

A GENERALIZED GEOMETRIC FACTOR FOR UNIFIED SCALING LAW FOR BIO-SENSOR BASED ON NANOSTRUCTURES OF GOLD

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Abstract- This paper presents a unified scaling law for biosensor using nanogolds in various structures of nanorods, nanoshells and nanoslits. Analytic formulas are developed by a generalized geometric factor (G) for the resonance wavelength and the associate sensitivity, where G depends on structure types and is defined by: the length and width ratio (for nanorod); the inner and outer diameter ratios of the gold-coated silica shell (for nanoshell); the period (for surface mode) and the ratio of slit height and slit width (for cavity mode). The general feature of the figure of merit and its optimal conditions are derived. The analytic formulas are justified by numerical solutions and show the nonlinear features for a wide range of resonance wavelength.

Keywords - Surface Plasmon Resonance; Biosensor Sensitivity; Nanogold; Nanoslit; Nanoshell; Scaling Laws.

I. INTRODUCTION

Bio-imaging, bio-sensing, drug delivery, diagnostics and selective phototherapeutics have been the focus of the applications of metal nanoparticles in biomedicine [1-4]. Various nanoparticles have been explored for the use of surface plasmon resonance (SPR) including shapes in spheres, rods, boxes, cages and shells [4-8]. By changing the shape of nanoparticles from spheres to nanorods, the absorption and scattering peaks change from visible to the near-infrared (NIR) regime. Comparing to the visible light, light in the NIR regime offers the advantages of larger absorption and scattering cross sections and much deeper penetration depth in tissues [1-5]. The red-shift of the absorption peak in nanorods is governed by the aspect ratio (defined by as the ratio of the length to the cross-sectional diameter), whereas it is governed by the shell thickness in nanoshells [6].

The performance of nanosensors is characterized by not only the index sensitivity (M), but more importantly, the figure of merit $FOM = M/FWHM$, where FWHM is the full width at half maximum of the extinction profiles of the nanoparticles. The index-sensitivity defined by the red-shift of the absorption peak per unit change of the refractive index of the sensing medium, has been studied for nanoparticles of various shapes [9,10]. Sensitivity and figure of merits for various nanostructures have been studied by the author numerically [11-13]. This paper presents, for the first time, the analytic formulas and a unified scaling law based on a generalized geometric factor which unifies various nanostructures.

II. THE UNIFIED THEORY

The Geometric Factor (G)

As shown in Figure 1, three type of nanostructures are unified by a geometric factor (G) defined by:

$G=B/A$, the ratio of rod length (B) and width (A);
 $G= r/R$, the ratio of the inner (r) and outer diameter (R) of the gold-coated silica shell;
 $G=P$ (for surface mode in nanoslit); and
 $G=h/d$ (for cavity mode in nanoslit).

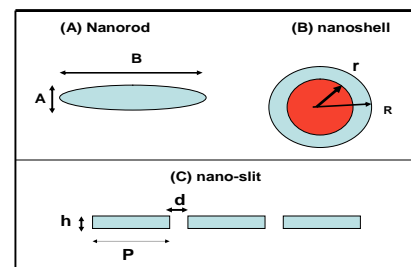


Fig. 1 A geometric factor (G) defined in various nanostructure of (A) nanorod, (B) nanoshell and (C) nanoslit.

The Permittivity of Gold

The real (ϵ') and imaginary part (ϵ'') of gold relative permittivity, reported by Johnson and Christy [7], may be fit to the following nonlinear equations [11,12]:

$$\epsilon'(\lambda) = 12.5 - 0.02\lambda - 0.0000333\lambda^2,$$

for wavelength range of (550-2000) nm;

$$\epsilon''(\lambda) = 0.00005\lambda^2 - 0.071\lambda + 25.65,$$

for short wavelength range of (500-700) nm;

$$\epsilon''(\lambda) = 0.000011\lambda^2 - 0.0127\lambda + 4.6,$$

for long wavelength >700 nm.

