Analytical Model for s-type SNOM of 2D Conducting Materials

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Abstract— *We present an analytical calculation of plasmon excitation in a 2D conducting material by a thin horizontally arranged polarized cylindrical tip. Due to its simplicity, our minimalistic model provides better understanding of scattering type surface near-field microscopy (s-SNOM) of 2D materials in term of operation and measurements.*

Introduction

s-SNOM is a powerful tool for exploring local electronic properties of surfaces and 2D materials in a few-nanometer-size domain [1, 2, 3]. Simulation of s-SNOM signal obtained in experiments is an important part of the technique for retrieving physical properties of a material being studied. For the moment, mathematical modeling of s-SNOM experiments is developed mainly in the cases of surfaces of homogeneous bulk materials [4, 5]. Recently, we performed calculations for the case of a bulk wafer covered by graphene and cylindrical exciting tip were published [6]. Here, we improve the theoretical approach presented in the latter research by analytical calculation of charge distribution in a conducting 2D material excited by a dipole line arranged parallel to the surface (see Fig. 1).

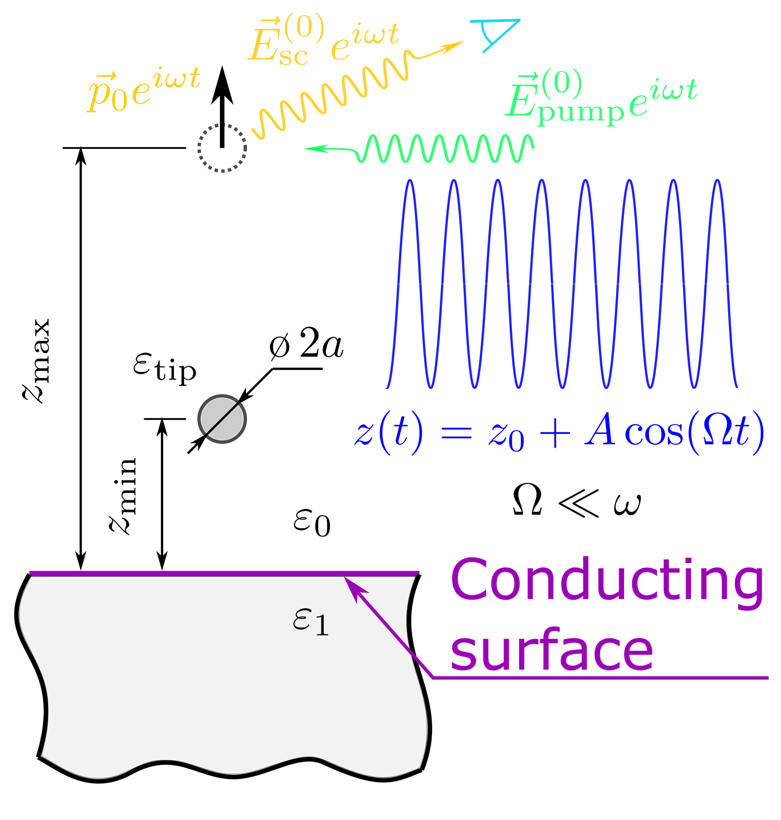

Fig. 1: Schematic view of s-SNOM of 2D conducting material

Basics of s-SNOM simulation

The s-SNOM measures E_{sc} electric field scattered by the tip which is proportional to the dipole amplitude $p^{(0)}$ oscillating in it. For cylindrical tip and electric field $\vec{E}^{(0)}$ acting on it which is directed perpendicularly to its axis, the dipole moment is given by

$$\vec{p}^{(0)} = \alpha \vec{E}^{(0)} \qquad (1)$$

where $\alpha = \frac{a^2 \varepsilon_0}{2} \frac{\varepsilon_{tip} - \varepsilon_0}{\varepsilon_{tip} + \varepsilon_0}$ — for a cylindrical tip. The total electric field $\vec{E}^{(0)}$ causing the tip's polarization consists of the two components:

