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Configuration-dependent enhancements of electric fields near the quadruple and the triple junction

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We investigated the behavior of electric field near the junction composed of metal, dielectric, and vacuum. By assuming that the junction is symmetric along one direction, we use the two-dimensional model to calculate the electric field near the junction as a function of configuration. For the triple junction of metal-vacuum-dielectric, the electric field is found to be enhanced and reduced according to the ratio of dielectric and vacuum portions. The use of the same model also leads to the result that the quadruple junction of metal-vacuum-dielectric-vacuum yields the much larger field enhancement than the triple junction. This dielectric enhancement results in the more profound effect in the field intensity at the junction by combining the shape enhancement of the metal.

Materials discussed: diamond, GaN, metal, dielectric

I. INTRODUCTION

Dielectric is considered to play the role only to reduce the electric field intensity. For a long time, however, the strongly enhanced electric field has often been observed in the vicinity of the contact between metal and dielectric.[1-4] Such an unexpected field enhancement or breakdown, called the triple junction effect, is considered to be due to dielectric. The most significant experiment to reveal the dielectric effect on the field

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enhancement was made by the Geis group.[5] They measured the enhanced field emission when the diamond portion was increased into the vacuum for the triple junction configuration. In the same sense, the contact angle of the junction and the volume conductivity of the media are considered to play a role in the enhancement mechanism.[6-8] The metal-dielectric contact with voids was found to result in the vacuum insulation breakdown.[9-11] Theoretically, Schächter[12] used a two-dimensional model of the triple junction to find that the field emission current density was proportional to the dielectric constant.

The field enhancement observed at the triple junction of metal-vacuum-dielectric is different from that produced by protrusion or sharpening of the edge in the emitting region.[13,14] At the contact of a sharp metal point with dielectric, there exist the enhancements due to not only shape and but also dielectric. The observed enhancement at the junction is the product of the two enhancements. This means the more importance of the exact description of the dielectric enhancement. According to the works of the author's group,[15,16] both the magnitude and direction of polarization determine what configuration leads to enhancement or reduction of the electric field near the triple junction. The same effect has also found near the quadruple junction of metal-vacuum-dielectric-vacuum (see Fig. 1). The quadruple junction is a more general configuration since it reduces the triple junction when one vacuum portion is removed. In addition, the quadruple junction is more probable to enhance the electric field if the dielectric polarization is responsible for the enhancement. Thus we consider the quadruple junction in the current work.

II. SOLUTIONS OF THE LAPLACE EQUATION

We consider a cylinder of length ℓ and radius R whose portions of metal, vacuum, dielectric, and vacuum meet at the axis (see Fig. 2). The angles subtended by each portion are represented by α, θ_1, θ_2 and θ_3, respectively, where $\theta_1+\theta_2+\theta_3=\theta_t=2\pi-\alpha$. To make analytic analysis of electric field near the junction, we assume that $\ell >> R$. Then the junction configuration can be considered to be two-dimensional and be described using the polar coordinates (r, θ).[14] The electric potential Φ which is the solution of the two-dimensional Laplace equation is written in the infinite r-power series. Since the lowest-power term only is dominant in the region of $r << R$, Φ near the junction can be given by[6,12]

$$\Phi_1 = A_1 r^{\nu} \sin\nu\theta, \qquad 0<\theta<\theta_1 \quad \text{(vacuum)}, \tag{1}$$

$$\Phi_2 = r^{\nu}\,(A_2 \sin\nu\theta + B_2\cos\theta), \qquad \theta_1<\theta<\theta_1+\theta_2 \quad \text{(dielectric)}, \tag{2}$$

$$\Phi_3 = A_3 r^{\nu} \sin\nu(2\pi-\alpha-\theta), \qquad \theta_1+\theta_2<\theta<\theta_1+\theta_2+\theta_3=\theta_t \quad \text{(vacuum)}, \tag{3}$$

where the subscripts 1, 2, and 3 represent the vacuum, dielectric, and vacuum regions, respectively. Coefficients A and B are determined by the boundary conditions. The electric field intensity, $F_i = |\nabla\Phi_i|$, is

