NANORESONATORS GET NEW TOOLS FOR THEIR CHARACTERIZATION

Nanoresonators offer optical science a new subwavelength tool to control light, and at Institut d'Optique d'Aquitaine, we have developed a method to gain new insights into their properties.

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AT THE LABORATOIRE PHOTONIQUE, Numérique, et Nanosciences of the Université de Bordeaux in France, we have been working to develop a method for understanding and predicting the interaction of light with matter at the subwavelength scale.

We have implemented a numerical tool based on electrodynamics equations using COMSOL Multiphysics®, its RF Module, and MATLAB®. Simulation is particularly useful for developing and operating the emerging technology known as nanoresonators, or optical nanoantennas. Theory, analytical solutions, and simulation provide great insights into how these devices operate and shorten their development time. This will favor the use of nanoresonators in applications ranging from photovoltaics to spectroscopy.

» WHY ARE NANORESONATORS USEFUL?

THE INTRODUCTION OF nanoresonators has been a relatively recent event in optics. These devices manage the concentration, absorption, and radiation of light at the nanometer scale in much the same way as it is accomplished with microwaves at much larger scales. An example of an optical nanoantenna is given in Figure 1, where a source, placed in between two gold nanospheres, is coupled to the far field more strongly than if it were alone in vacuum. Typically, the shape of the antenna can control the radiation. For example, Figure 2 shows how a silver sphere illuminated by a plane wave influences the scattered near-field.

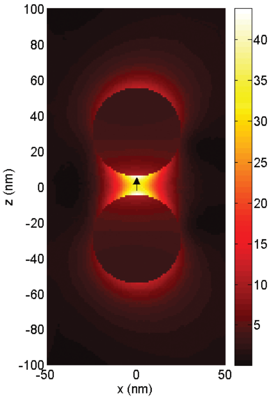

FIGURE 1: Example of nano-antenna: Intensity of electric field radiated by a gold sphere doublet coupled to a dipolar source (represented with a black arrow). The sphere radii are only 25 nanometers, and the distance between the spheres is 10 nm. The power radiated by the source is much larger than the power that would be radiated by the same source in the absence of the spheres. The radiation diagram in the far field can be controlled by tailoring the shape of the antenna. All dimensions are much smaller than the emission wavelength of 505 nm.

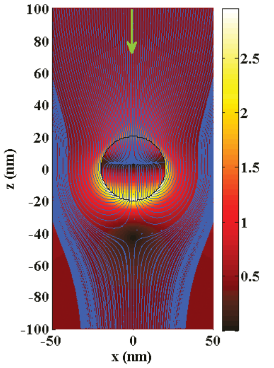

FIGURE 2: Intensity of the electric field around a single silver sphere with a radius of 20 nm illuminated by a plane wave incident from the top (the green arrow indicates the direction of propagation). The flux lines are represented in blue.

» MODELING ELECTRODYNAMICS IN NANORESONATORS

SINCE NANORESONATORS are essentially made of metal and can have different shapes, their simulation should rely on a software that can represent their geometry and model their electromagnetic properties accurately.

However, the electromagnetic properties of metal are not so easy to model, especially when you are solving for problems in the time domain and with complicated shapes like small, oddly shaped objects with curves and sharp corners that are also very close together. To model such complex nanoresonators, we rely on the finite element method (FEM) to achieve accurate predictions. And with COMSOL, one can get very good numerical representations of the curved surfaces and corners and of the volume involved in the computation, so it's quite convenient and appropriate.

Until very recently, the state of the art was to solve Maxwell's equations for a particular excitation, i.e., for a given incidence, wavelength, and polarization of a light beam impinging on a resonator.

However, when using such an approach, the whole numerical simulation has to be redone each time the excitation field changes. The numerical load may then be too heavy to fully characterize the nanoresonator, and above all, the computed results obtained with brute-force calculations may still hide a great deal of knowledge about the physical mechanisms at play.