$$\vec{E}^{(0)} = \vec{E}^{(0)}_{pump} + \vec{E}^{(0)}_{ind} \qquad (2)$$

where $\vec{E}^{(0)}_{pump}$ is the fixed amplitude of the external source of radiation, and $\vec{E}^{(0)}_{ind}$ is the electric field induced by the sample being sensed. Due to we consider $\vec{E}^{(0)}_{pump} \perp$ to the sample, all the vectors $\vec{E}^{(0)}_{pump}$, $\vec{E}^{(0)}_{ind}$ and $\vec{p}^{(0)}$ are parallel and one can relate the amplitudes of the latter two as

$$E^{(0)}_{ind} = \beta(z)\, p^{(0)} \qquad (3)$$

where $\beta(z)$ is the coefficient *to be determined.*

Combining the Eqs. (1)-(3), we obtain

$$p^{(0)} = \frac{\alpha E^{(0)}_{pump}}{1 - \alpha\beta(z)}, \qquad (4)$$

i.e. the value $\alpha / [1 - \alpha\beta(z)]$ in arb. units measured by the s-SNOM setup. To decrease the influence of background and tip's shape, it's forced to oscillate as depicted in the Fig. 1, and the *instantaneous* signal (4) is averaged by Fourier transform

$$S_n = \frac{2}{T} \int_0^T \frac{\alpha \cos n\Omega t\, dt}{1 - \alpha\beta[z(t)]}, \quad \Omega = \frac{2\pi}{T}, \qquad (5)$$

which is done by the setup analogously.

Excitation of plasmons in 2D conducting plane material by a parallel dipole line

We start from the Coulomb field produced by the linear dipole of the tip, whose components on the exploring surface are:

$$E_x(x) = \frac{-4phx}{(x^2+h^2)^2}, \quad E_z(x) = \frac{2p\left(h^2 - x^2\right)}{(x^2+h^2)^2},$$

where h is height of the dipole above the surface. Theirs Fourier transforms are: $e_{xq} = -2\pi i \cdot pqe^{-|q|h}$, $e_{zq} = 2\pi \cdot p|q|\, e^{-|q|h}$.

Solution of Poisson equation can be found as:

$$\varphi^{(r)} = \int_{-\infty}^{\infty} \varphi_q^{(r,0)} e^{i\omega t - iqx - |q|z} \frac{dq}{2\pi}, \quad \varphi^{(t)} = \int_{-\infty}^{\infty} \varphi_q^{(t,0)} e^{i\omega t - iqx + |q|z} \frac{dq}{2\pi},$$

where $\varphi^{(r)}$ is the potential distribution above the surface (excluding the tip's dipole compound), and $\varphi^{(t)}$ is below it.

From the boundary conditions at the surface:

$$\begin{aligned} &-p \cdot 2\pi i q e^{-|q|h} + iq\varphi_q^{(r,0)} = iq\varphi_q^{(t,0)} \\ &\varepsilon_0 \left[p \cdot 2\pi |q|\, e^{-|q|h} + |q|\, \varphi_q^{(r,0)}\right] + \varepsilon_1 |q|\, \varphi_q^{(t,0)} = 4\pi\sigma_{\omega,q} \end{aligned}, \qquad (6)$$

where $\sigma_{\omega,q}$ is the Fourier components of the charge density $\sigma(x,t)$ induced on the surface, $\sigma(x,t) = \int_{-\infty}^{\infty} \sigma_{\omega,q} e^{i\omega t - iqx} \frac{dq}{2\pi}$.

Then, using continuity Eq. $\frac{\partial\sigma}{\partial t} + \frac{\partial j}{\partial x} = 0$, where $j(x,t)$ is the linear current in the surface given as $j_{\omega,q} = \gamma_\omega E_{x,\omega,q}$, where γ_ω is the surface conductivity, $E_{x,\omega,q} = iq\varphi_q^{(t,0)}$ is the E-field component producing the current in the surface, one can obtain $\varphi_q^{(r,0)}$ and:

$$\beta = \int_{-\infty}^{\infty} \frac{\varepsilon_1 - \varepsilon_0 - 4\pi|q|\, i\gamma_\omega/\omega}{\varepsilon_1 + \varepsilon_0 - 4\pi|q|\, i\gamma_\omega/\omega} |q|\, e^{-2h|q|} dq \qquad (7)$$

