Nonlocal hydrodynamic Drude model of nano-plasmonic optical devices

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Summary. As optical devices get much smaller than the wavelength of the operating light, local material models for metallic structures like the Drude model and the Lorentz model become inadequate to describe accurately the light-matter interactions. To overcome this, a sophisticated nonlocal hydrodynamic Drude model has been proposed. We discuss a weak formulation of the nonlocal hydrodynamic Drude model in the frequency domain and apply the finite element method for scattering and propagating mode problems to demonstrate the dramatic impact of non-local effects on the device characteristics.

1 Introduction

The dispersive material properties of plasmonic structures are usually described by the Drude model and the Lorentz model. These material models take into account spatially *purely local* interactions between electrons and the light. Recent investigations have shown that these local models are inadequate as the size of the plasmonic structure becomes much smaller than the wavelength of the exciting light [1, 2]. To overcome this, a sophisticated *nonlocal* material model is required, such as the hydrodynamic model of the electron gas [3].

The hydrodynamic model is formulated by coupling macroscopic Maxwell's equations with the equations of motion of the electron gas. This gives rise to a hydrodynamic polarization current. Considering only the kinetic energy of the free electrons, it yields the nonlocal hydrodynamic Drude model, which is given in frequency domain by a coupled system of equations

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

$$\beta^2 \nabla(\nabla \cdot \mathbf{J}_{\mathrm{HD}}) + \omega(\omega + i\gamma)\mathbf{J}_{\mathrm{HD}} = i\omega\omega_{\mathrm{p}}^2 \varepsilon_0 \mathbf{E}, \quad (2)$$

where $\mathbf{E}$ is the electric field, $\mathbf{J}_{\mathrm{HD}}$ is the hydrodynamic current, $\varepsilon_{\mathrm{loc}}$ is the relative permittivity due to the local-response, β^2 is a term proportional to the Fermi velocity, γ is the damping constant, and $\omega_{\mathrm{p}}^2 = \frac{e^2 n_0}{\varepsilon_0 m_{\mathrm{e}}}$ is the plasma frequency of the free electron gas, c.f. [6, 7].

The hydrodynamic current is non-zero only in a region Ω_{m} filled with metal. We assume that Ω_{m} is bounded and contained in the computational domain Ω. *Transparent boundary conditions* such as PML (Perfectly Matched Layers) are required to model the coupling of the light field with the exterior domain [9].

2 Weak formulation

Appropriate Sobelev spaces for the electric field $\mathbf{E}$ and the hydrodynamic current $\mathbf{J}_{\mathrm{HD}}$ are $H(\mathrm{curl}, \Omega)$ and

$$H_0(\mathrm{div}, \Omega_{\mathrm{m}}) = \{\mathbf{J}_{\mathrm{HD}} \in (L^2(\Omega_{\mathrm{m}}))^3 \mid \nabla \cdot \mathbf{J}_{\mathrm{HD}} \in (L^2(\Omega_{\mathrm{m}}))^3,\ \mathbf{n} \cdot \mathbf{J}_{\mathrm{HD}} = 0 \text{ on } \partial\Omega_{\mathrm{m}}\},$$

respectively. This restricts the hydrodynamic current to the metallic domain, and imposes a zero normal component on the boundary of the metal.

One can use textbook Nédélec finite element spaces to discretize $H(\mathrm{curl}, \Omega)$ and $H_0(\mathrm{div}, \Omega_{\mathrm{m}})$, leading to a consistent discretization of the problem, fulfilling the required boundary and material interface conditions [8, Ch. 5].

Special geometries such as z-invariant structures or with a rotational symmetry, can be treated as in the standard Maxwell case. This allows for the computation of plasmon-polarition waveguide modes of a z-invariant structure on a 2D cross-section domain. In this case it is assumed that the electric field and the hydrodynamic current depend harmonically on z :

$$\mathbf{E}(x,y,z) = \mathbf{E}(x,y)e^{ik_z z},$$

$$\mathbf{J}_{\mathrm{HD}}(x,y,z) = \mathbf{J}_{\mathrm{HD}}(x,y)e^{ik_z z}$$

Replacing all $z-$derivatives in the coupled system (1), (2) with ik_z yields a quadratic eigenvalue problem for the propagation constant k_z.

3 Numerical examples

3.1 Cylindrical plasmonic nanowires

We validate the present approach by simulating a test case of cylindrical nanowire as in [1], for which an analytical solution based on Mie theory is available.

Consistent with the observations in [1], peaks due to nonlocal interactions are present *only* beyond the bulk plasma frequency, c.f. Fig. 1. The positions of the surface plasmon resonance and the nonlocal hydrodynamic Drude resonances agree very good with the analytical Mie results.