$$F_1 = A_1 \nu\, r^{\nu-1}, \tag{4}$$

$$F_2 = ({A_2}^2 + {B_2}^2)^{1/2}\, \nu\, r^{\nu-1}, \tag{5}$$

$$F_3 = A_3 \nu\, r^{\nu-1}. \tag{6}$$

By Eqs. (4)-(6), the configuration-dependence of field F is mostly characterized by ν. Coefficients A and B play a minor role in determining the configuration-dependence of F. Using the boundary conditions imposed on the potential and its angular derivative at $\theta=\theta_1$ and $\theta_1+\theta_2$, we have the transcendental equation

$$\frac{(1-\varepsilon)\tan\nu\theta_1}{1+\varepsilon\tan^2\nu\theta_1} = \frac{\varepsilon\tan\nu\theta_3 + \tan\nu(\theta_1+\theta_2)}{1-\varepsilon\tan\nu\theta_3\tan\nu(\theta_1+\theta_2)}, \tag{7}$$

where ε is the dielectric constant. By solving Eq.(7), ν is obtained as a function of α, θ_1, θ_2, and ε, or any two angles and ε. It is recalled that ν is the smallest of the positive numbers which satisfy Eq. (7). In the form of Eq. (7), θ_1 and θ_3 are not exchangeable. However, the exchange of θ_1 and θ_3 do not make any affect on the result that ν is obtained as a function of θ_2 at given α and ε. It is meaningful that when θ_3=0, Eq. (7) reduces the equation for the triple junction[15,16]

$$\varepsilon \tan \nu\theta_1 = -\tan \nu\theta_2 . \qquad (8)$$

The solution of Eq. (7) becomes more meaningful by comparing with that in the absence of dielectric. For ε =1, Eq. (7) is satisfied at

$$\nu = \nu_0 = \frac{\pi}{\theta_1 + \theta_2 + \theta_3} = \frac{\pi}{\theta_t} = \frac{\pi}{2\pi - \alpha} . \qquad (9)$$

If it is obtained in the absence of dielectric, ν_0 is also the solution in the absence of vacuum. For $1 < \varepsilon < \infty$, i.e., in the presence of dielectrics, we make numerical calculations of Eq. (7) to find ν as a function of α, θ_2, θ_3 and ε. We choose θ_3 = 0 (triple junction), 15^o (asymmetric quadruple junction), and θ_1 (symmetric quadruple junction) at α = 180^o. We make the calculations at several values of α. Then we have found that all the graphs are the same irrespective of α if ν and θ_2 are given in units of ν_0 and θ_t. This implies that the α-dependences of ν_0 and ν are exactly cancelled. As expected, ν/ν_0 changes with θ_2/θ_t. It seems clear that the cases of $\nu > \nu_0$ and $\nu < \nu_0$ correspond to the enhancement and reduction of the electric field, respectively. Further, the lower ν represents the larger enhancement of the field. The important feature to see is the value and location of the minimum ν, ν_{min} in short. The value of ν_{min} becomes smaller with increasing ε for both triple and quadruple junction.

It is seen that ν_{min} becomes less in order of θ_3 = 0, 15^o, and θ_1. This implies that ν has lowest values for the symmetric quadruple junction of $\theta_3 = \theta_1$. This is also confirmed by the fact that the quadruple junction of θ_3=15^o shows ν_{min} at θ_2=165^o (i.e., θ_1 = 15^o = θ_3). It is interesting that ν is always lower than ν_0 for the symmetric quadruple junction, while ν can be higher and lower than ν_0 for the triple junction. Further, the location ν_{min} is fixed at $\theta_2 = \theta_t / 2 = \theta_1 + \theta_3 = 2\theta_1 = 2\theta_3$ irrespective of change in ε for the quadruple junction. For the triple junction, instead, it moves to the larger θ_2 as ε increase.