After transformations, Eq. (7) is reduced to

$$\begin{aligned} &\beta = \frac{1}{2\varepsilon_0 h^2}\left[1 - \frac{2\varepsilon_0}{\varepsilon_0 + \varepsilon_1}\mathcal{F}(2q_p h)\right], \; q_p = \frac{(\varepsilon_0+\varepsilon_1)\,\omega}{4\pi i \gamma_\omega}, \\ &\mathcal{F}(\zeta) = \zeta^2 e^{-\zeta}\left[\mathrm{Ei}(\zeta) + \pi i\right] - \zeta, \; \mathrm{Ei}(\zeta) = \int_{-\infty}^{\zeta} \frac{e^u}{u} du, \end{aligned} \qquad (8)$$

that for $\gamma_\omega = 0$ gives the result similar to [4]: $\beta = \frac{\varepsilon_1 - \varepsilon_0}{\varepsilon_0(\varepsilon_1+\varepsilon_0)} \frac{1}{2h^2}$.

Below, we consider γ_ω as Drude model for graphene conductivity: $\gamma_\omega = \frac{e^2 \mathcal{E}_F}{\pi\hbar^2(i\omega + \nu)}$, where $\mathcal{E}_F$ is the Fermi energy, and ν is electron scattering rate. Unless otherwise stated, in our calculations we take: $\omega = 120$ meV, $\mathcal{E}_F = 300$ meV, $\nu = 10$ meV, $\varepsilon_1 = 3.9$, $a = 30$ nm (tip's radius), $h_{min} = z_{min} - a = 5$ nm, and $h_{min} = z_{max} - a = 50$ nm (see Fig. 1).

