Optics Communications ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Optical response in subnanometer hollow sodium nanowires

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ARTICLE INFO

Article history:
Received 18 September 2015
Received in revised form
6 April 2016
Accepted 21 June 2016

Keywords:
Surface plasmons
Nonlocal effects
Sodium hollow nanowire
Nanofocusing

ABSTRACT

We simulate and analyze the influence of nonlocal effects on the optical properties of thin metal hollow nanowires by finite element method. Nonlocal effects in hollow nanowires with both nm-sized overall volume and a tiny metal shell are considerable for extinction cross section but more for field enhancement, resulting in nonlocal plasmonic modes excited. Then, we show the dependence of extinction effects of a hollow super-nanowire on its parameters, including the metal shell thickness, the average radius and the optical constant of the hollow core. We find that nonlocal quadrupolar mode is very sensitive to the thickness of metal layer but with great stability as increasing the hollow nanowire dimension or changing the hollow core. Furthermore, the eccentricity of the hollow nanowire brings out new physical phenomena, such as nanofocusing and multimodes. The proposed structure promises a great of applications in nanoscale, such as designing nanoplasmonic antenna, sensing and nonlinear optics, etc.

1. Introduction

Localized surface plasmonic resonance (LSPR) is the electron cloud collectively oscillating at metallic surface which is exposed to the field of the p-polarized wave. Since it is a resonant interaction of light with metallic nanostructure beyond the traditional diffraction limit, it triggers off the study of nanoscience in optical region [1–3] and has found enormous applications, including optical nanoantennas [4], surface-enhanced Raman spectroscopy [5,6], optoelectronics in hybrid devices [7], optical trapping [8,9], the design of broad-band light harvesting nanostructures [10,11], etc.

The limit of nanofabrication has been pushed to new levels of precise control, e.g. electron beam lithography (EBL) is capable of obtaining very small nanogaps between nanoparticles [12]. Helium ion milling (HIM), a gentle method but with more control over the precise nanoscale, was used to obtain narrow (<5 nm) nanoplasmonic structure [13,14]. Once a tiny structure appears in a plasmonic configuration, nonlocal dielectric response of nanostructures becomes pronounced, e.g. nonlocal effects of metallic plasmonic tips modify its ability of electromagnetic nanofocusing [15]; nonlocal effects make less loss and better nanoconfinement for a hybrid plasmonic waves propagated in a hybrid plasmonic waveguide [16]; nonlocal effects modify nanowire dimers' field enhancement and optical extinction [17]; and nonlocal effects lead to less enhancement and blue-shift of surface-enhanced Raman scattering (SERS) peaks of nanoparticles [18]. However, there are few works about super-nanosystem with both a nm-sized overall volume and a nanometer structure details, where larger nonlocal and quantum effects play an important role. Moreover, it costs much to explore fundamental characteristics of surpernano plasmonic configuration with experimental methods. To reflect the emergence of strong electronic interactions in this sub-nanometer length scale, the implementation of nonlocal (spatially dispersive) dielectric functions for metals is required.

In this work, we investigate interesting optical effects of a metallic hollow nanowire by adopting a reliable nonlocal model – nonlocal hydrodynamic Drude model [19] based on finite element method. We consider a hollow nanowire of both a nm-sized overall volume and a nanometer thickness of metal shell, which is different from core-shell nanowires [20,21] where the nanowire radius is too large to cause nonlocal effects. We expect that such nanosystem would exhibit great non-local effects once both the hollow nanowire overall size and the metal layer thickness are small as nanometers, resulting in the field of the plasmonic mode in such metal nanostructure to be largely modified. We also calculate extinction spectrum of hollow nanowires, where the magnitude and position of nonlocal LSPR are related to the hollow nanowire parameters including the thickness of the hollow

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http://dx.doi.org/10.1016/j.optcom.2016.06.058
0030-4018/

nanowire, the average radius and the optical constant of the hollow core. Furthermore, the process of EM nanofocusing and the formation of multimodes take place in a nonconcentric hollow nanowire as a consequence of both local surface plasmon resonance and nonlocal effects together. The proposed structure is feasible by using modern fabrication methods, which may be of interest in future applications including nanoantenna, optical absorption in nanoscale, nanosensing and nanoscale nonlinear optics and so on.

2. Computational method and implementation

The nonlocal dielectric function of a material $\epsilon(k, \omega)$ is a function of both the wave vector k and angular frequency ω, where the k dependence is responsible for the nonlocal effects.

Nonlocal material response distinctively changes the optical properties of nanoscale plasmonic structures. Since the electron gas in metal behaves analogous to a hydrodynamic flow, the equations governed the motion of electron gas could be described by hydrodynamic Drude model which could be derived from macroscopic Maxwell's equations via inserting $\epsilon(k, \omega)$ in them, and as consequence of that, in frequency domain (with time dependence $e^{i\omega t}$), the hydrodynamical model consist of a coupled system of equations for the electric field $\mathbf{E}$ and the nonlocal hydrodynamic current density $\mathbf{J}_{HD}$ [19]:

$$\nabla \times \mu_0^{-1}(\nabla \times \mathbf{E}(\mathbf{r}, \omega)) - \omega^2\varepsilon_0\varepsilon_{loc}(\mathbf{r}, \omega)\mathbf{E}(\mathbf{r}, \omega) = i\omega\mathbf{J}_{HD}(\mathbf{r}, \omega) \quad (1)$$

