Simulation of orientation dependent chirality in plasmonic structures

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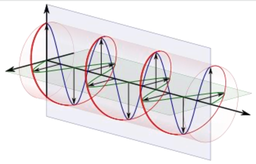
Introduction

Plasmonics is the study of the interaction between electromagnetic field and free electrons in a metal. Free electrons in the metal can be excited by the electric component of light to have collective oscillations.

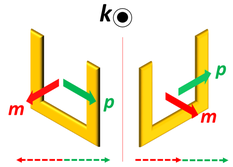


In physics, chirality can be found in the spin of a particle, where the handedness (left or right) of the object is determined by the direction in which the particle spins.

Circular dichriosm (CD) spectroscopy is used to detect chirality for a compound in a solution. In particular, nonzero response is measured only for chiral compounds, which may have nonvanishing rotational strength[1] for molecular states *n,0*, electric dipole **p**, and magnetic dipole **m**. However, this method loses its selectivity for samples that are not rotationally averaged. Indeed, achiral nanostuctures have demonstrated nonzero signals in CD experiments.2,3

$$R_{n0} = \Im\left(\mathbf{p}_{0n} \cdot \mathbf{m}_{n0}\right)$$

A structure that we looked at is the U-shaped Au split ring resonator (SRR).[4] So-called "extrinsic chirality" occurs when the SRR is tilted out of the plane perpendicular to vector **k** and is determined by projection of **p** and **m** onto the plane.[5]



SRR Backscattering: Method

We created a simulation in MATLAB that would allow us to theorize the extinction cross section (extinction is the phenomena of light either being absorbed by the dimer or scattered in a different direction, i.e. not passing through). We follow the point-dipoles-approximation approach and the unit system of Sersic et al.[6] Take the static polarizability of a single SRR to be:

$$\overline{\overline{\alpha}}^{static} = \begin{pmatrix} \overline{\overline{\alpha}}_{EE} & \overline{\overline{\alpha}}_{EH} \\ \overline{\overline{\alpha}}_{HE} & \overline{\overline{\alpha}}_{HH} \end{pmatrix} = \frac{\omega_0^2 V}{\omega_0^2 - \omega^2 - i\omega\gamma} \begin{pmatrix} \eta_E & 0 & 0 & 0 & 0 & i\eta_C \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -i\eta_C & 0 & 0 & 0 & 0 & \eta_H \end{pmatrix},$$

where V = l x w x h = 200 x 200 x 30 nm3, ω0 = 400π THz, ω = ω0, γ = 1.25 x 1014 Hz, ηE = 0.7, ηH = 0.3, ηC = 0.4. Then, apply the optical theorem to obtain the dynamic polarizability by modifying each eigenvalue α0 of the static polarizability by:

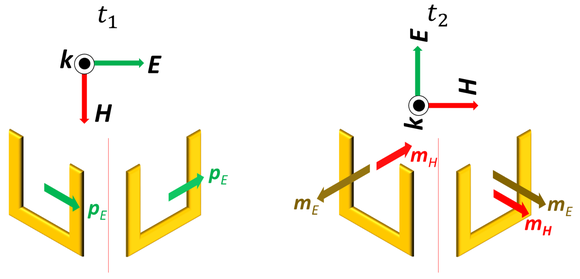
$$\alpha_0 \to \left(\frac{1}{\alpha_0} - \frac{2ik^3}{3}\right)^{-1}$$

Last, compute the backscattering cross section for **k** = k**z**:

$$\sigma_{backscattering} = \frac{k^4}{|\mathbf{E}|^2}\left|\begin{pmatrix} p_y \\ -p_x \end{pmatrix} + \begin{pmatrix} m_x \\ m_y \end{pmatrix}\right|^2$$

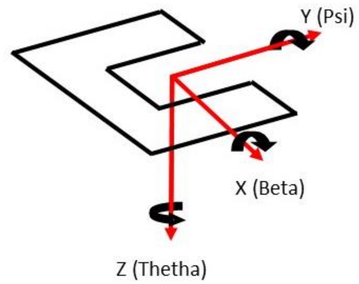
SRR Extrinsic Chirality: Heuristic Model

The extrinsic chirality of an SRR is represented by the interference of the ***H***-induced $\boldsymbol{m}_H$ and ***E***-induced $\boldsymbol{m}_E$ The ***E***-induced $\boldsymbol{p}_E$ is also shown:



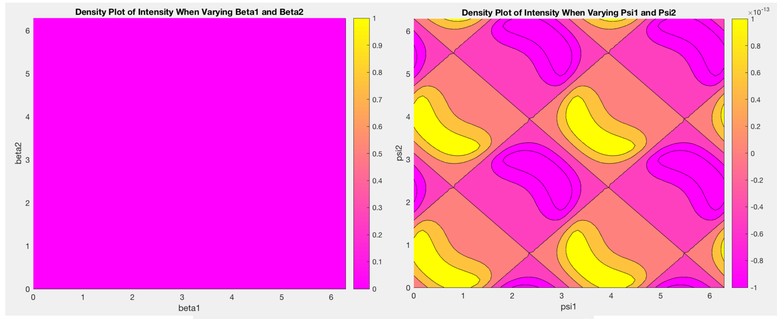
Results

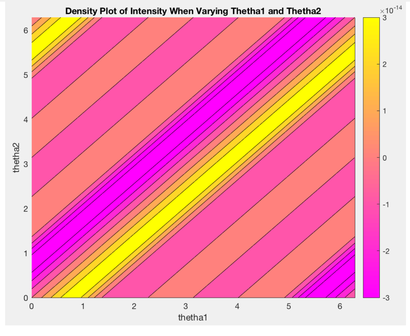
In our simulation, we declared the orientation of the Cartesian coordinate system with the right-hand rule. Declaring Z as the downwards direction, Y as the forwards direction, and X as the rightward direction. Then we assigned each axis with an angle label. Z being Thetha, X being Beta, and Y being Psi.



Our simulation would allow us to alter all three angles for two split ring resonator, one on top of the other, for a total of six different inputs. While the simulations could take in six different inputs, the graphs that we created could only display two inputs and one output. So we limited our inputs for each graph.

The graphs are displaying the scattered light from the split ring resonator, with the amount of scattered light from right-handed light being subtracted from scattered light from left-handed light. This can indirectly inform us of how much light is being transmitted through the split ring resonator and how the chiral light interacts with the chiral resonators. The angles are in radians.

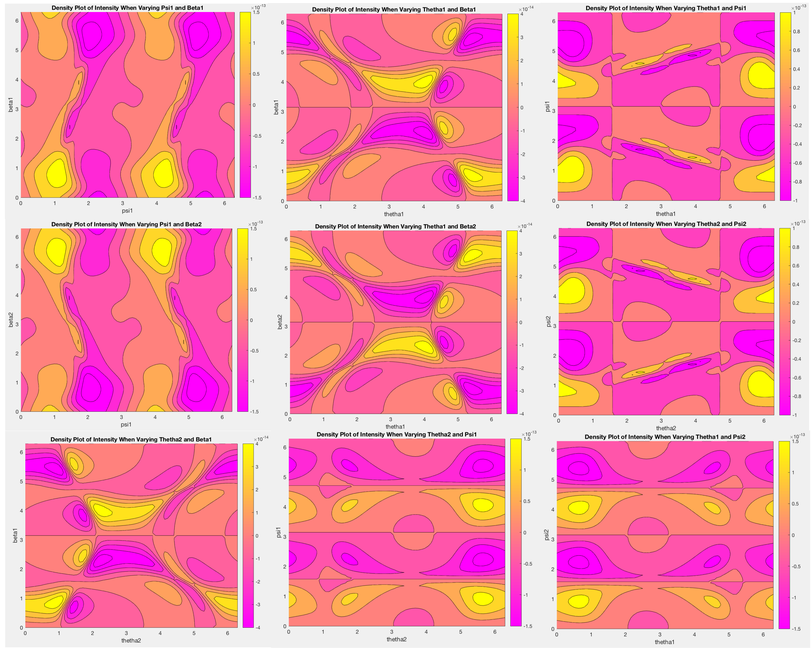




In the three graphs above, the same angle for both resonators were being manipulated at the same time. The graphs comes out as one expects from a logical stand point, and many patterns can be seen and drawn from the coloration of the graphs. So far the patterns are quite easy to see and explain.

For example, in the graph where the Beta angles are being changed, it makes sense that the graph would be one solid color indicating zero. Keep in mind that the graph shows the amount of light scattered by left hand light subtracting the scattered light from right hand light. It does not mean that there is zero interaction between the light and the split ring resonators, but rather that the lights interact with the resonators in the same way. With this information in mind, it is now clear why the graph is one solid color: rotating the split ring resonator being rotated along the X-axis does not influence how the chiral lights interact with the split ring resonators in terms of right hand light and left hand light.

For the other two graphs, the patterns are clear, with the one graphs of Thetha being changing from positive to negative with clear cut lines across key angles incriminates, such as zero and pi. The reason the sides are mirror images from each other is due to the relative angles of the split ring resonator on top is to the one on the bottom. The same is true of the graph involving the changes of the Psi angle. The patterns are much easier to see for these simple angle comparison, but moving onto changing two different angles for the two different resonators, or changing two different angles on one resonator while leaving the other at a starting position, the patterns get more bizarre.



Discussion and Conclusions

The simulation for detecting the interaction of chiral light with objects with chirality can help with problems that are present in pharmaceuticals. A molecule can have chirality (left and right-hand) and different handiness in molecules can have different effects on a biological system. For example, a hormone with a left-handed form can have a positive effect on a biological system, where as a right-handed form could have no effect or even a negative effect on a biological system. Telling the difference between the different forms of molecules can difficult and time consuming. With this method, using chiral light, one can plot the interaction the light has with a molecule as the molecule is rotated around its "center". But to read the plot of the interaction of chiral light with chiral molecules and deciding the chirality of the molecule will require a baseline measurement, which can be found through simulations, like the one that we have created. In the future, more specific simulations can be used on structures that are not as uniform as the split-ring resonators used in this simulation.

References

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