III. CALCULATIONS OF ELECTRIC FIELDS AND ENHANCEMENTS

Now we consider only the symmetric quadruple junction and the triple junction which are the quadruple junctions of $\theta_3 = \theta_1$ and $\theta_3 = 0$, respectively (see Fig. 2). For both two junctions, we calculate the enhancements of the electric field due to dielectric. We assume that the free negative charge Q is distributed on the surface of the metal of the quadruple junction. The total field energy W is stored in the field region of $0 < \theta < \theta_t$, $0 < r < R$, and $0 < z < \ell$ shown in Fig. 2. Then we can obtain Q and W in terms of the coefficient A_2 and the geometrical quantities using the form of F given in Eqs. (4)-(6). The use of the capacitance relation $W = (1/2)CV^2 = (1/2)QV$ leads to the effective potential[12,16]

$$V = 2W / Q = -\eta \nu R^{\nu} A_2, \tag{10}$$

$$\eta = \frac{\eta_1^2 \theta_1 + \varepsilon(1+\eta_2^2)\theta_2 + \eta_3^2 \theta_3}{8\pi(\eta_1 + \eta_2)} \tag{11}$$

where

$$\eta_1 \equiv A_1 / A_2 = \frac{\varepsilon(1+\tan^2 \nu\theta_1)}{1+\varepsilon \tan^2 \nu\theta_1}, \tag{12}$$

$$\eta_2 \equiv B_2 / A_2 = \frac{(\varepsilon - 1)\tan \nu\theta_1}{1+\varepsilon \tan^2 \nu\theta_1}, \tag{13}$$

$$\eta_3 \equiv A_3 / A_2 = \frac{\sin \nu(\theta_1 + \theta_2) + \eta_2 \cos \nu(\theta_1 + \theta_2)}{\sin \nu\theta_3}. \tag{14}$$

Combining Eqs. (10)-(14) with Eqs. (4) and (6), we have

$$F_1(r) = (\eta_1/\eta)\left(\frac{R}{r}\right)^{1-\nu}\left(\frac{-V}{R}\right), \qquad (15)$$

$$F_2(r) = \left((1+\eta_2{}^2)^{1/2}/\eta\right)\left(\frac{R}{r}\right)^{1-\nu}\left(\frac{-V}{R}\right), \qquad (16)$$

$$F_3(r) = (\eta_3/\eta)\left(\frac{R}{r}\right)^{1-\nu}\left(\frac{-V}{R}\right), \qquad (17)$$

All the fields F_i are given in unit of V/R. Eqs. (15-17) show the dependence of F_i on both configuration and position. The dependence is evaluated with respect to the reference field F_0, which is defined as F_1 when dielectric is replaced with vacuum. This is F_1 at $\theta_1 = \theta_3 = \theta_t/2$ for the symmetric quadruple junction, where we have $\nu = \nu_0$ and $\eta = \theta_t/(16\pi)$. This also implies that $\theta_2 = 0$ and $\varepsilon = 1$. From Eq. (12), we have

$$F_0 = 15\nu_0\left(\frac{R}{r}\right)^{1-\nu_0}\left(\frac{-V}{R}\right). \qquad (18)$$

The dielectric enhancement is represented by the field enhancement factor β, which is defined as the ratio of F_1 and F_0:

$$\beta(r) = F_1(r)/F_0(r) = \frac{\eta_1/\eta}{16\nu_0}\left(\frac{R}{r}\right)^{\nu_0-\nu}, \qquad (19)$$

where r is the distance from the junction to the point at which field emission or breakdown occurs. It is cleat that β is strongly dependent on both ε and the ratio R/r. If we consider the ferroelectric materials, ε varies from 1 to 1000. Realistically, we consider two materials, diamond (ε =5.7) and GaN(ε =10.4). Incidentally, ε increases twice. It is found that β increases more than twice with the double increase of ε. It seems that r has the values of a few angstroms or less, whereas R changes much with the choice of the system. For the corrugations shown in the contact between metal and dielectric, R is a few tenths of microns.

Sometimes, R may become a few microns for the triple junction geometries in the tip fabrication,. This argument leads to the choice of $R/r = 10^3 – 10^4$. In the current work, we take $R/r = 10^4$.

