Coupling mechanisms in nano-U dimers

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Abstract

In this paper we explore the electric and magnetic coupling mechanisms in nano-U dimers comprising of two identical nano-U elements in the axial arrangement twisted relative to each other by an arbitrary angle. In our analytical model the electric and magnetic coupling can be expressed through the self and mutual terms for magnetic and electric field energy. In addition, we incorporate the effect of kinetic inductance due to the inertia of the electrons. The analytical results agree with numerical simulations (CST Microwave Studio). Our approach should enable an effective design of metamaterial structures with desired properties.

1. Introduction

The main advantage of metamaterials over naturally occurring materials is that their electromagnetic properties can be designed and controlled by choosing the shape of the elements and the way they are arranged within the structure. Obviously, to be able to effectively employ metamaterials for the manipulation of the electromagnetic fields, it is important to understand their 'microscopic' properties, i.e. the way how the electric and magnetic fields are created and the details of the coupling mechanisms between the elements [1,2]. We first introduce a method for calculating the electric and magnetic coupling analytically from the charge and current distributions in coupled resonators and then employ this method to dimers [3], pointing out the importance of kinetic inductance and retardation.

2. Analytical model for electric and magnetic coupling

Assume two metallic elements with arbitrary mutual orientation that can interact both electrically and magnetically through mutual inductance and capacitance. The magnetic and electric coupling between them can be expressed through the self- and mutual terms for the magnetic and electric energy of the system [2,4,5]. The magnetic (κ_H) and electric (κ_E) couplings of two elements can be expressed in terms of the fields, produced by the elements:

$$\kappa_H = \frac{2M}{L} = 2\frac{\int \vec{H}_1 \vec{B}_2 dV}{\int \vec{H}_1 \vec{B}_1 dV}, \quad \kappa_E = \frac{2C}{K} = 2\frac{\int \vec{E}_1 \vec{D}_2 dV}{\int \vec{E}_1 \vec{D}_1 dV}, \tag{1}$$

where L and C are the self inductance and capacitance, M and K are the mutual inductance and capacitance, $\vec{E}, \vec{H}, \vec{D}, \vec{B}$ are the electric field, magnetic field, displacement field and magnetic flux density, respectively. Subscripts denote fields attributed to either first or second element. The total coupling constant is a combination of electric and magnetic coupling constants, $\kappa_{total} = \kappa_H + (-\kappa_E)$. In our recent publication [5], we have shown that for split rings, resonating at microwave frequencies, the fields under the integrals can be replaced by the field sources, i.e. via the charge and current distributions. These distributions are highly non-uniform so the coupling coefficients κ_H and κ_E are anisot-

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ropic. Unlike in [5], we are going to explore nano-scaled resonators here. Therefore, the kinetic energy of conduction electrons becomes important. It can be characterized by the kinetic inductance, an additional term to the self inductance [6]. This term increases the magnetic self energy, but not the mutual energy of two elements. One of the consequences is that the resonant frequency $\omega_0 = (LC)^{-1/2}$ saturates as the resonator is being downscaled to

$$\omega_{sat} = \left((L_{kin} + L)C\right)^{-1/2} = \left((L_{kin}/L + 1)LC\right)^{-1/2} = \omega_0/\sqrt{\alpha}\,, \tag{2}$$

where L_{kin} is the kinetic inductance and $\alpha = L_{kin}/L + 1$. As a further consequence the expression for the magnetic coupling (1) should be redefined as

$$\kappa_H = \frac{2M}{L_{kin} + L} = 2\frac{\int \vec{H}_1 \vec{B}_2 dV}{\alpha \int \vec{H}_1 \vec{B}_1 dV}. \tag{3}$$

For large resonators, α is 1 and the magnetic coupling resembles the low-frequency form (1). However, as we approach the saturation frequency, the magnetic coupling is drastically reduced.

