_L^2-\omega_T^2}{\omega_T^2-\omega^2-i\omega\gamma}\right), \qquad (11)$$

where ϵ_∞ is the high-frequency permittivity, ω_T is the transverse optical phonon frequency, ω_L is the longitudinal optical phonon frequency, and γ is the loss. In the remaining sections of this paper the material is assumed to be $LiTaO_3$, which has a static permittivity of $\epsilon_0 = 41.4$, $\epsilon_\infty = 13.4$, and $\omega_T = 2.67\times10^{13}$ rad/s [7], and it is assumed that $\gamma = \omega_T/30$. The longitudinal optical phonon

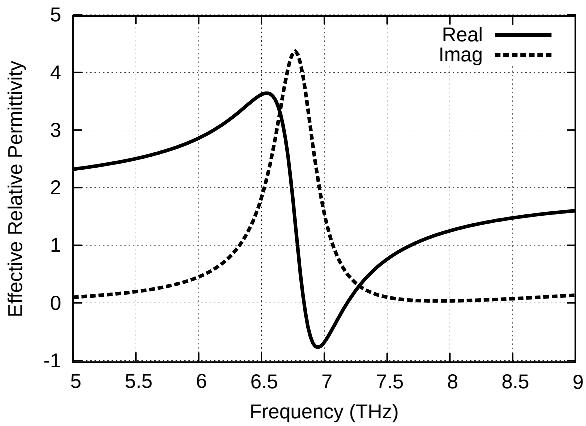

Figure 2. Effective relative permittivity for a collection of $LiTaO_3$ spheres. The radius of the spheres is $4\,\mu$m. The filling fraction is 26.81%.

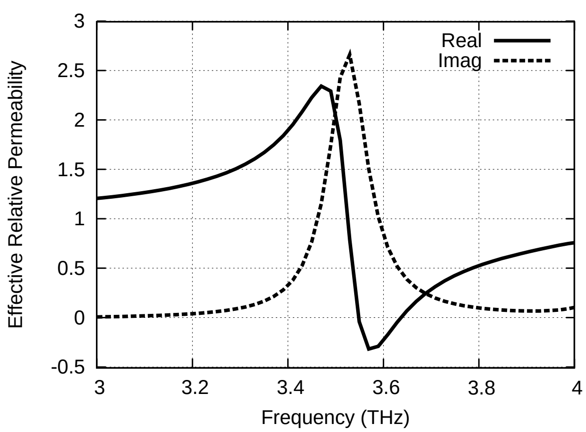

Figure 3. Effective relative permeability for a collection of $LiTaO_3$ spheres. The radius of the spheres is $4\,\mu$m. The filling fraction is 26.81%.

frequency is found from the Lyddane-Sachs-Teller relation

$$\frac{\omega_L^2}{\omega_T^2} = \frac{\epsilon_0}{\epsilon_\infty}. \tag{12}$$

Figure 1 shows the relative dielectric permittivity of bulk $LiTaO_3$. The phonon resonance at 4.25 THz is easily seen.

The choice of $LiTaO_3$ was made due to its large static permittivity ϵ_0. This makes it easier to create a strong resonance in the effective permeability. Other materials, such as SiC, may have higher resonant frequencies, which would result in the resonances being even further into the infrared range, however this would be at the cost of having weaker resonance amplitudes.

The effective electromagnetic parameters of a large collection of spheres are presented in Fig. 2 and Fig. 3. The radius of the spheres is $4\,\mu$m and the filling fraction is chosen to be 26.81%. These effective medium values are expected to be appropriate since the transverse phonon wavelength exceed the diameter of the spheres by a factor of 8.8, which is in the long-wavelength regime.

As expected, Fig. 2 shows that the effective permittivity of the collection is resonant at approximately 6.75 THz. where the material permittivity is around -2. The effective permeability in Fig. 3 shows a resonance around 3.53 THz, which is below the transverse phonon frequency and happens to be where the material permittivity becomes quite large. Note that the resonance in both effective parameters is strong enough that they become negative over a range of frequencies above the resonance.

3.2 Multiple scattering results

Since the effective permeability and permittivity that have been found are within the long-wavelength limit, the actual lattice structure, if any, should have little impact on the effective dispersion. Even so, it is desirable to verify the theory with a full multiple scattering approach. The Clausius-Mossotti relation is supposed to account for dipole-dipole interations, and although it can be derived by assuming a simple cubic lattice of dipoles, it should be appropriate for other lattices also [9]. In addition, as the free-space wavelength approaches the length scale of the lattice, periodic scattering effects become important.

A photonic crystal band structure calculation was needed in order to verify the theory, as well as to determine how these periodic effects deviate from the calculated effective parameters. To this end, software from Ref. [12] was modified and used. This software can calculate the complex band structure and transmission through a composite of arbitrary layers of planes of spheres as well as homogeneous layers. It takes the full multiple scattering approach into account, and the only approximations used are in the angular momentum cutoff in the spherical scattering coefficients and the number of reciprocal lattice vectors taken in each of the planes of spheres. This method is a frequency-domain solver which easily accommodates the material dispersion of the polaritonic spheres.