» *A NEW ANALYTICAL-NUMERICAL METHOD FOR CHARACTERIZING NANORESONATORS*

USING THE STRIKING of a bell as an analogy for light excitation of a nanoresonator, it is possible to understand that any hammer stroke will more or less excite the same vibration modes of a bell. The latter represents an intrinsic characteristic of the resonator that does not depend on the excitation. If one is able to find these modes and understand how they are excited, then it is possible to describe the interactions between the resonator and its environment much more easily and intuitively and without the need to rely on brute-force calculations. Very rapidly, we realized how helpful it was to have a modal theory to describe our resonators.

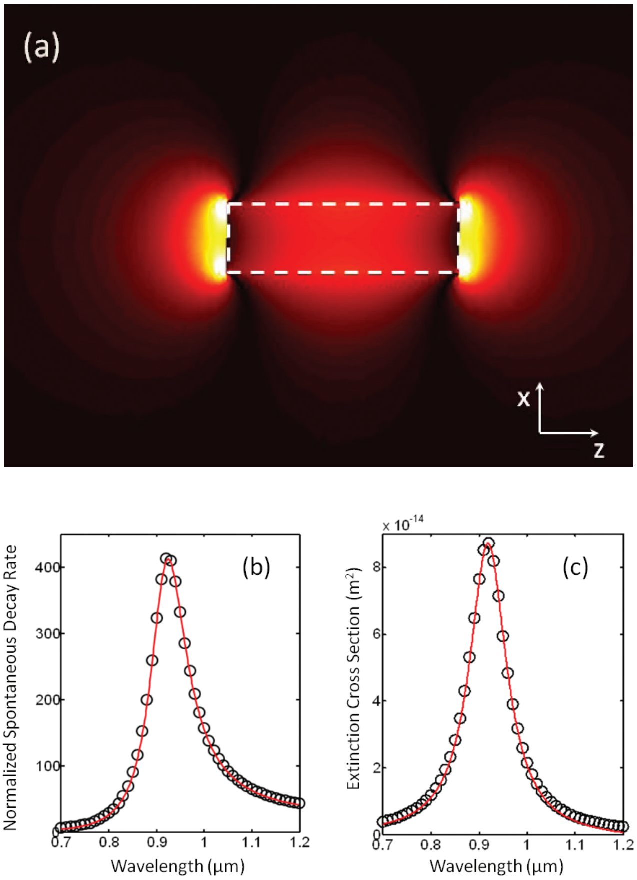

FIGURE 3: (a) Distribution of z-component of the electrical field |Ez| for the normalized quasinormal mode of a cylindrical gold nanorod with a diameter of 30 nm and a length of 100 nm. The white dashed line represents the rod contour. (b) Spontaneous decay rate of a cold molecule located on the rod axis at a 10 nm distance from the rod. (c) Attenuation cross section of the rod under illumination by a plane wave polarized along its axis. In (b) and (c), black circles are fully vectorial computational results obtained with COMSOL. Each point requires an independent calculation. Simulation results are in good agreement with the predictions of the analytical model represented by the solid red curves.

Our initial contributions were more theoretical. We knew that if you hit a nanoresonator with light, you are going to excite its resonance modes, which is obvious. Defining what the excitation strength is analytically, however, was not obvious. Using COMSOL, we created a tool that calculates the modes and their excitations quite easily and solved this long-standing problem.

We were able to use COMSOL both to compute the response of the system to a particular excitation and to compute the modes of the nanoresonator. The fact that COMSOL can easily be interfaced with MATLAB® was an essential point for us, as our COMSOL simulation could be integrated as the field-computing engine of a theoretical procedure.

When we adapted our mathematical theory to COMSOL, it permitted the normalization of the modes and allowed us to compute their excitation coefficients simply by evaluating a volume integral. This part was crucial, as it further resulted in a rapid and analytical method to calculate the electromagnetic field scattered by the resonator along with all the associated physical quantities, such as the scattering and absorption cross sections and the radiation diagram, as depicted in Figure 3.

Now that a method has been developed to understand how light is scattered by nanoresonators, we expect that this will assist in the spread of nanoresonators in a number of optical applications, ranging from sensors and defense applications to computers and electronics. A new breed of devices called nanoelectromechanical systems (NEMS) will soon see the light, thanks to simulation. ◎