By Eq. (19), it seems that the case of $\nu < \nu_0$ implies $\beta > 1$, implying the enhancement of field. It is clear that the maximum field enhancement β_{max} occurs slightly away from the location of ν_{min} due to the prefactor of Eq. (19). However, it makes only a slight change in the both location and value of β_{max}. This is the same for all F_i given by Eqs. (15)-(17). In general, β changes with ν/ν_0, i.e., θ_2/θ_t for $\varepsilon > 1$. According to Fig. 3, β is larger or less than unity for the triple junction but is always larger than unity for the symmetric quadruple junction.

For the triple junction, the dielectric field enhancement is made in the region of $1/2 < \theta_2/\theta_t < 1$, whereas the reduction in the region of $0 < \theta_2/\theta_t < 1/2$. As θ_2 increases from $\theta_t/2$ to θ_t, the prefactor in Eq. (19) increases approximately from unity to 5.5. For $R/r = 10^4$, where $r = 0.1$ nm and R = 1 μm, we calculate β as a function of θ_2/θ_t for the triple junction. The obtained β are shown in Fig. 4. Since $F_1 = \beta F_0$ and $F_2 = \eta_1 \beta F_0$, the vacuum field F_1 has the maximum at a little larger θ_2 in comparison with ν_{min}, whereas the dielectric field F_2 just at a littler less θ_2. For $\varepsilon = 5.7$, β_{max} is 19.8 in vacuum and 6.9 in dielectric. These values increases with increasing both ε and R/r. With the increase of ε from 5.7 to 10.4, β_{max} increases from 19.8 to 47.1 in vacuum and from 6.9 to 11.3 in dielectric.

For the symmetric quadruple junction, the dielectric effect makes only the enhancement of the field. This feature is not true for a general quadruple junction. It is seen in Fig. 3 that ν becomes larger than ν_0 at the beginning for the quadruple junction of $\theta_3 = 15^o$. Another important feature is that β is much larger than that for the triple junction, as seen in Figs. 4 and 5. For ε = 5.7, β_{max} = 66.1 in vacuum and = 26.1in dielectric for R/r =10^4. With increase of ε from 5.7 to 10.4, β_{max} increases from 66.1 to 207.6 in vacuum and from 26.1 to 57.8 in dielectric. In addition, the field enhancement in dielectric is considerable for the quadruple junction, whereas it is not for the triple junction.

It is noted that F_0 itself represents the field enhancement due to the curvature of the metallic tip. Since $\nu_0 = \pi/\theta_t = \pi/(2\pi-\alpha)$, F_0 (in unit of V/R) increases with decreasing α. Thus field has the two types of enhancement. One is due to the sharpness of the metallic portion. The other is due to the dielectric polarization. Thus the total enhancement of the electric field at the junction is the product of the two enhancements due to dielectric as well as the shape of the metallic emission portion.

It is clear that the polarization is responsible for the difference between enhancements shown in the quadruple and triple junctions. The current results surely give rise to a new concept that dielectric can enhance the electric field. The new type of the field enhancement is attributed to the polarization of dielectric. The field enhancement is resulted from the accumulation of the free charges on the metal around the junction. In the absence of dielectric, the surface charge is distributed on the metal depending on the curvature. If dielectric is introduced to be in contact with metal, the surface charge causes dielectric to polarize. The magnitude and direction of polarization depends on the angle configuration of the constituents. Then the free surface charge on metal is redistributed under the two factors, the curvature and the polarization of dielectric. If the polarization attracts the free surface charge on the metal to the junction, more free charge is accumulated at the junction. This process goes on until the perfect polarization of dielectric, yielding the very large surface charge density near the junction. The larger surface charge means the stronger field around the junction. Such strong fields lead to the enhanced field emission or the dielectric breakdown at the triple junction.

IV. CONCLUSIONS

We have found that dielectric enhance the electric field near the symmetric quadruple junction, whereas it enhance or reduces the field the triple junction. The field enhancement is much larger for the quadruple junction than for the triple junction, being more profound in dielectric field. By this reason, the dielectric breakdown may occur near the quadruple junction, if any, rather than near the triple junction. It is noted that the total enhancement of the electric field at the junction is the product of the two enhancements due to dielectric and the shape of the metallic emission portion.

