Enhancement of electromagnetic fields caused by subwavelength rectangular cavities

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Outline :

1. Introduction : A model problem for diffraction by rough surfaces
2. Integral representation of the Green function
3. Asymptotics as the width of the cavity tends to 0
4. Interaction of 2 close cavities
5. Conclusions and perspectives

1. Diffraction by rough surfaces

- Ebbesen et al (Nature, 1998) have shown that, at certain frequencies, the rugosity of metallic surfaces can create fields with intensities that can be very large locally (up to a factor 10^3)

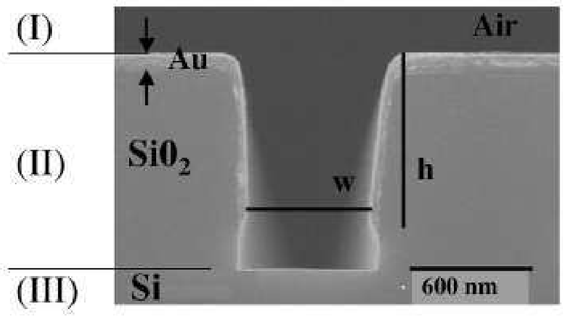
- The localization of the fields is due to resonance phenomena in the sub-wavelength cavities formed by the non-smooth surface, or to surface waves $\longrightarrow$ SERS

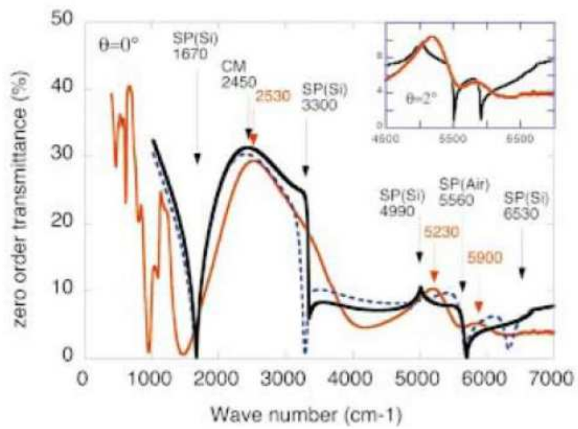
- Because it is sensitive to lengthscales smaller than the wavelength, this phenomenon has many potential applications : imaging of single molecules, optical filters, . . .

- However, control of SERS requires great care in the design of the gratings (instability of the hot spots)

- This work was started following discussions with A. Barbara and P. Quémerais (Institut Néel Grenoble).
  Goal : Design of surfaces with structured rugosities that allow good control of the amplified fields

Experimental results

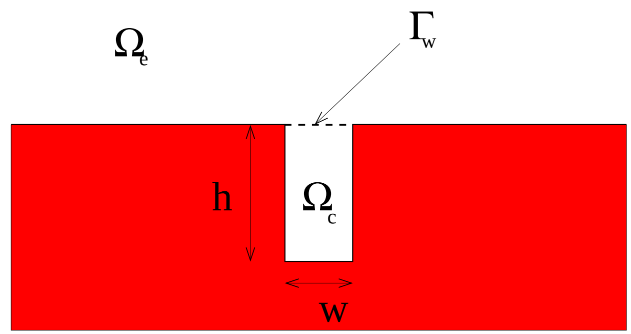




A. Barbara, P. Quémerais, E. Bustarret, T. Lopez-Rios, PRB 66, 161403(R) (2002)

G.A. Kriegsmann, SIAP, 65, 24-42 (2001)

The geometry of a model problem



The metallic surface is assumed to be perfectly conducting. The width of the cavity is small compared to the wavelength.

