Non-local optical response in silver-silicon-silver heterostructure system

Min S. Choi
Department of Electrical and Computer Engineering, University of Illinois at Chicago, Chicago, IL 60607, USA
Email: mchoi29@uic.edu

Gautam D. Stroscio
Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, USA

Introduction

Surface plasmon polaritons (SPP) in a thin metal film has been studied extensively in recent years due to their unique properties such as a huge increase of intensity [1], non-locality [2], etc. Recently, Trolle et al. [4] suggested a mechanism of optical excitation in silicon with photon energy below the direct bandgap using the non-locality of SPP in a silver thin film embedded in crystalline silicon. With a quantum mechanical point of view, this can be explained by the uncertainty principle, which asserts a wider spread of uncertainty in momentum space with high confinement in spatial space. In this abstract, we examine the indirect optical absorption in a silicon nanowire coupled with silver nanocavity.

Electric field in Ag-Si-Ag heterostructure

In this abstract, we perform a one dimensional analysis to calculate the optical power absorption rate in the structure shown in Figure 1. By solving the 2D wave equation assuming $\mathbf{E}(\mathbf{r},t) = E(\mathbf{r})e^{i\omega t}$, we get

$$E_x(z) = \begin{cases} -iA\frac{s_1}{\omega\epsilon_1\epsilon_0}e^{-s_1 z}e^{i\beta x} & \text{z} > h/2 \\ i\frac{A}{2}\frac{1}{\omega\epsilon_0}\left[\left(\frac{s_2}{\epsilon_2}-\frac{s_1}{\epsilon_1}\right)e^{(-s_1-s_2)h/2}e^{s_2 z}-\left(\frac{s_2}{\epsilon_2}+\frac{s_1}{\epsilon_1}\right)e^{(-s_1+s_2)h/2}e^{-s_2 z}\right]e^{i\beta x} & -h/2 < \text{z} < h/2 \\ i\frac{A}{2}\frac{1}{\omega\epsilon_0}\frac{s_1\epsilon_2}{s_2\epsilon_1}\left[\left(\frac{s_2}{\epsilon_2}-\frac{s_1}{\epsilon_1}\right)e^{-s_2 h}-\left(\frac{s_2}{\epsilon_2}+\frac{s_1}{\epsilon_1}\right)e^{s_2 h}\right]e^{s_1 z}e^{i\beta x} & \text{z} < -h/2 \end{cases} \quad (1)$$

and

$$E_z(z) = \begin{cases} -A\frac{\beta}{\omega\epsilon_1\epsilon_0}e^{-s_1 z}e^{i\beta x} & \text{z} > h/2 \\ -\frac{A}{2}\frac{1}{\omega\epsilon_0}\frac{\beta}{s_2}\left[\left(\frac{s_2}{\epsilon_2}-\frac{s_1}{\epsilon_1}\right)e^{(-s_1-s_2)h/2}e^{s_2 z}+\left(\frac{s_2}{\epsilon_2}+\frac{s_1}{\epsilon_1}\right)e^{(-s_1+s_2)h/2}e^{-s_2 z}\right]e^{i\beta x} & -h/2 < \text{z} < h/2 \\ -\frac{A}{2}\frac{\beta}{\omega\epsilon_0}\frac{\epsilon_2}{s_2\epsilon_1}\left[\left(\frac{s_2}{\epsilon_2}-\frac{s_1}{\epsilon_1}\right)e^{-s_2 h}-\left(\frac{s_2}{\epsilon_2}+\frac{s_1}{\epsilon_1}\right)e^{s_2 h}\right]e^{s_1 z}e^{i\beta x} & \text{z} < -h/2 \end{cases} \quad (2)$$

where A is incident field intensity, s_i and β decay constants, ϵ_i dielectric functions, and ω the energy. With appropriate boundary conditions in each region, we get a dispersion relation

$$s_i^2 = \beta^2 - k_0^2\epsilon_i \ \ (i = 1, 2), \quad (3)$$

and the continuity of E_x at $z = -h/2$ gives the dispersion equation

$$s_2\epsilon_1 - s_1\epsilon_2 e^{s_1 h} = 0 \quad (4)$$

which has to be satisfied in order for solutions to exist. The equations () and () are solved numerically. The frequency- and wavevector- dependent dielectric function of silicon, ϵ_2, is obtained empirically using time-dependent density functional theory [5], and the dielectric function of silver, ϵ_1, is calculated using Drude-Lorentz model. [6]

The time-averaged optical power absorption rate is given by

$$P_{abs} = \frac{\omega}{2}\int \mathbf{P}(\mathbf{r},\omega)\cdot\mathbf{E}^*(\mathbf{r},\omega)d\mathbf{r} \quad (5)$$

where the polarization density, $\mathbf{P}$, is given by $\mathbf{P}(\mathbf{r},\omega) = \epsilon_0\tilde{\chi}\mathbf{E}(\mathbf{r},\omega)$. The non-local optical power absorption can be computed by Fourier-transforming the equation (5) to get the sum of contributions of SPP over the momentum space.