3. Coupling mechanisms for nano-U dimers

In this Section we consider a periodic 2D structure with the unit cell comprising of two identical nano-U elements which are twisted relative to each other by an angle ϕ in the axial configuration. Fig.1 shows a single nano-U resonator and a dimer arrangement. To explore the coupling mechanism in a nano-U dimer we performed CST Microwave Studio simulations of pairs of nano-U resonators using the Drude model for gold [7] and relying on absorbing boundary conditions. We fixed one element and varied the twisting angle of another element from 0 to 180^0. We shall show that the filament current and charge distribution model, used in [5] also works for nano-U resonators if modified as described in Section 2. Therefore, we calculated the coupling from Eqs. (1), (3), using the mean radius of 75 nm and a gap of 50 nm. The results are shown in Fig.2.

(a) (b)

Fig. 1: (a) Nano-U element with geometrical parameters: b = 230 nm, l = 230 nm, w = 90 nm, g = 50 nm and h = 50 nm, f_0 = 211.8 THz and Q = 14; (b) nano-U dimer unit cell with twisting angle ϕ and the axial vertical distance between nano-U elements is 100 nm.

As mentioned above, the total coupling as well as the electric and magnetic couplings depend on the relative orientation of the two nano-U elements in the dimer. Fig.2 (a) shows the behavior of the electric, magnetic and total coupling and their phases as a function of the twisting angle ϕ calculated from the analytical model. As one can see the magnetic coupling continuously decreases reaching its minimum at 180^0, when the bottom parts of the U are furthermost. The retardation effect is also strongest there. The electric coupling monotonically increases and changes sign from negative to positive going through zero at a twisting angle $\phi = 84^0$ in contrast to the 90^0, predicted by the dipole approximation. Magnetic coupling is dominant in the angle range from $\phi = 45.9^0$ to 108.5^0. When $|\kappa_E| = |\kappa_H|$ at the twisting angle of $\phi = 47^0$ the total coupling has a non-zero minimum. This can be understood in terms of retardation effects which provide us with complex coupling coefficients as could be seen from the phase behaviour [8]. Fig. 2 (b) shows comparison of calculated coupling coefficients and

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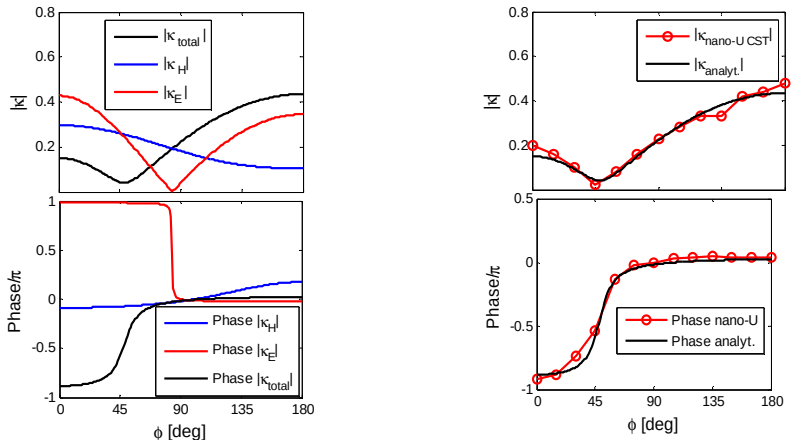
phases with those, extracted from simulations for U-element. As one can see results calculated for U-elements are in good agreement with theoretical model.



(a) (b)

Fig. 2: (a) Analytical calculated coupling constants and their phases versus twisting angle; (b) total coupling constant, phase from CST for U-element (red) and calculated total coupling, phase (black) versus twisting angle.

4. Conclusions

We have presented a detailed analysis of coupling mechanisms between two metamaterial elements of nano-U type in a dimer. We have shown that depending on the relative angle between elements the total coupling is a combination of magnetic and electric coupling. We have shown that our theoretical model very well describes the U-elements. Also our model allows us to define changes in magnetic coupling due to the inertia of the electrons. All this enables us to provide effective design of metamaterial structures with desired properties that is extremely useful for developing metamaterial devices for optics and photonics.

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