3D configuration with invariance along x_3 direction, $k = \omega\sqrt{\varepsilon\mu}$

$\Omega_e = \mathbf{R}^{2,+}, \quad \Omega_c = (-w/2, w/2) \times (-h, 0)$

We are interested in the Green function G_w defined in $\Omega := \Omega_e \cup \Omega_i \cup \Gamma_w$, solution to

$$\begin{cases} (\Delta + k^2)G_w(X,Y) = \delta_Y(X) & X \in \Omega \\ \dfrac{\partial}{\partial n_X} G_w(X,Y) = 0 & X \in \partial\Omega \\ \text{radiation condition} & \end{cases}$$

2. Representation of G_w

G_e = Green function in the upper half-plane

$$\begin{cases} G_e(X,Y) &= \frac{-i}{4}\left(H_0^{(1)}(k|X-Y|) + H_0^{(1)}(k|X-\tilde{Y}|)\right), \qquad \tilde{Y} = (y_1, -y_2) \\ \frac{\partial}{\partial n_X} G_e(X,Y) &= 0 \qquad X \in \partial \mathbf{R}^{2+} \\ |X|^{1/2}(\partial_r - ik)G_e(X,Y) &\to 0 \qquad |X| \to \infty \end{cases}$$

G_c = Green function in the cavity

$$\begin{cases} G_c(X,Y) &= \frac{4}{hw}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\cos(\frac{m\pi}{w}(x_1+w/2))\cos(\frac{m\pi}{w}(y_1+w/2))}{k^2-(\frac{m\pi}{w})^2-(\frac{n\pi}{h})^2} \\ & \quad \times \cos(\frac{n\pi}{h}(x_2+w))\cos(\frac{n\pi}{h}(y_2+w)) \\ \frac{\partial}{\partial n_X} G_c(X,Y) &= 0 \qquad X \in \partial\Omega_i \end{cases}$$

Representation for G_w : for $Z \in \mathbf{R}^{2+}$

$$\left\{ \begin{array}{lclr} G_w(Y,Z) & = & G_e(Y,Z) \; + \displaystyle\int_{\Gamma_w} \frac{\partial}{\partial n_e} G_w(x_1,0,Z) G_e(x_1,0,Y) dx_1, & Y \in \mathbf{R}^{2+} \\ G_w(Y',Z) & = & \displaystyle\int_{\Gamma_w} \frac{\partial}{\partial n_i} G_w(x_1,0,Z) G_c(x_1,0,Y') dx_1, & Y' \in \Omega_i \end{array} \right.$$

We obtain an integral equation for $\phi(y) = \dfrac{\partial}{\partial x_2} G_w(wx,0,wy,0)$

$$S_w(k)(y)\phi(x) \quad = \quad \frac{-1}{w} G_e(wy,0,Z)$$

with $\qquad S_w(k)\phi(y) = \displaystyle\int_{-1/2}^{1/2} \phi(x)(G_e + G_c)(wx,0,wy,0)dx$

3. Asymptotics as $w \to 0$

$$G_e(wx,0,wy,0) = \frac{-i}{2} H_0^{(1)}(kw|x-y|)$$

$$\sim \frac{1}{\pi}\ln|kw(x-y)| \;+\; \frac{1}{\pi}(\gamma - \ln(2)) \;-\; i/2$$

$$G_c(wx,0,wy,0) = \frac{4}{hw}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\cos(\frac{m\pi}{w}(wx+w/2))\cos(\frac{m\pi}{w}(wy+w/2))}{k^2-(\frac{m\pi}{w})^2-(\frac{n\pi}{h})^2}$$

$$\sim \frac{4}{hw}\sum_{n=0}^{\infty}\frac{1}{(k^2-\frac{n\pi}{h})^2}$$

$$+\frac{1}{\pi}\left(2\ln(2)+\ln\left|\sin(\frac{\pi}{2}(x+y+1))\;\sin(\frac{\pi}{2}(x-y))\right|\right)$$

$$+\frac{4h}{\pi^2 w}\sum_{m=1}^{\infty}\cos(m\pi(x+1/2))\cos(m\pi(y+1/2))\;O(\left(\frac{w}{m}\right)^2)$$

The first term in the expansion of G_c has the form

$$\frac{4}{hw}\sum_{n=0}^{\infty}\frac{1}{k^2-(\frac{n\pi}{h})^2} \quad = \quad \frac{2}{kw}\left(\frac{1}{hk}+\mathrm{cotan}(hk)\right) \;=:\; \frac{\alpha_k}{w}$$