The Resonance Wavelength and Sensitivity (M)

As shown in Fig. 2, the resonance wavelength versus the geometric factor (G) and medium refractive index (n) for the linear case (B-1) and nonlinear case (B-2). Fig. 3. shows the

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sensitivity (M) associate to Fig. 2 which is based on a nonlinear equation of G and n,

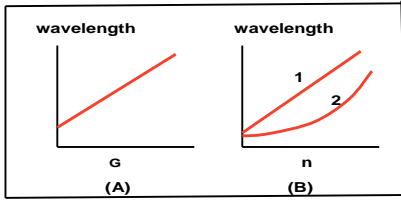


Fig. 2 Resonance wavelength versus G and medium index (n) for the linear case (B-1) and nonlinear case (B-2).

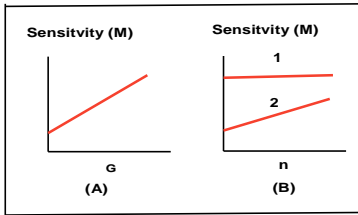


Fig. 3. The sensitivity (M) associate to Fig. 2.

$$\lambda = a + (b + cn + dn^2)G \quad (1)$$

which is linear in G but nonlinear in n. The associate sensitivity defined by the derivative of Eq. (1) $M = d\lambda / dn$

$$M = (c + 2dn)G \quad (2)$$

which is shown in Fig.3 for both linear and nonlinear cases. We will show later that the above general formulas are based on our early published numerical results [11,12].

The Figure of Merit (FOM)

As shown in Fig. 4, given the spectral of gold, one may find the full width at half maximum (FWHM) in wavelength which is then converted to the geometric factor (G) based on the linear relationship of Eq. (1). The FWHM may be expressed by $FWHM = e + (G-f)^2$ which combined with Eq. (2) for M gives us the figure of merit (FOM)=M/FWHM. The optimal G^* for maximum FOM is given by $d(FOM)/dG (G=G^*)=0$ to obtain

$$G^* = f / (1 + 0.5c^2 / FWHM) \quad (3)$$

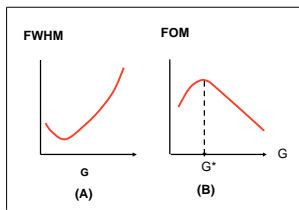


Fig. 4. Full width at half maximum (FWHM) of gold and the figure of merit (FOM) showing an optimal value at $G=G^*$

The Numerical Results

Fig. 5 and 6 show FWHM and FOM versus the gold nanorod aspect ratio $G=B/A$ based on numerical calculations [11], which shows the optimal G^* about 4.0 corresponding o a resonance wavelength about 810 nm. A diode laser at 810 nm is recommended for biosensor using gold-coated fiber sensor [13]. The resonance wavelength in nanogold rods given by a fit equation [11]

$$\lambda = 395 + (86.5n + 3.5n^2 - 28)R + 5n^3 \quad (4)$$

which gives the fit equation for the sensitivity (M)

$$M = (86.5 + 7n)R + 15n^2 \quad (5)$$

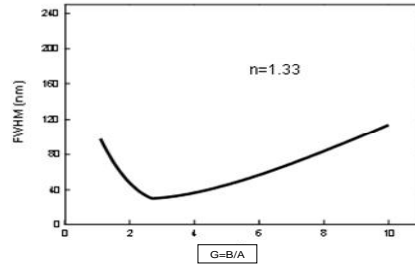


Fig. 5. Full width at half maximum (FWHM) versus the gold nanorod aspect ratio $G=B/A$ based on numerical calculations, after Lin [11].

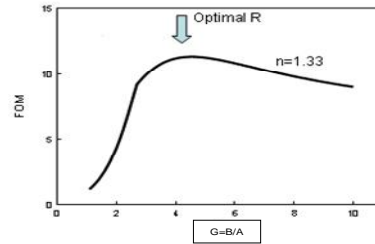


Fig. 6 Same as Fig. 5, but for FOM versus G, after Lin [11].

NANOSHELL

Fig. 7 shows the FOM versus the reduced thickness $T=t/R=1/G - 1$, based on numerical calculations [12]. which shows the optimal T^* about 0.15 (or thickness about $t=0.13R$) or G^* about 0.88, corresponding o a resonance wavelength about 810 nm.

The resonance wavelength in nanoshell is given by a fit equation [12]

$$\lambda = a + b \exp(-T/c) \quad (6)$$

with $a = 568.2$, $b = 761.5$ and $c = 0.11117$, which is more accurate than that of Jain and El-Sayed [3] ignoring the nonlinear term in Eq. (3). It should be noted that the scaling fit coefficients (a,b,c) are slightly influenced by the refractive index of the core and the sensing medium. The fit equation for the sensitivity (M) is given by

$$M = a' + b' \exp(-T/c'), \quad (7)$$

where $a' = 127.68$, $b' = 596.18$, and $c' = 0.1023$ for a silica core ($n_1 = 1.45$) in water medium ($n = 1.33$).