Results

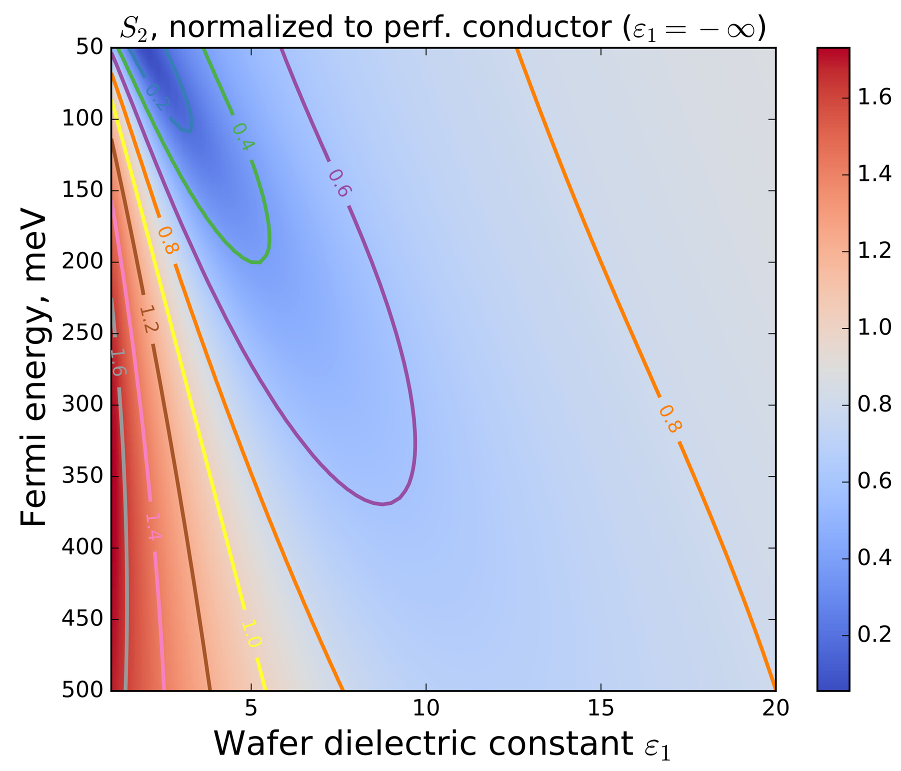

Fig. 2: Normalized S_2 value of signal for $a = 30$ nm

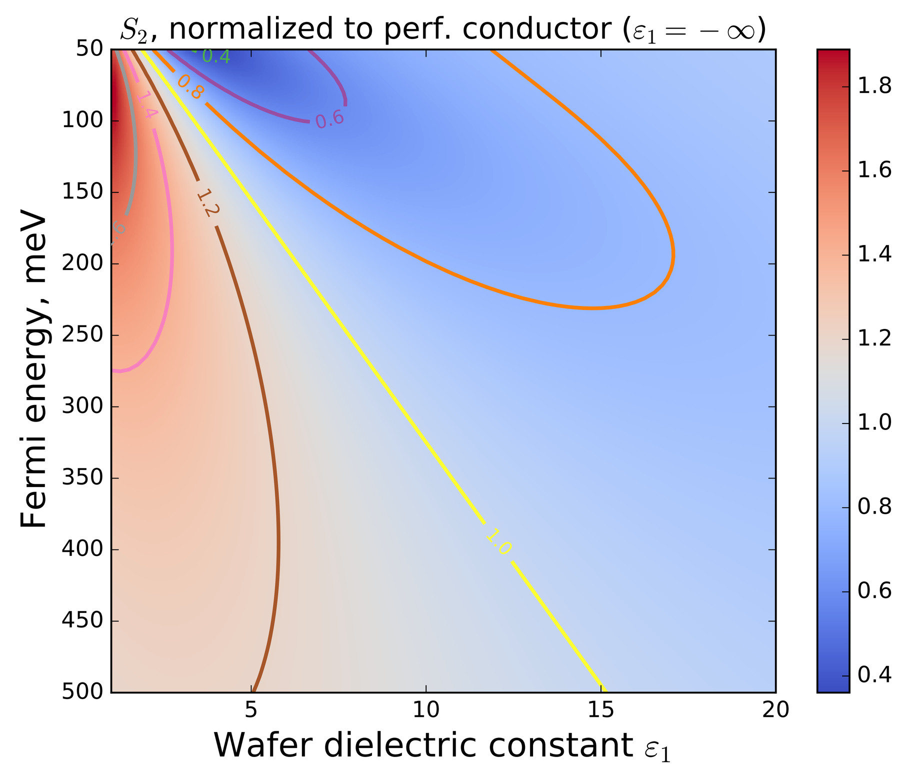

Fig. 3: Normalized S_2 value of signal for $a = 5$ nm

Scaling

In Fig. 4, $\lambda_{p0} = \mathrm{Re}\left\{2\pi/q_p\right\}$ and $Q = \omega/\nu$. The case $Q = 0$ is calculated for $\gamma_\omega = e^2\mathcal{E}_F/\pi\hbar^2\nu$ and $\lambda_{p0} = \mathrm{Im}\left\{2\pi/q_p\right\}$.