Its poles are the resonances of a 1-d cavity of length h

We decompose the kernel as

$$\begin{aligned}(G_e+G_c)(wx,0,wy,0) \quad &= \quad \theta_w(k) \;+\; s_1(x,y) \;+\; s_2(x,y)w \\ &\quad + s_3(k,x,y)w^2\ln(w) \;+\; s_{4,w}(k,x,y)w^2\end{aligned}$$

where

$$\begin{cases} \theta_w(k) \quad = \quad \dfrac{\alpha_k}{w} + \dfrac{1}{\pi}\ln|kw| + \dfrac{1}{\pi}(\ln(2)+\gamma) - i/2 \\ s_1(x,y) \quad = \quad \dfrac{1}{\pi}\ln\left|(x-y)\sin(\dfrac{\pi}{2}(x+y+1))\sin(\dfrac{\pi}{2}(x-y))\right| \end{cases}$$

The integral equation and resonances

$$S_w(k) \quad = \quad \theta_w(k) < 1, . > + S_1 + wS_2 + w^2(\ln(w)S_3(k) + S_{4,w}(k))$$

$S_1 : \tilde{H}^{-1/2} \longrightarrow H^{1/2}$ is invertible
$S_j : \tilde{H}^{-1/2} \longrightarrow H^{1/2}, 2 \leq j \leq 4$ are compact

$$\begin{aligned} S_w(k) &= \theta_w(k) < 1, . > + \left[I + w \left(S_2 + w^2(\ln(w)S_3(k) + S_{4,w}(k)) \right) S_1^{-1} \right] S_1 \\ &= \theta_w(k) < 1, . > + I_w(k) \end{aligned}$$

with $I_w(k)$ invertible for w small enough.

$$S_w^{-1}(k) \quad = \quad I_w^{-1}(k) - \frac{\theta_w(k) \ < I_w^{-1}., 1 >}{\theta_w(k) < 1, I_w^{-1}(k)(1) > +1} < I_w^{-1}(k), 1 >$$

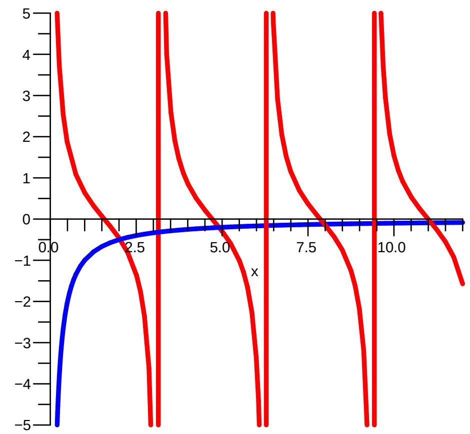
The resonances are the zeros of $\quad \theta_w(k) < 1, I_w^{-1}(k)(1) > +1$

Recall that

$$\theta_w(k) \quad = \quad \frac{\alpha_k}{w} - \frac{1}{\pi}\ln|kw| - \frac{1}{\pi}(\ln(2)-\gamma) + i/2$$

$$\alpha_k \quad = \quad \frac{4}{h}\sum_{n=0}^{\infty}\frac{1}{k^2-(\frac{n\pi}{h})^2} = \frac{2}{k}\left(\frac{1}{hk} + \mathrm{cotan}(hk)\right)$$

Let k_0^n denote a zero of α_k :



The k_0^n's are the resonances of a limiting one-dimensional cavity $(-h,0)$

$$\begin{cases} g''(s)+k^2 g(s) & = & \delta_0(s) \quad \text{in } (-h,0) \\ g'(-h)=g'(0) & = & 0 \end{cases}$$

then $\quad \alpha_k = g(0)$

The Rouché theorem shows that when w is small enough, there is a unique resonance of the open cavity k_w^n near k_0^n.

$$k_w^n - k_0^n \quad = \quad -\frac{1}{2i\pi} tr \int_{|k-k_0^n|=r_n} (k - k_0^n) S^{-1}(w,k) \frac{dS}{dk}(w,k)\, dk$$

Moreover, we have the following asymptotics for k_w^n :

$$\begin{aligned} k_w^n \quad &= \quad k_0^n \ + \ \frac{\sin^2(hk_0^n)}{1+\cos^2(hk_0^n)} \frac{k_0^n}{4\pi h}\, w \ln(w) \\ &+ \ \left(\frac{1}{\pi} (\ln(2) + \gamma) - i/2 + \frac{1}{\pi} \ln(k_0^n) + < 1, S_1^{-1}(1) >^{-1} \right) \frac{\sin^2(hk_0^n)}{1+\cos^2(hk_0^n)} \frac{k_0^n}{2h}\, w \ + \ o(w) \end{aligned}$$

