Interplay of various loss mechanisms and ultimate size limit of a surface plasmon polariton semiconductor nanolaser

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Abstract: The issue of an ultimate size limit of a surface plasmon polariton (SSP) nanolaser is investigated by a systematic simulation study. We consider a prototypic design of a metal-insulator-semiconductor multi-layer structure with finite, varying lateral sizes. Our focus is on the design of such lasers operating at room temperature under the electrical injection. We find that there is an interesting interplay between the facet loss and the SPP propagation loss and that such interplay leads to the existence of a minimum-threshold mode in each mode group. The red-shift of the minimum-threshold mode with the decrease of device thickness leads to a further reduction of threshold gain, making the threshold for the SSP nanolaser achievable for many semiconductors, even at room temperature. In addition, we find that the threshold can be further reduced by using thinner metal cladding without much exacerbated mode leakage. Finally, a specific design example is optimized using Al$_{0.3}$Ga$_{0.7}$As/GaAs/Al$_{0.3}$Ga$_{0.7}$As single quantum well sandwiched between silver layers, which has a physical volume of $1.5 \times 10^{-4}$ $\lambda^3_0$, potentially the smallest semiconductor nanolasers designed or demonstrated so far.

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have been fabricated.

3. Introduction

Metallic cavity nanolasers [1–13] and spasers [14, 15] with ever shrinking cavity sizes down to tens of nanometers have attracted a great deal of attention recently due to progress in the nano-fabrication technology and in the understanding of semiconductor-metal interactions at nanoscales. Metals such as Ag and Au have been widely adopted in the past several years in metallic cavity nanolasers [1–13] and spasers [14, 15] with cavity sizes down to tens of nanometers have attracted a great deal of attention recently due to progress in the nano-fabrication technology and in the understanding of semiconductor-metal interactions at nanoscales. Metals such as Ag and Au have been widely adopted in the past several years in the design and fabrication of nano-scale semiconductor lasers [1–13], even though non-metals such as heavily doped semiconductors are also receiving attention [16]. With the cladding of metals, semiconductor lasers with a physical cavity volume of 0.019 $\lambda_0^3$ have been fabricated [8], and a design of nanolaser with a cavity volume smaller than 0.01 $\lambda_0^3$ has been proposed [9], where $\lambda_0$ is the corresponding wavelength of the cavity mode in vacuum. One of the reasons of using metals in nano-scale lasers is to take the advantage of the very small modal volume of surface plasmon polariton (SPP) modes [17], formed at the interface of metals and dielectric materials. However, only a few papers showed nanolasers operating near the SPP resonances [4–6] with only one under electrical pumping at room temperature [4] and mostly...
under optical pumping [5, 6] at low temperature, mainly due to the large intrinsic modal loss of SPP modes. Although efforts have been made on compensating the modal loss by incorporating gain medium in various structures that support SPP modes [18–22], the material gain required to overcompensate the loss is often large and not achievable in common semiconductors, especially near the SPP resonance [13, 21]. While several experiments reporting spaser operation with very small sizes, such structures are not compatible with electrical injection. Several questions remain unanswered: Is it practically possible to operate a nanolaser or spaser near the SPP resonance at room temperature under electrical injection? Can or to what extent the required laser threshold be further reduced through the realistic consideration and optimization? What is the ultimate, practically achievable smallest size of the SPP lasers or spasers, especially under the electrical injection? In order to answer such questions and to realize the electrical injection SPP lasing at room temperature, we carried out a systematic study of various loss mechanisms and focus on the design and optimization of the structure of a plasmonic nanolaser with the smallest possible sizes.