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Figure Captions

Fig. 1 Natural formation of triple and quadruple junctions. The contact of metal and dielectric makes triple junctions of metal-vacuum-dielectric (small circle) and quadruple junctions of metal-vacuum-dielectric-vacuum (large circle).

Fig. 2 Cylindrical quadruple junction. The quadruple junction is the axis of the cylinder of radius R and length ℓ which is composed of metal, vacuum, dielectric and vacuum subtended by angle α, θ_1, θ_2, and θ_3, respectively. Here, $\theta_1 + \theta_2 + \theta_3 = \theta_t = 2\pi - \alpha$.

Fig. 3 Enhancement parameters ν. The ν are obtained for $\theta_3 = 0$(triple junction, red line), 15^o(asymmetric quadruple junction, green line), θ_1 (symmetric quadruple junction, blue line). When ν and θ_2 are given in units of ν_0 and θ_t, plots of ν vs θ_2 are independent of α. In fact, the calculation is made $\alpha = 180^o$.

Fig. 4 Field enhancement β for the triple junction. The β represents the enhancement for the vacuum field F_1 (solid line) and the dielectric field F_2 (dotted line). We take ε = 5.7 (lower line) and 10.4 (upper line)

Fig. 5 Field enhancement β for the symmetric quadruple junction. The β represents the enhancement for the vacuum field F_1 (solid line) and the dielectric field F_2 (dotted line). We take ε = 5.7 (lower line) and 10.4 (upper line)