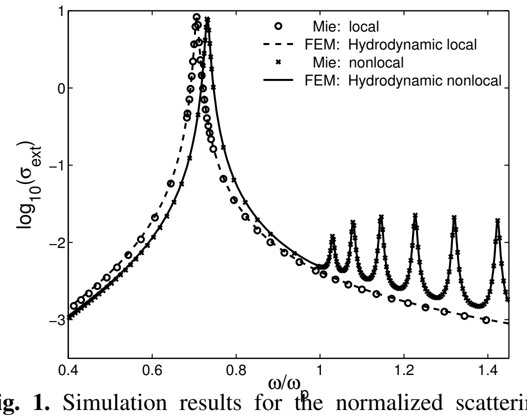

Fig. 1. Simulation results for the normalized scattering cross section σ_{ext} of the cylindrical nanowire in [1]. The curves show comparison of the numerical finite element solutions for the nonlocal and the local hydrodynamic model with the corresponding analytical solutions based on Mie theory.

3.2 V groove channel plasmon-polariton resonances

To demonstrate capability of the method to handle an arbitrary shaped geometry, we simulate a channel plasmon-polariton (CPP) waveguide with a V groove.

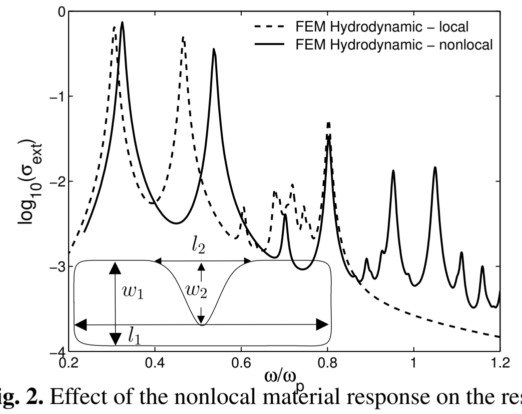

Fig. 2. Effect of the nonlocal material response on the resonance modes of V groove CPP waveguide. The waveguide parameters are: $l_1 = 7$ nm, $w_1 = 1$ nm, a groove of length $l_2 = 0.7$ nm, width $w_2 = 0.7$ nm is placed in the center. The material and the hydrodynamic parameters are taken as in the case of cylindrical nanowires in [1]. The sharp corners of the waveguide are rounded with corner radius of 0.1 nm. Resonances are excited by a unit amplitude, x-polarized plane wave propagating in the direction of minus y-axis.

We consider a V groove configuration as shown in clip of Fig. 2. First we simulated it for the local Drude model. As seen from the dashed curve in Fig. 2, several resonance modes are excited. When this setting is simulated with the nonlocal Drude model, the mode spectrum changes significantly (solid-line curve). Some of the local Drude model modes such as at $\omega/\omega_{\text{p}} = 0.306332$ and $\omega/\omega_{\text{p}} = 0.80262$ experience small shifts towards high frequency, whereas others like at $\omega/\omega_{\text{p}} = 0.466485$ and $\omega/\omega_{\text{p}} = 0.605087$ undergo noticeable shifts towards high frequency. As in the case of the cylindrical nanowires, also for the V groove waveguide a completely new set of resonances appear at the frequencies beyond the plasma frequency. For the present simulation setting, some of these hydrodynamic resonance modes are more prominent than the higher order waveguide resonance modes. It gives the indication that the modal properties of the CPP waveguides change significantly with the inclusion of nonlocal effects.

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References

1. R. Ruppin. Extinction properties of thin metallic nanowires. *Optics Communications*, 190(1-6):205–209, 2001.
2. S. Palomba, L. Novotnyb, and R. E. Palmer. Blue-shifted plasmon resonance of individual size-selected gold nanoparticles. *Optics Communications*, 281(3):480–483, 2008.
3. A. D. Boardman. *Electromagnetic surface modes*, chapter Hydrodynamic theory of plasmon-polaritons on plane surfaces, pages 1–76. John Wiley and Sons Ltd., 1982.
4. J. M. McMahon, S. K. Gray, and G. C. Schatz. Calculating nonlocal optical properties of structures with arbitrary shape. *Physical Review B*, 82:035423, 2010.
5. S. Raza, G. Toscano, A. P. Jauho, M. Wubs, and N. A. Mortensen. Unusual resonances in nanoplasmonic structures due to nonlocal response. *Physical Review B*, 84:121412, 2011.
6. G. Toscano, S. Raza, A.-P. Jauho, N. A. Mortensen, M. Wubs, Modified field enhancement and extinction by plasmonic nanowire dimers due to nonlocal response, Opt. Express 20 (4) (2012) 4176–4188.
7. K. R. Hiremath, L. Zschiedrich, and F. Schmidt. Numerical solution of nonlocal hydrodynamic Drude model for arbitrary shaped nano-plasmonic structures using Nédélec finite elements. arXiv:1201.1527v2 (submitted to J. Comp. Phys.), 2012.
8. P. Monk. *Finite Element Methods for Maxwell's equations*. Oxford Science Publications, 2003.
9. L. Zschiedrich Transparent boundary conditions for Maxwell's equations: Numerical concepts beyond the PML method, Ph.D. thesis, Freie Universität Berlin (2009). http://www.diss.fu-berlin.de/diss/receive/FUDISS_thesis_000000013994