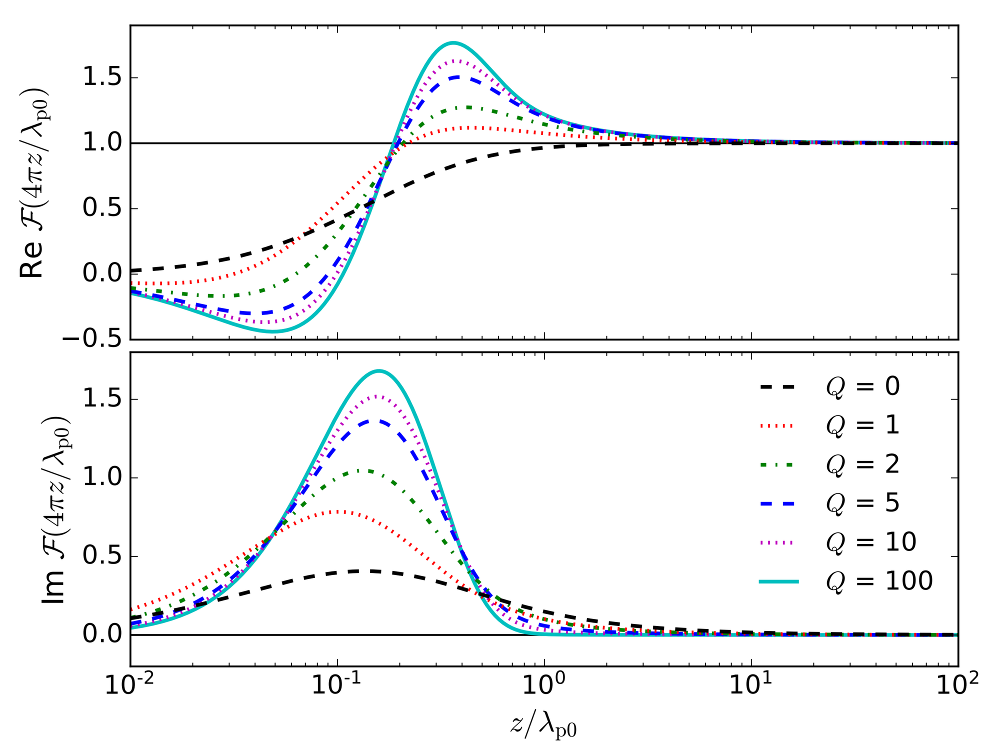

Fig. 4: Variable part's of β scaling versus normalized z calculated for different values of Q.

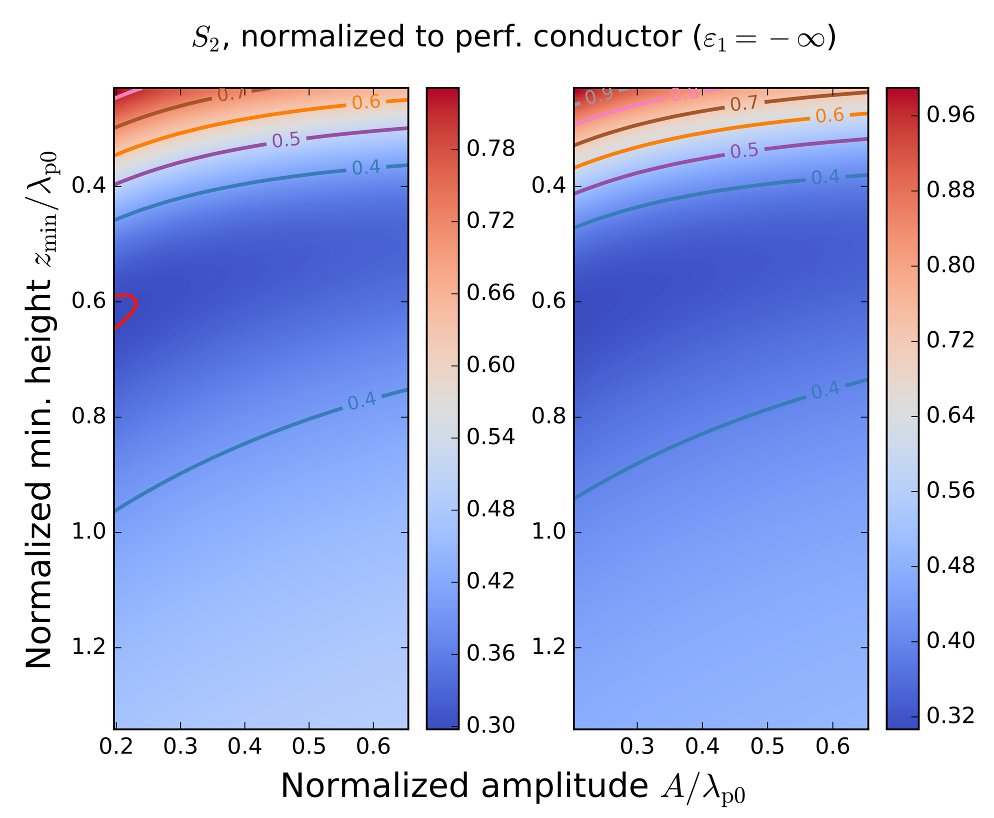

Fig. 5: Normalized S_2 value of signal for $a = 30$ nm (left panel) and 5 nm (right) panel versus z_{min}/λ_{p0} and A/λ_{p0}.

Conclusions

- s-SNOM response highly depends on the size of the tip and its regime of oscillation (z_{min} and z_{max}).
- If $z_{min}/\lambda_{p0} \gtrsim 0.4$, the normalized to perfect conductor (or to some other reference) response is almost independent of the size of the tip.
- Scaling dependence $\mathcal{F}(\zeta)$ may be used for selecting of s-SNOM tip's oscillation regime that best suites the explored surface.

References

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