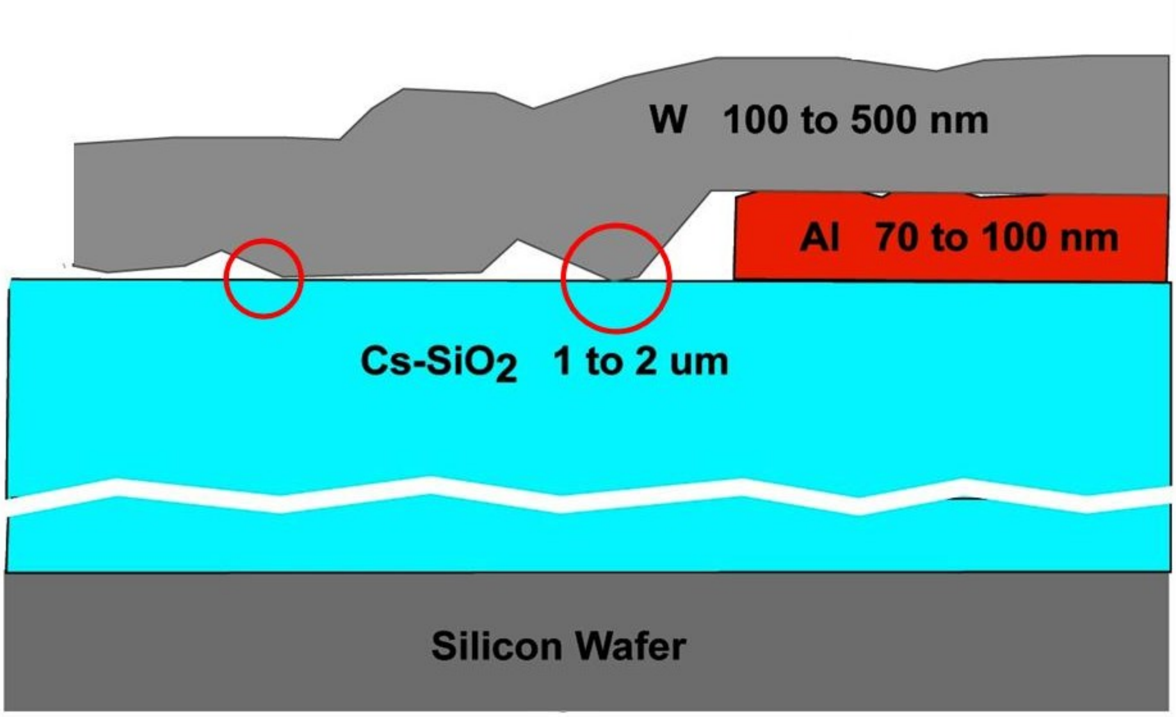
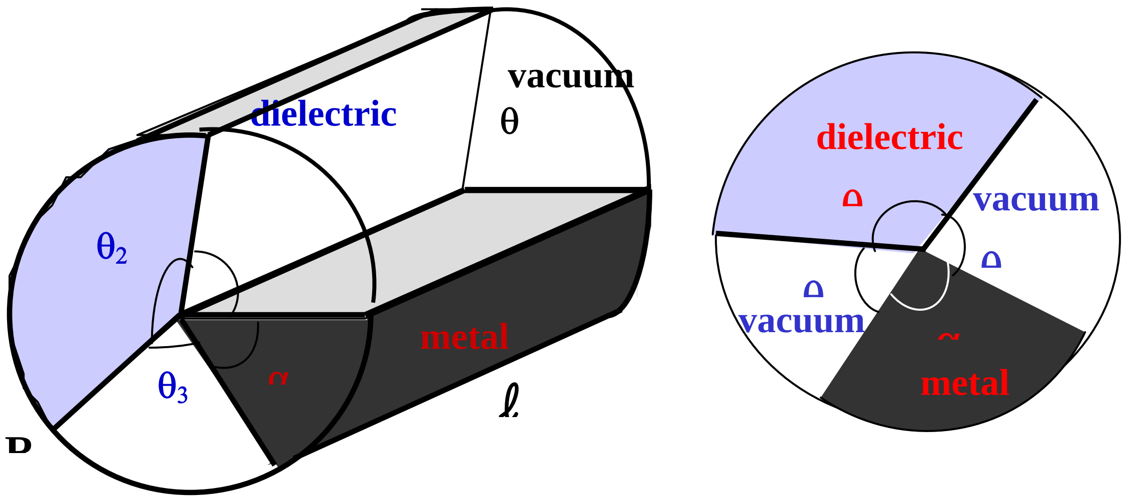
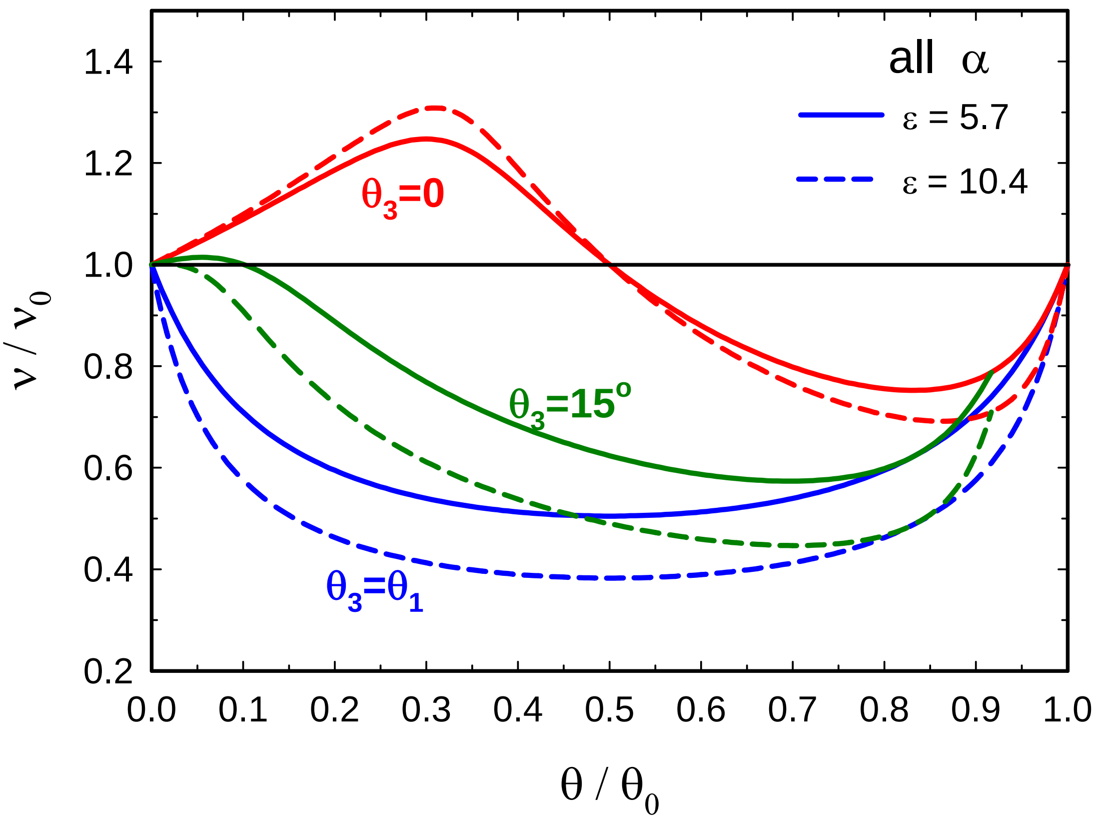