The resonances are located in the lower-half of the complex plane

$$Im(k_w^n) \quad = \quad \frac{-\sin^2(hk_0^n)}{1+\cos^2(hk_0^n)} \frac{k_0^n}{4h} w \ + \ o(w) \ = \ \eta(h, k_0^n) w + o(w)$$

Main result (far field)

Let $X, Y \in \mathbf{R}^{2+}, X \neq Z$

Away from the resonances (i.e., for some $r > 0$, $|k - k_0^n| > r$ for all $n \in \mathbf{N}$)

$$G_w(X,Y) \quad = \quad G_e(X,Y) \; - \; \frac{w}{4\alpha_k} \frac{S_1^{-1}(1)}{< 1, S_1^{-1}(1) >} H_0^{(1)}(k|X|) H_0^{(1)}(k|Y|) \; + \; o(w)$$

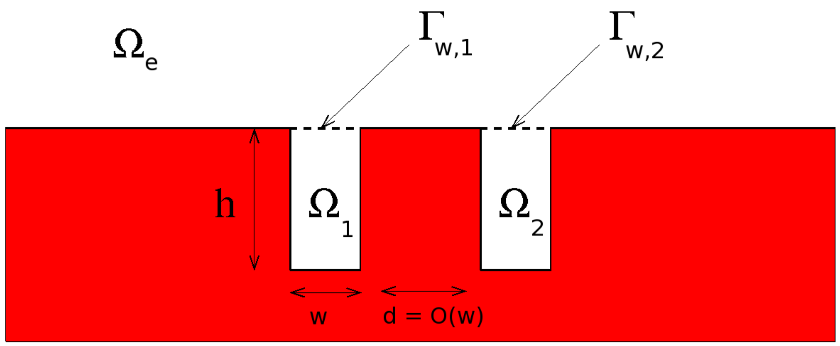
In the resonance zone

$$G_w(X,Y) \quad = \quad G_e(X,Y) \; + \; \sum_{n=0}^{\infty} \frac{c_w^n \, g_w^n(X) g_w^n(Y)}{k - k_w^n} \; + \; F_w(k, X, Y)$$

where

- c_w^n is a constant, that only depends on h
- g_w^n satisfies $(\Delta + k^2) g_w^n(X) \; = \; d_w^n(x_1)\delta_0(x_2)$, $\quad d_w^n$ expressed in terms of $I_w^{-1}(k_w^n)$
- $F_w(k, X, Y)$ holomorphic
- The amplification is proportionnal to $\dfrac{c_w^n}{\eta(h, k_0^n)} \ln(w)$

4. Talking cavities



Given $f \in L^2(\Omega_e)$ with compact support, find u s.t.

$$\begin{cases} \Delta u + k^2 u = f & \text{in } \Omega = \Omega_e \cup \Omega_1 \cup \Omega_2 \\ \partial_\nu u = 0 & \text{on } \partial\Omega \\ \lim_{|x|\to+\infty} \sqrt{|x|}\,(\partial_r u(x) - iku(x)) = 0 & \end{cases}$$

$(\varphi_1, \varphi_2) = (\partial_\nu u_{|\Gamma_{w,1}}, \partial_\nu u_{|\Gamma_{w,2}})$ solution to the system of integral equations

$$S_w(k) \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \int_{\Gamma_{w,1}} \begin{pmatrix} G_1 + G_e \\ G_e \end{pmatrix} \varphi_1 + \int_{\Gamma_{w,2}} \begin{pmatrix} G_e \\ G_2 + G_e \end{pmatrix} \varphi_2 = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$$

Asymptotics $\Gamma_{w,i} \to \Gamma$

$$\begin{aligned} S_w(k) &= \Theta_w(k) + S_1 + S_2 w + \text{remainder} \\ &= \Theta_w(k) + L_w(k) \end{aligned}$$

where S_1 is invertible
S_2 and the remainder are compact $\quad (\tilde{H}^{-1/2}(\Gamma))^2 \longrightarrow (H^{1/2}(\Gamma))^2$

and where

$$\Theta_w(k) \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \begin{pmatrix} \frac{\alpha_k}{w} + \delta_2 + \frac{\ln(wk)}{\pi} & \delta + \frac{\ln(wk)}{\pi} \\ \delta + \frac{\ln(wk)}{\pi} & \frac{\alpha_k}{w} + \delta_2 + \frac{\ln(wk)}{\pi} \end{pmatrix} \int_\Gamma \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

