Assigning Effective Parameters to Amorphous Metamaterials

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Abstract

We summarize our efforts to assign effective parameters to amorphous metamaterials. To this end we rely on a multipole analysis of the scattered field of individual meta-atoms. If only electric and magnetic dipole moments contribute to the scattered field, effective parameters can be assigned to the metamaterial by considering these multipole moments and an adequate filling fraction for the bulk metamaterial. Results are compared to rigorous simulations of amorphous metamaterials and the predictive accuracy of the method is evaluated.

1. Introduction

Metamaterials (MMs) are artificial structures comprising unit cells, called meta-atoms. These meta-atoms may exhibit a magnetic scattering response; being often in the focus of interest since it cannot be observed for natural materials in the visible. A possible way to describe the interaction of light with MMs is to assume them to act as an effective homogeneous material which requires the meta-atoms to be sufficiently small and to be arranged sufficiently dense. If these assumptions hold, effective wave parameters like impedance and refractive index can be assigned to the MM. Wave parameters can be retrieved by various means; an example consists in inverting the scattering data (reflection, transmission) of a slab. Assuming specific constitutive relations these wave parameters can be finally related to effective material parameters; where usually an effective permittivity and permeability are at the focus of interest.

However, for most MMs fabricated by top down methods such a strategy to introduce effective material parameters turned out to be inadequate. The strictly periodic arrangement of meta-atoms with a mesoscopic size leads to a nonlocal response that in fact is identical to strong spatial dispersion. Then, the isofrequency surfaces of the dispersion relation, i.e. the dependence of the longitudinal wave vector component on the transverse components, takes such complicated functional dependency that it cannot be mapped on even bi-anistropic constitutive relations being the most general constitutive relation amenable for an analytical treatment by using the usual Maxwell's boundary conditions.

Evidently, this is not a satisfying situation since the proper theoretical description in terms of effective properties is very desirable if MMs shall serve as building blocks of functional devices. One possible strategy to overcome these difficulties is to use amorphous MMs. There meta-atoms are randomly arranged and spatial dispersion, at least that caused by the periodic arrangement, is suppressed. Effective properties can be assigned to the bulk material while considering only the electric and magnetic dipole contributions to the scattered field from individual meta-atoms. However, spatial dispersion may arise from higher order multipoles. Thus the meta-atoms have to be probed for the existence of these multipoles. For a perfect amorphous arrangement and orientation of all meta-atoms, genuine isotropic MMs seem to be in reach. Therefore the aim of this contribution is the exploration of strategies for assigning effective properties to amorphous MMs.

We describe here how to analyze the scattering response of individual meta-atoms. Such analysis allows identifying whether the dipolar contributions dominate or whether higher order multipoles equally contribute to the scattered far-field. Implications of the existence of higher order multipoles for the assignment of effective properties will be discussed. In addition to the study of the scattering response of meta-atoms we also show how effective bulk parameters may be introduced by using the

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Clausius-Mossotti equation. We will compare these predictions with rigorous results taking into account all the fine details of the structure.

In a first part we concentrate on meta-atoms composed of a small number of spheres. Such MMs are of particular interest because they are amenable for a fabrication with bottom-up approaches of colloidal nanochemistry. We will use experimental results to motivate our theoretical efforts. At second we will lift this restriction and investigate arbitrarily shaped meta-atoms.

2. Spherical Meta-Atoms

The optical response of meta-atoms made from a finite number of spheres is investigated using Mie theory. All fields are decomposed into a finite series of vector spherical harmonics with complex amplitudes. By imposing the usual boundary conditions it is possible to solve for these amplitudes. The scattered field of the entire cluster is expanded into elementary multipoles in spherical coordinates. It is possible to transform the multipole moments from spherical to Cartesian coordinates by comparing the field contributions of them in the respective coordinate systems [2]. This allows revealing the multipolar contributions to the scattered field in terms of electric and magnetic dipoles and quadrupoles; and any arbitrary higher order multipole. Figure 1 shows the excited multipole moments for a meta-atom consisting of two gold spheres, sometimes termed a dimer, for three distinct illumination scenarios.

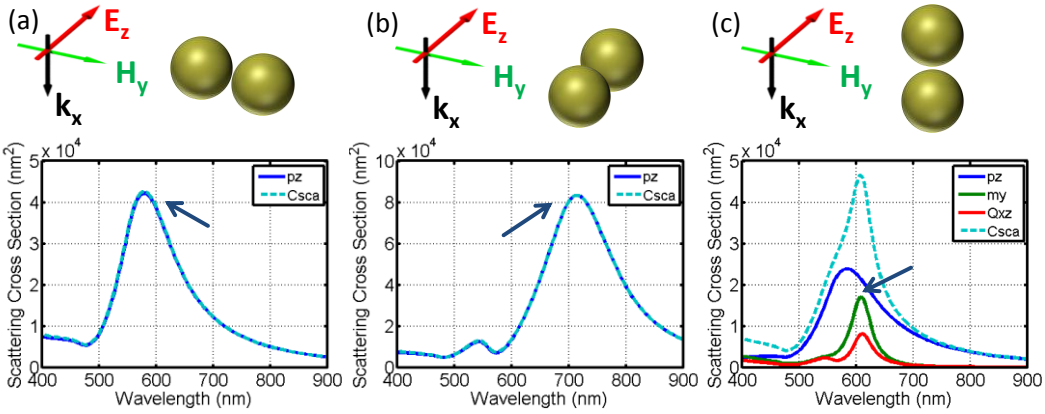

Fig. 1: Contributing multipole moments to the scattered field of a dimer structure (radii = 40 nm, center-to-center distance = 83 nm) embedded in a dielectric host material ($\varepsilon = 2.25$) for three distinct illumination scenarios with a plane wave (a)-(c). Amplitudes of multipole moments are shown as they contribute to the scattering cross section of the dimer. The blue arrows depict resonances as predicted from dipole-dipole coupling models [3].