Fig. 1



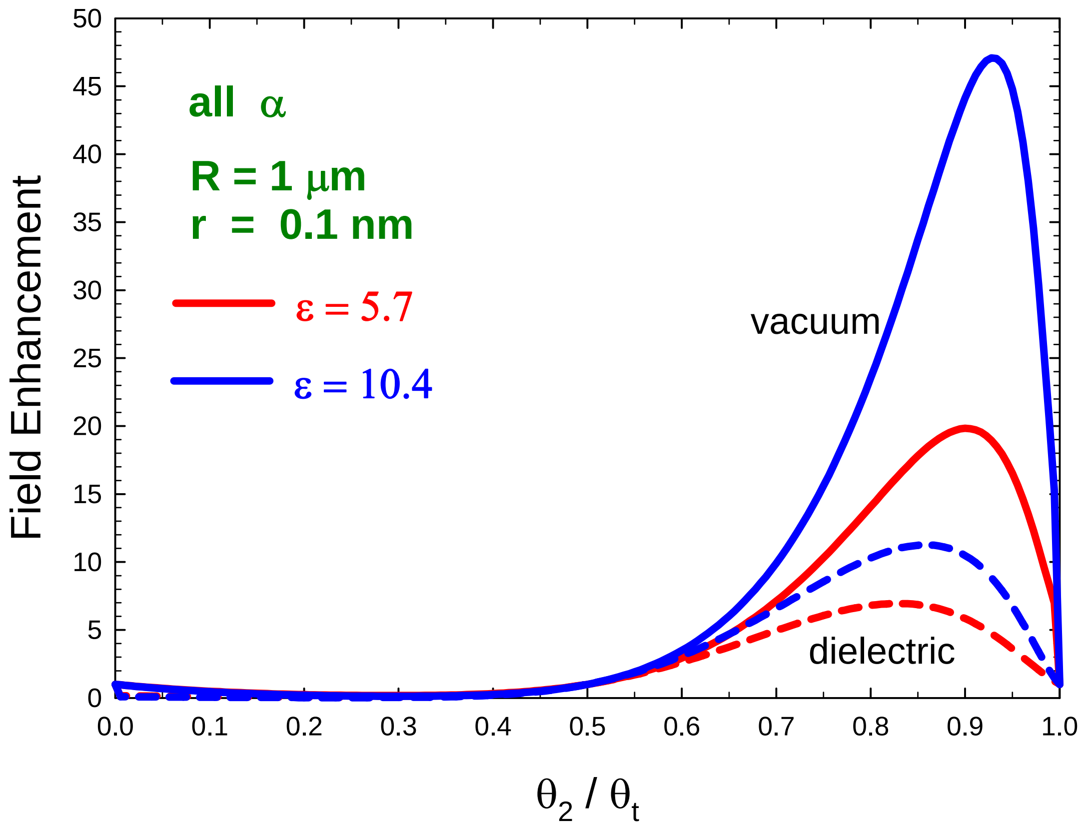
dielectric
vacuum
θ
θ_2
θ_3
metal
ℓ
dielectric
vacuum
vacuum
metal