A simple cubic lattice with lattice constant $a = 10\,\mu$m of $LiTaO_3$ spheres of radius $r_0 = 0.4a$ was simulated. These values match the filling fraction of 26.81% used earlier. The Bloch wavevector was oriented along the ΓX direction. The results are shown as dots in Fig. 4. The solid line compares the effective photon dispersion from the relation

$$\omega^2 = \frac{c^2 k^2}{\epsilon_r^{\text{eff}}(\omega)\mu_r^{\text{eff}}(\omega)}, \tag{13}$$

in the long-wavelength regime, where $\mu_r^{\text{eff}}(\omega)$ and $\epsilon_r^{\text{eff}}(\omega)$ were obtained from (9) and (10). Indeed, the curves match very closely for small ω and small k_z. Only near the Brillouin zone edge ($k_z a/2\pi = 0.5$) do the curves begin to differ. This indicates that it is appropriate to define the effective permittivity and permeability as derived in Section 2. Note that the effective photon dispersion need not be confined to the first Brillouin zone, as shown in Fig. 4 around

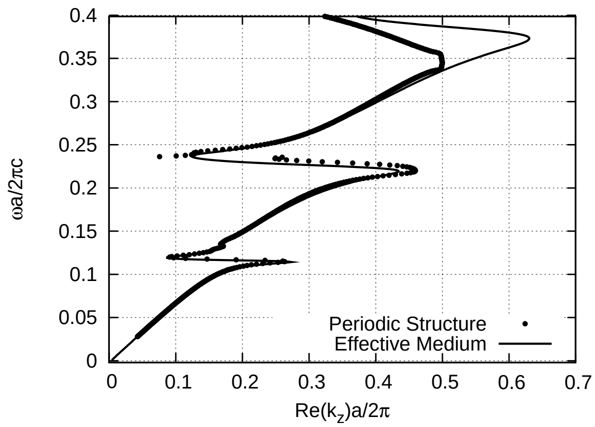

Figure 4. Band structure for a simple cubic lattice of $LiTaO_3$ spheres. The lattice constant is $a = 10\,\mu$m, the radius of the spheres is $r_0 = 0.4a$. The Bloch wavevector is in the ΓX direction.

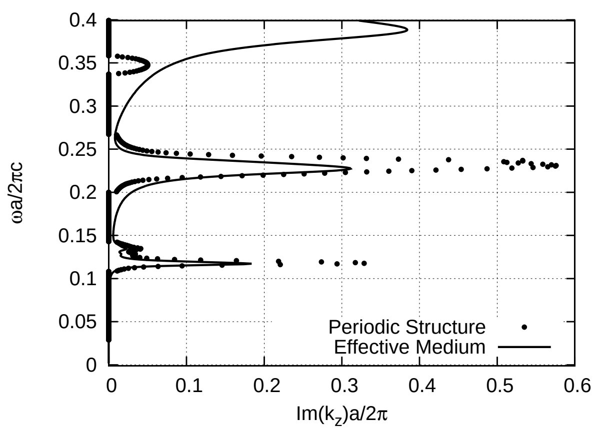

Figure 5. Extinction for a simple cubic lattice of $LiTaO_3$ spheres. The lattice constant is $a = 10\,\mu$m, the radius of the spheres is $r_0 = 0.4a$. The Bloch wavevector is in the ΓX direction.

$\omega a/2\pi c = 0.35$. The first "kink" around $\omega a/2\pi c = 0.12$ in the band structure is due to the permeability resonance, and the second feature around $\omega a/2\pi c = 0.23$ is due to the permittivity resonance. The first Bragg resonance occurs around $\omega a/2\pi c = 0.35$.

The two regions which result from the effective resonances are seen to have negative group velocity, since $v_g = \partial\omega/\partial k_z < 0$ at resonance. This is physically acceptable, since there is also notable extinction in those frequency ranges [13, 14]. This extinction is shown in Fig. 5 as the imaginary part of the Bloch wavevector. Both regions of negative group velocity are within noticeable bandgaps.

4 Conclusion

It has been shown that the effective permittivity and permeability can be derived for a collection of small spheres of arbitrary material permittivity. The results for sphere of $LiTaO_3$ have been presented. The theory has been verified by a comparison of the effective photon dispersion to the band structure of an equivalent sample with a simple cubic lattice.

The results presented have shown that not only can effective media with substantial paramagnetism, or diamagnetism, be created for the infrared regime, but that these new materials can even have a negative permeability. This simple method might also be used as one of the components in a composite with a negative index of refraction.

Future work will include determining the effect of the lattice structure on the effective media values, and the extent to which these values are isotropic. Work is underway to determine how these results may be used to make a simple composite with a negative index of refraction in the infrared regime.

5 Acknowledgments

This work was supported by the Natural Sciences and Engineering Research Council of Canada under Grant No. 249531-02, and in part by Photonic Research Ontario, Funded Research No. 72022792.

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