$$\beta^2\nabla^2\mathbf{J}_{HD}(\mathbf{r}, \omega) + \omega(\omega + i\gamma)\mathbf{J}_{HD}(\mathbf{r}, \omega) = i\omega\omega_p^2\varepsilon_0\mathbf{E}(\mathbf{r}, \omega)) \quad (2)$$

where ε_0 is the vacuum permittivity, and γ and ω_p are the damping coefficient and the plasma frequency, respectively. The nonlocal parameter β, which measures approximately the speed of sound in Fermi-degenerate plasma of conduction electrons, is proportional to the Fermi velocity V_F of the metal. In the limit $\beta \to 0$, the nonlocal hydrodynamic Drude model become a local Drude model. To excite plasmonic effects, a TM-polarized plane wave is chosen to be incident on a nano-plasmonic structure surrounded by free space. The nanoscale structure is made up of a dispersive material sodium with $\varepsilon_{loc}=1$, bulk plasma resonance frequency $\omega_p = 8.65 \times 10^{15}\ \mathrm{s}^{-1}$, damping constant $\gamma = 0.01\omega_p$. The system constant $\beta = \sqrt{\frac{3}{5}}V_F$ is computed for the Fermi velocity $V_F = 1.07 \times 10^6\ \mathrm{m\ s}^{-1}$. We solve the coupled equations (1)–(2) self-consistently, with the ordinary Maxwell's boundary conditions for electric field at all the interfaces except the metal surfaces where the vanishing normal component of the hydrodynamic current $(\mathbf{J}_{HD})_n = 0$ are applied. The metallic nanostructures were enclosed by a spherically symmetric perfectly matched layer (PML) that efficiently absorbs scattered EM waves. Highly non-uniform tetrahedral discretization meshes were used to resolve accurately the different length scales involved in the solution of the coupled set of equations. The finest details of the nanostructures were mapped manually using grid spacings as narrow as 0.01 nm.

3. A single cylindrical nanowire

Cylindrical nanowire is a simple nonlocal configuration due to its cylindrical symmetry, which allows us to easily understand the phenomenon. Ruppin had extended the mie theory for the nonlocal response and formulated the analytical solution for this problem [22]. The changed optical properties of nanowire due to nonlocal effects also have been shown in detail by various numerical methods based on different theory frameworks [23,19,24]. Hydrodynamic Drude model based on finite element method (2D nonlocal FEM model) adopted by this work is a great reliable and flexible implementation for any arbitrary shaped nonlocal structures.

For validation of the nonlocal FEM model and making a comparison with hollow nanowires studied in the next section, we simulate a spatially dispersive sodium nanowire with a diameter of 4 nm in vacuum. A light of plane wave with unit amplitude of electric field ($E_0 = 1$) impinges normally on the Na cylindrical plasmonic nanowire, which leads to incoming and scattered electromagnetic fields outside the nanowire (with induced longitude hydrodynamic current inside). We calculate the optical extinction cross section σ_{ext} normalized by the nanowire diameter. Fig. 1(a) plots the extinction spectrum for the local (black rectangle-marked curve) and nonlocal responses (red circle-marked), which is consistent with the observations in Ref [19]. The main peak appears in the extinction spectrum around $\omega/\omega_P = 0.705$ ($\omega = 4.014$ eV) for a local response and $\omega/\omega_P = 0.7308$ ($\omega = 4.17$ eV) for a nonlocal response with a noticeable blue shift of 0.0258 (0.156 eV). The relative difference in the cross section under the

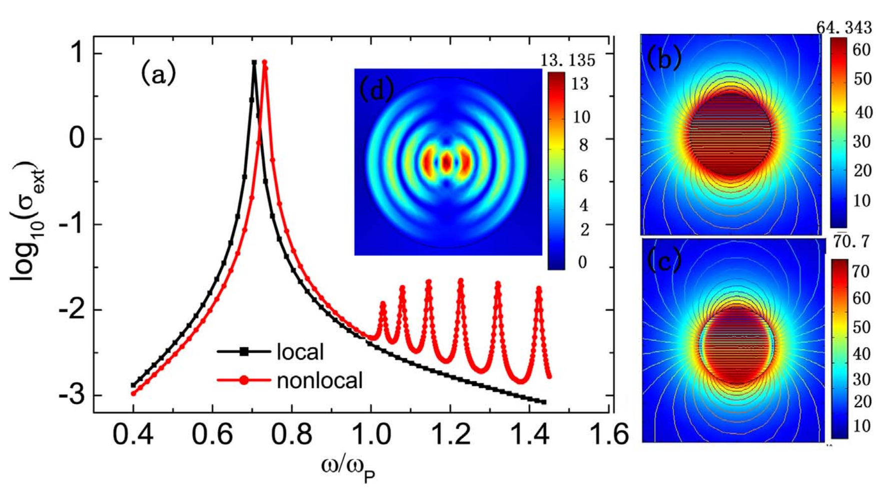

Fig. 1. (a) Extinction cross sections σ_{ext} as a function of frequency for TM-polarized light normally incident on a sodium cylindrical plasmonic nanowire (r=2 nm) in vacuum. Black rectangle-marked curve is under the local theory and red circle-marked is under the nonlocal theory. Snapshot of field distributions (color map represents |E| and contour lines represent |H|) at the main peak of the extinction spectrum, with (b) the local and (c) the nonlocal response included, respectively, and (d) the fourth order nonlocal resonance. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

Please cite this article as: B. Sun, et al., Optics Communications (2016), http://dx.doi.org/10.1016/j.optcom.2016.06.058