Inversion of $S_w(k)$

$$S_w^{-1}(k) = L_w^{-1}(k) - L_w^{-1}(k)\theta_w(k)F_w^{-1}(k) \begin{pmatrix} < \cdot, L_w^{-1}(k)e_1 > \\ < \cdot, L_w^{-1}(k)e_2 > \end{pmatrix}$$

where $\quad F_w(k) = I + \theta_w(k) \begin{pmatrix} < e_1, L_w^{-1}(k)e_1 > & < e_1, L_w^{-1}(k)e_2 > \\ < e_1, L_w^{-1}(k)e_2 > & < e_2, L_w^{-1}(k)e_2 > \end{pmatrix}$

The resonances (the poles of $S_w^{-1}(k)$) are the poles of the matrix-valued function $F_w^{-1}(k)$

In the neighborhood of each zero of α_k there are exactly 2 resonances

$$\begin{aligned} k_w^{n,+} &= k_0^n + \eta_{1,1}^+ w \ln(w) + \eta_{1,0}^+ w + o(w) \\ k_w^{n,-} &= k_0^n + \eta_{1,0}^- w + \eta_{2,0}^- w^2 + \eta_{3,1}^- w^3 \ln(w) + \eta_{3,0}^- w^3 + o(w^3) \end{aligned}$$

and in particular

$$\begin{aligned} Im(k_w^{n,+}) &= \frac{w}{\alpha'(k_0^n)} + o(w) \\ Im(k_w^{n,-}) &= Im(\eta_{3,0}^-) w^3 + o(w) \end{aligned}$$

Asymptotics of the field

For a fixed $y \in \Omega_e$, if k is close to a resonance, then

$$u(y) \quad = \quad u_e(y) + \sum_n \frac{\kappa_w^{n,+}(y)}{k - k_w^{n,+}} + \sum_n \frac{\kappa_w^{n,-}(y)}{k - k_w^{n,-}} + \text{holomorphic}(k, y)$$

The functions $\kappa_w^{n,\pm}$ solve the Helmholtz equations in Ω_e

$$\begin{cases} (\Delta + k^2)\kappa_w^{n,+} & = & c_n^+ w \delta_0 \\ (\Delta + k^2)\kappa_w^{n,-} & = & c_n^- w^3 \partial_{x_1} \delta_0 \end{cases}$$

The spatial singularity sensed in the far field when k is close to $k_w^{n,+}$ is asymptotically that of a dipole placed on the metallic plane

When k is close to $k_w^{n,-}$, the singularity is that of a quadripole

The near field concentrates near the top of the cavities : in the cavities it behaves like

$$u(y) \quad = \quad \sum_n \frac{\gamma_w^{n,+}(y)}{k - k_w^{n,+}} + \sum_n \frac{\gamma_w^{n,-}(y)}{k - k_w^{n,-}} + \text{holomorphic}(k, y)$$

When k is close to $k_w^{n,+}$

$$\frac{\gamma_w^{n,+}(y)}{k - k_w^{n,+}} \quad = \quad \frac{c^{n,+}}{w}(1 + O(w\ln(w))), \qquad y \in \Omega_1 \cup \Omega_2$$

while when k is close to $k_w^{n,+}$

$$\frac{\gamma_w^{n,-}(y)}{k - k_w^{n,-}} \quad = \quad \begin{cases} \dfrac{c^{n,-}}{w^2}(1 + O(w)) & y \in \Omega_1 \\[2ex] -\dfrac{c^{n,-}}{w^2}(1 + O(w)) & y \in \Omega_2 \end{cases}$$

Consistent with the results of Le Perchec et al (Phys. Rev. Letter, 97 (2006), 036405)

Perspectives

- periodic and quasi-periodic system of cavities

- coupling with a small object placed on top of the cavity (and inverse problem)

- can one consider the substrate as a real metal ?

- design problems