Fig. 2



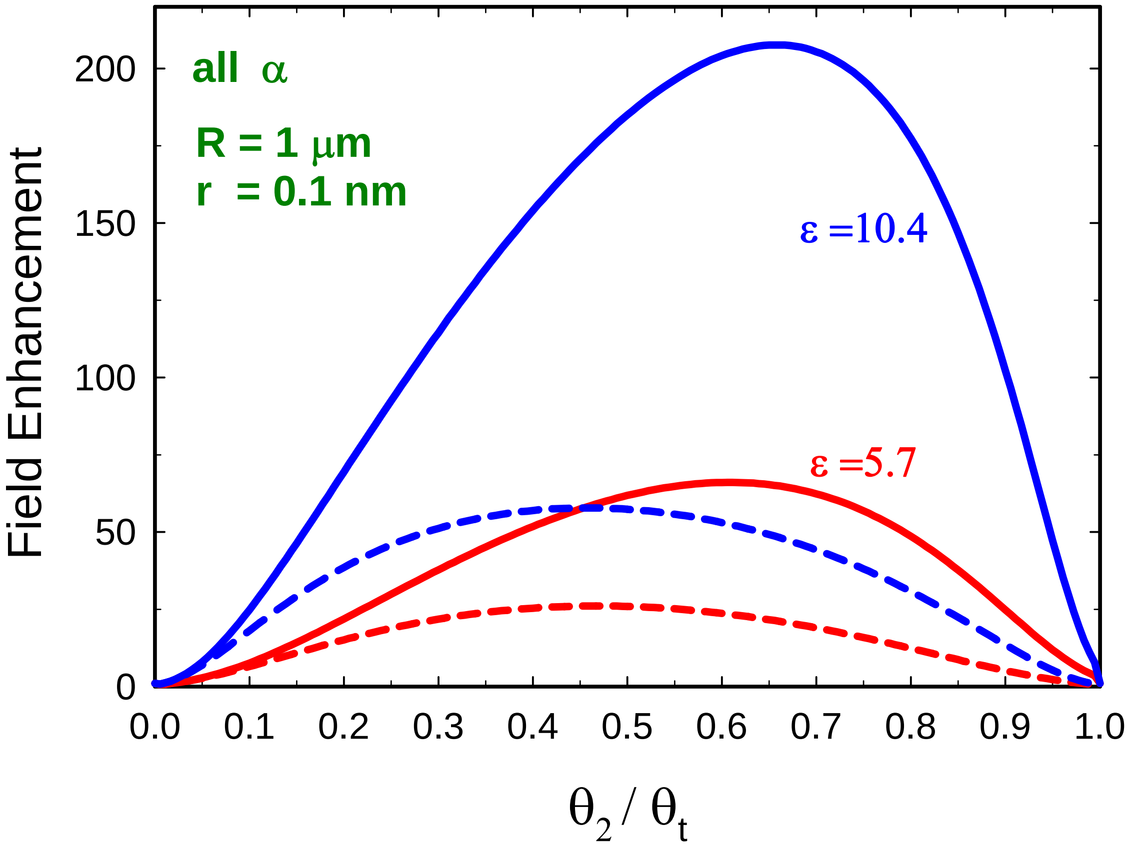
all α
ε = 5.7
ε = 10.4
θ3=0
θ3=15°
θ3=θ1
1.4
1.2
1.0
0.8
0.6
0.4
0.2
ν / ν0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
θ / θ0

Fig. 3



all α
R = 1 μm
r = 0.1 nm
ε = 5.7
ε = 10.4
vacuum
dielectric
Field Enhancement
θ2 / θt
0
5
10
15
20
25
30
35
40
45
50
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Fig. 4



all α
R = 1 μm
r = 0.1 nm
ε =10.4
ε =5.7
Field Enhancement
200
150
100
50
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
θ2 / θt

Fig. 5