2. Interplay of loss mechanisms and parametric dependent study

We study a prototype of a metal-semiconductor-metal (MSM) cavity as shown in Fig. 1(a) through the design and simulation by using COMSOL Multiphysics [23]. Such MSM configuration can be easily extended to more practical situations including electrical injection and can be scaled down in three dimensions separately for optimization. In a realistic electrical injection device, an insulator layer is usually sandwiched between the metal and semiconductor layers. Such structure can be approximated by the MSM structure for the purpose of modal property study. As shown in Fig. 1(a), the cavity has length $L$ in the $z$ direction, width $W$ in the $y$ direction and thickness $h_s$ of semiconductor core layer and $h_m$ of metal (silver) cladding layer in the $x$ direction. The semiconductor has a dielectric constant $\epsilon_s$ with a real part of 12, and the silver dielectric function $\epsilon_m(\omega)$ is taken from [24] and curve fitted for our numerical solution. Since we only study the possibility of SPP mode (as opposed to optical modes) lasing in the cavity, the modes are always decaying in the $x$ direction from the metal-semiconductor interface. By exciting the cavity with a transverse magnetic (TM)-polarized incident wave, we can obtain the intensity spectrum of the SPP modes. The cavity modes are denoted by TM$_{0nm}$. The first index, “0”, means that there is no half-cycle variation of field in the $x$ direction (to avoid dielectric or optical modes), the second and the third indices stand for the number of half-cycle variations in the $y$ and $z$ direction, respectively. Figure 1(b) shows the intensity spectrum of a MSM cavity with $W = L = 50$ nm and $h_s = h_m = 10$ nm. The inset of Fig. 1(b) is the field pattern of the TM$_{012}$ mode in the $x$-$z$ plane. The material gain spectrum in a semiconductor can be calculated by using a microscopic theory [25] and can be added to the imaginary part $\epsilon_s''$ of the dielectric function, and is given by the following formula at frequency $\omega$.

$$G_0 = \frac{\epsilon_s''\omega}{n_s c}$$

(1)

where $n_s$ is the refractive index of semiconductor and $c$ is the speed of light in vacuum. The metal loss is defined in a similar way as Eq. (1) with a positive sign by using the imaginary part of the metal dielectric function. The semiconductor material gain and the metal loss are then used as input parameters of COMSOL to find the lasing mode. In the linear regime, the material gain will increase with pumping. When the modal gain (material gain × confinement factor) is equal to the overall loss of the cavity experienced by a mode, which is the sum of modal (internal) loss and facet (transmission or radiation) loss, this mode reaches its lasing threshold. The corresponding material gain is called threshold gain. In the linear theory of lasers, spectral width of a mode is proportional to the net gain or loss. Thus the spectral linewidth approaches zero at the threshold. This fact can be used to obtain the threshold numerically by following the spectral width with increasing gain in the semiconductor.
Our study is focused on the loss mechanisms and their parametric dependence on nanolaser geometries. Such study will allow us to determine the smallest size of the laser cavity and the corresponding threshold gain that is practically achievable. In a nanolaser cavity of a finite size, there are several loss processes: 1) The cavity transmission or radiation to the outside through facets; 2) The SPP modal (propagation) loss; and 3) The so-called lossy surface waves as a result of pair-excitations in the electron gas [26, 27]. The pair excitation loss leads to the strong quenching of dipole emissions near the metal surface. But since the pair excitation wave-vector is on the order of $10^9 - 10^{10}$ m$^{-1}$ in Au or Ag, such quenching layer is extremely thin. Our calculation showed that such quenching layer is around 1 to 2 nm in a MSM structure. The dipole quenching can be easily avoided by adding a thin layer on the order of 1-2 nm between the gain medium and metal. Since the SPP wave-vector is at least 10 times smaller, strong interaction can still be maintained between the metal and gain medium through the SPP modes. Thus in the following discussions, we will first focus on the first two loss mechanisms, while assuming that the last loss mechanism can be avoided by adding a very thin layer. Later, we will use a quantum-well heterostructure to include such a thin layer in our design.

2.1 Dependence on gain layer thickness

To study the effect of the middle gain layer thickness, we first fix the in-plane size $W$ and $L$ both at 50 nm and the metal layer thickness at $h_m = 10$ nm, and then vary the thickness of the core layer. The threshold gain for each cavity mode with different core layer thicknesses is shown as a function of photon energy ($\omega = h\omega$) in Fig. 2. First, we notice that in the cavity with $h_s = 10$ nm, $TM_{02m}$ and $TM_{03m}$ modes have higher threshold than $TM_{01m}$ modes. It is true in general that, as we vary the middle layer thickness, the threshold gain is higher for mode $TM_{0nm}$ with larger mode index $n$. Therefore, we will discuss from now on $TM_{01m}$ modes ($n = 1$) only. Second, it is important to realize that for each mode group $TM_{01m}$, there is a mode index $m$ with a given photon energy, for which the threshold gain is minimum. That is because the threshold gain for lower order modes (smaller $m$) is dominated by the large facet loss while the threshold gain for higher order modes by the large SPP modal loss. As photon energy increases, the facet loss decreases since higher order mode is more tightly confined inside the cavity while the SPP modal loss increases monotonically as the photon energy approaches the SPP resonance [21]. The threshold gain, proportional to the sum of the facet loss and SPP modal loss, thus has a minimum value at an intermediate photon energy. Third, we see in Fig. 2 that the minimum threshold gain decreases with the core layer thickness which is mainly due to the reduction of facet loss, and the details will be shown later. The red-shift of the modes with minimum threshold with decreasing core layer thickness further reduces the threshold gain. We emphasize that the delicate interplay between the SPP modal loss and the facet transmission loss leads to the existence of a minimum-threshold mode.
2.2 Dependence on in-plane sizes