Results and Discussion

The non-local optical power absorption in silicon and silver are plotted in Figures (2) and (3), respectively. In silicon, several distinct peaks are appeared at $\hbar\omega$ =1.4 eV, 2.35 eV, 2.5 eV, and 2.7 eV. These results overlap well with our previous calculation of the local density of states of plasmons in silver

ISBN 978-0-692-50554-0

[7], and also with an experiment of hot luminescence from a similiar structure. [8]

References

[1] M. Kerker et al. ”Surface enhanced Raman scattering (SERS) by molecules absorbed at spherical particles.”, *Appl. Optics.* Vol 19, No 19, 3373 (1980).

[2] Ru, E., and Etchegoin, P. ”Principles of surface-enhanced Raman spectroscopy and related plasmonic effects.” *Amsterdam: Elsevier* (2009).

[3] S. Maier. *Plasmonics: Fundamentals and Applications.* New York: Springer, (2007).

[4] M. Trolle. ”Microscopic Theory of Linear & Nonlinear Optical Response: Zinc-blende Semiconductors.” *Thesis*. Aalborg University, (2011).

[5] ”The Elk FP-LAPW Code.” *The Elk FP-LAPW Code.* Web. ¡http://elk.sourceforge.net/¿.

[6] Rakic et al., ”Optical properties of metallic films for vertical-cavity optoelectronic devices”, *Applied Optics*, Vol. 37, 22, 5271 (1998)

[7] Choi et al., ”Numerial analysis of local density of state of plasmons in Si-SiO2-silver nanocavity system” *Proceedings of IEEE International Workshop on Computational Electronics*. (2014)

[8] Chang-Hee Cho, Carlos O. Aspetti, Joohee Park and Ritesh Agarwal, *Nature Photonics*, 2013.

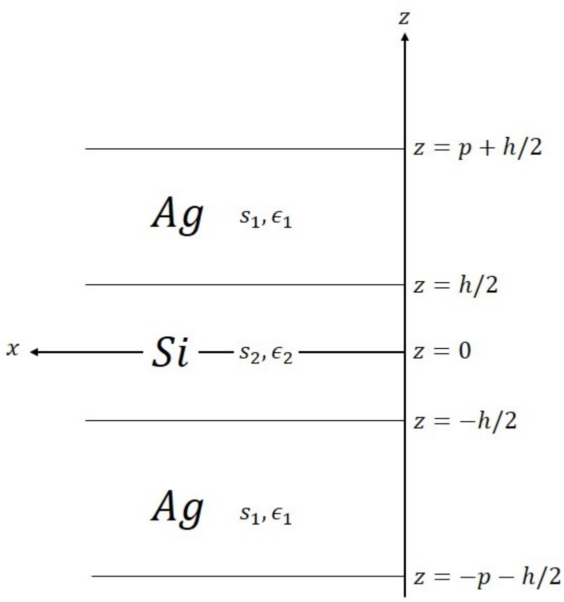

Fig. 1: Si-Ag-Si heterostructure

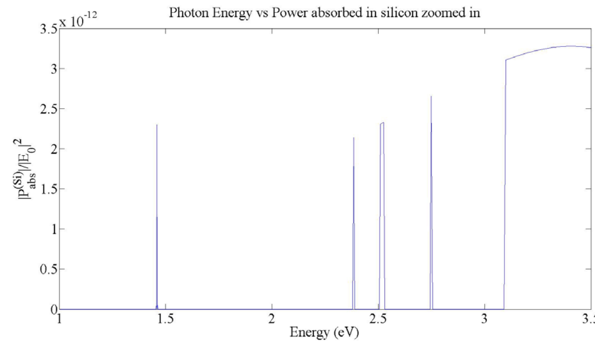

Fig. 2: Power absorption rate in silicon nanowire vs energy of photon

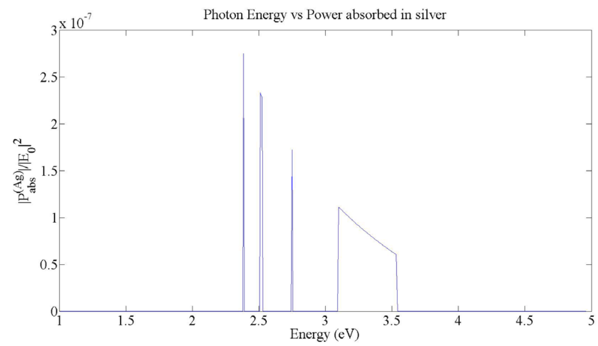

Fig. 3: Power absorption rate in silver vs energy of photon