Whereas the scattered field for an illumination direction perpendicular to the connecting line of the dimer [Fig 1 (a), (b)] is dominated by an electric dipole contribution, an illumination parallel to that line evokes a significant magnetic dipole contribution. The three main resonances highlighted by blue arrows in Fig 1. can be equally predicted by means of hybridization theory for the dimer, see e.g. [3]. Interestingly, the illumination scenario in Fig. 1 (c) shows an unexpected broad electric dipole resonance and, furthermore, a non negligible contribution of an electric quadrupole at the magnetic dipole resonance. Especially this quadrupole contribution is usually neglected when effective parameters are assigned to a MM made of dimers. Normally one wants to exploit this magnetic resonance to affect light propagation in a MM but the quadrupole contribution that usually gives rise to spatial dispersion should be suppressed. Therefore the assignment of effective parameters tends to be questionable and a simple description of the light propagation in this MM is not feasible.

3. Arbitrarily Shaped Meta-Atoms

In this section we extend the multipole analysis towards arbitrarily shaped meta-atoms. To this end the scattered field of the meta-atom will be calculated by an appropriate numerical method as e.g. the fi-

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nite-difference time-domain method for rectangular shaped structures. The multipole coefficients (as they appear in Mie theory) can be calculated as follows. The product of the scattered field with the complex conjugate of the vector spherical harmonics is integrated over the surface of a virtual sphere enclosing the meta-atom, i.e., the scattered field is projected onto the eigenfunctions of Mie theory. The resulting coefficients are the multipole coefficients of the scattered field in spherical coordinates which can be transformed into Cartesian coordinates. In Fig. 2 (b) the excited multipole moments are shown for a cut-plate pair (two gold plates with an MgO spacer in between). The structure is illuminated by plane wave as sketched in Fig. 2 (a).

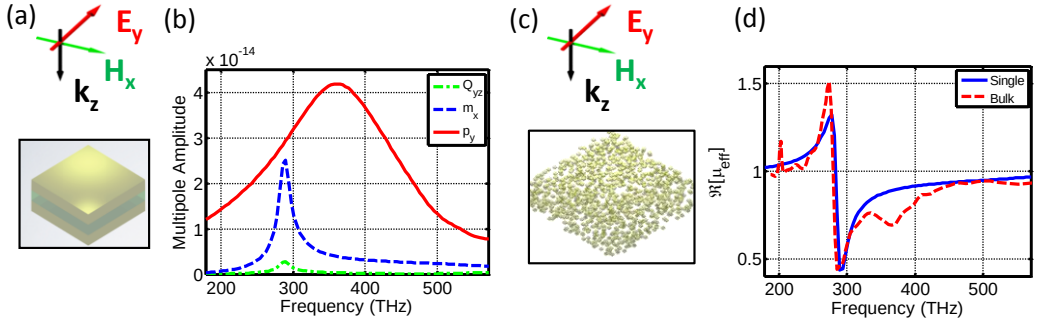

Fig. 2 (a) A cut-plate pair consisting of two gold plates (which have a thickness of 30 nm and a lateral extension of 180 nm) and an MgO spacer (thickness 45 nm) in between is illuminated by a plane wave as sketched. (b) Contributing multipole moments to the scattered field of the structure specified in (a). (c) Amorphous arrangement of the meta-atom from (a). (d) Assigned effective permeability when only the scattering response of the single meta-atom is considered (blue-solid curve) and for a rigorous simulation of the structure sketched in (c) [red-dashed curve].

Similar to the dimer structure of Fig. 1 (c), a magnetic dipole resonance can be observed for a propagation direction perpendicular to the Au plates. Interestingly, the quadrupole contribution is very minor. The Clausius-Mossotti relation links the molecular polarizabilities to effective parameters for a given volume filling fraction. Therefore, if the scattered field of the investigated meta-atom can be fully described by electric and magnetic dipole contributions, one can assign effective properties to the structure by simply applying the Clausius-Mossotti equation [2, 4]. The blue curve in Fig. 2 (d) shows the effective permeability of the structure specified in Fig. 2 (c) when only the magnetic dipole moment of Fig. 2 (b) is considered in the Clausius-Mossotti equation and a realistic volume filling fraction [see Fig. 2 (c)] is chosen. To evaluate the predictive accuracy of the these effective parameters we rigorously simulated the scattered field of the structure in Fig 2 (c) by a large scale FDTD calculation and inverted reflection and transmission data to arrive at the effective Parmeters. The good agreement with the effective permeability achieved from the Clausius-Mossotti equation is shown in Fig. 2 (d).

4. Conclusions

In conclusion we introduce a method to assign effective parameters to MMs consisting of amorphous arranged meta-atoms. It is based on a multipole analysis of the scattered field of a single meta-atom. If the scattered field could be fully described by electric and magnetic dipole contributions we revealed that effective parameters could be assigned by simply applying the Clausius-Mossotti relation instead of a rigorous simulation of the amorphous MM. Referential examples for amorphous metamaterials are discussed and predicted effective properties are compared to those obtained by classical means.

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