We next fix the thickness of the core and metal layer both at 10 nm, and vary the in-plane size \( W \) and \( L \) by assuming \( W = L \). Figure 3 shows the threshold gain of consecutive modes with different in-plane sizes as a function of photon energy. The overall behavior is similar to that in Fig. 2: There is a mode with a minimum threshold gain for each given in-plane size. The photon energy with the minimum threshold is red-shifted as the in-plane size increases and the minimum threshold gain decreases accordingly. Note that for \( W = L = 200 \) nm, the TM\(_{015}\) mode (with a photon energy of 1.2 eV) has a threshold gain around 2000 cm\(^{-1}\), a low enough value achievable in many common semiconductors.

By reorganizing the results from Fig. 2 and Fig. 3, we plot the minimum threshold gain as a function of (a) core layer thickness and (b) in-plane size in Fig. 4. We can see from Fig. 4(a) that the minimum threshold gain drops quickly if the core layer thickness is smaller than 30 nm and keeps decreasing even if the core size is as thin as 5 nm. The reason for this has been
explained by the reduction of facet loss in the previous paragraph. The facet loss, defined as the threshold modal gain subtracting the SPP modal loss, is shown in Fig. 4(a) for the modes with minimum threshold at different core layer thicknesses. The SPP modal loss can be calculated using the method given in Ref [21]. We can see the facet loss coincides with the threshold gain very well except the case with $h_s = 10$ nm. In the cavity with $h_s = 10$ nm, TM$_{012}$ mode has the minimum threshold, while in other cavities with larger $h_s$, TM$_{013}$ mode has the minimum threshold. Although TM$_{013}$ modes in some cavities with $h_s > 10$ nm may have less facet loss than the TM$_{012}$ mode at $h_s = 20$ nm, their threshold is still higher due to their high modal frequency. Therefore, there is no low limit on core layer thickness to achieve minimum threshold gain for core thickness down to 5 nm. The dashed curve in Fig. 4(a) shows the minimum threshold by including the influence of the pair-excitation quenching near the metal interface. To include the effect of dipole quenching on the material gain, we calculated the possibility of dipole emission into all electromagnetic modes as a function of the distance between the dipole and the metal surface by using the method given in Ref [26]. A non-uniform semiconductor gain, $G_0(x)$, is then obtained and used in the simulation. We can see that the minimum threshold gain is larger than that without pair excitation. The difference is less than 5% when core layer is thicker than 30 nm, but is over 70% when the core is 5 nm. The minimum threshold gain reaches the smallest value at a core thickness about 6 nm. Therefore the core thickness of the MSM structure has a lower limit due to the existence of the pair-excitation loss. In Fig. 4(b), the minimum threshold becomes practically constant for in-plane size larger than 200 nm. Although in-plane size over 200 nm $\times$ 200 nm is on the same order of magnitude as reported [7], the advantage of scaling down of the core layer thickness enables significant reduction of the overall size of the cavity. The corresponding cavity volume (in $\lambda_0^3$) is also shown in Fig. 4(b). Taking the cavity with 200 nm in in-plane size and 10 nm in core layer thickness as an example, the cavity volume is only $3.6 \times 10^{-4} \lambda_0^3$ and the required threshold gain is as low as 2000 cm$^{-1}$, achievable with many semiconductors, especially with semiconductor quantum wells.

Fig. 4. The minimum threshold gain vs. core layer thickness (a) with (dashed line) and without (solid line) pair-excitation loss, and vs. in-plane size (b). We also include the facet loss in Fig. 4(a) and the cavity volume (in $\lambda_0^3$) in Fig. 4(b).