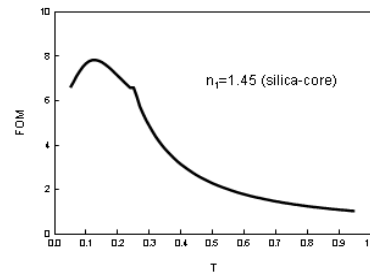


Fig. 7. FOM versus the reduced thickness $T=t/R=1/G -1$, based on numerical calculations, after Lin [12].

Nanoslit

The extraordinary transmission of a TM wave in nanoslits was explained by two resonances: the surface plasmon wave propagating along the metallic interface and the gap resonance inside the nanoslit cavity (cavity mode) [14-16].

(a) Surface modes [14]

Fig. 8 and 9 show the FWHM and FOM versus the slit period (P) based on numerical calculations (J.T. Lin, unpublished), which shows the optimal P* about 500 nm, corresponding to a resonance wavelength about 660 nm.

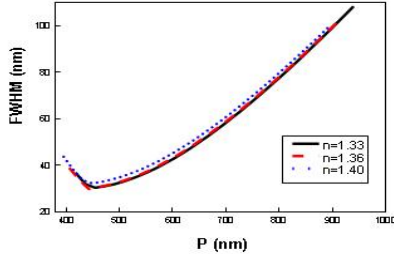


Fig. 7. FWHM versus the slit period (P), based on numerical calculations for the surface plasmon mode (after Lin, unpublished).

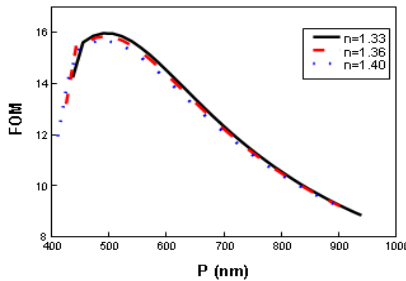


Fig. 8 Same as Fig. 7, but for FOM.

The resonance wavelength for the surface mode is given by a fit equation

$$\lambda = nP + 3.73n^2 \tag{8}$$

which gives the fit equation for the sensitivity (M)

$$M = P + 7.46n \tag{9}$$

Eq. (8) and (9) show that the surface mode resonance is characterized by a geometric factor given by $G=P$.

(b) Cavity modes [15]

In the asymptotic approximation, the resonance wavelength is given by [15]

$$\lambda = \left(\frac{2N_0h}{q} \right) (1 + h_0/h) \tag{10}$$

Where N_0 is an effective refractive index and q is the number of resonance mode. From above equation, one expects $[N_0h]$ will be the universal ratio for the resonance wavelength. Moreover, this scaling ratio can be further reduced to a geometric factor $[nh/d]$, since N_0 is proportional to n/d .

The refractive index sensitivity, in the asymptotic regime, can be easily derived from Eq. (10) as follows,

$$M_n = \frac{\partial \lambda}{\partial n} = \frac{2}{q} (h - h_0) F(d) - \frac{2N_0}{q} \left[\frac{\partial}{\partial n} h_0 \right] \tag{11}$$

which is an increasing function of the nanoslit geometric factor $G= (h/d)$. Therefore, one shall also expects an optimal ratio h/d for the FOM of the cavity mode. Greater details based on numerical calculation will be shown elsewhere [15].

III.CONCLUSIONS

A unified scaling law for biosensor using nanogolds in various structures is presented. Analytic formulas, Eq. (1) and (2), based on a generalized geometric factor (G) for the resonance wavelength and the associate sensitivity is derived, where G is defined by the length and width ratio in nanorod; the ratio of the inner and outer diameter of the gold-coated silica shell; the period (for surface mode) and the slit height and width ratio (for cavity mode). The general feature of the figure of merit the figure of merit (FOM)=M/FWHM. The optimal G^* for maximum FOM is derived, Eq. (3). The analytic formulas are justified by numerical solutions and show the nonlinear features for a wide range of resonance wavelength.

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