2.3 Dependence on metal layer thickness

The metal cladding layers are usually designed to be thick enough to prevent mode leakage from the core. However, as we will show later, using thin metal layer is crucial in reducing
lasing threshold gain further. Therefore it is necessary to study the influence of the thickness of metal layer. Figure 5(a) shows the energy profile in the x-z plane for three different values of metal layer thickness. We can see that, as the metal layer thickness increases from 5 to 20 nm, less energy leaks through the metal claddings and most of the light comes out from the side of the cavity in the z direction. The percentage of the energy leaked through the metal cladding as a function of metal layer thickness is plotted in Fig. 5(b). We can see that the leakage decreases exponentially as metal layer thickness increases linearly, and less than 0.1% of the energy leaks through the metal cladding if the thickness of metal layer is 15 nm and thicker. Figure 5(c) shows the relation between the minimum threshold gain and metal layer thickness. The minimum threshold gain increases rapidly from $h_m = 5$ nm to 15 nm and keeps nearly constant as $h_m > 20$ nm. The reduction of the minimum threshold gain with decreased metal thickness is partly due to the decreased metal loss, but mainly due to the red shift of the mode with the minimum threshold (TM$_{014}$ mode). The red-shift of the mode is probably caused by the coupling between the modes inside the core and those outside the metal.

2.4 Effects of insulating layer between metal and gain layers

In an actual metal-semiconductor nanolaser design, an insulating layer is usually inserted between the metal cladding and the semiconductor active region (thus forming a MISIM structure) to prevent charge transfer from active region to metal layer. Such insulating layer can be SiO$_2$ or Si$_3$N$_4$ [3, 4, 7] or wide-gap semiconductors [8, 28]. It was reported that [7, 29] there is an optimal thickness of the insulating layer, for which the laser has the smallest threshold gain. The conclusion is correct only for TE-like modes which have a very weak electric field component vertical to the insulating or metal layer. The low-index insulating layer can push the field towards the high-index core and away from the metal cladding, thus reducing the metal confinement factor [1, 30] and the metal modal loss. However, for TM-like modes such as SPP mode, there is a strong electric field component vertical to the insulating layer or metal layer, so that a slot mode [31] will be formed with a strong field intensity inside the insulating layer due to the low index of the insulating layer and the continuity of the displacement vector. The slot mode will mix with SPP mode, resulting in the strongest mode intensity located at the metal-insulating layer interface, as shown in the inset of Fig. 6(a), the field thus cannot be pushed away from the metal cladding.
If the dielectric constant of the insulating layer, \( \varepsilon_d \), is too small compared to \( \varepsilon_s \), as is the case for many insulators, the electric field in the insulating layer will be much larger than that in the core, resulting in a small mode volume in the active core region. The weak field intensity inside the active layer will lead to a small gain confinement factor and an increased threshold material gain. Therefore, it is preferable to use materials with dielectric constant close to that of the semiconductor core to enhance the modal gain. An ideal choice is a quantum well structure with a narrow gap semiconductor sandwiched between two layers of wide gap semiconductor. Usually the index difference between the well and barrier material is relatively small and the quantum well structure provides both the required index profile and the mechanism for electrical injection and confinement. Assume \( \varepsilon_d = 10 \). Fig. 6(a) shows the minimum threshold gain as a function of insulating layer thickness with a fixed total thickness \( h_s + h_d = 20 \) nm. Note that the pair-excitation loss is not included here. It is shown [26] and confirmed by our calculation that pair-excitation has less than 5% influence on the material gain if the dipole or the active material is 1.5-2 nm away from the metal surface in the MSM structure. Since the insulator thickness studied in our work is at least 1.5 nm, we ignore the pair-excitation for simplicity. We can see the thinner the insulating layer is, the smaller the minimum threshold gain will be. Therefore the insulating layer should be made as thin as possible for SPP mode lasing. Once the thickness of the insulating layer is determined, the thickness of the semiconductor core is the only parameter that needs to be optimized. Remember we showed in Fig. 4(a) that the minimum threshold gain decreases as core thickness is reduced if the total thickness of the layers between metal layers is smaller than 30 nm. On the other hand, with a fixed thickness of the insulating layer, the decrease of the active core thickness as the total size between metals decreases will lead to the increase of the threshold gain. Therefore, there will be an optimal value for the thickness of the active core at which the threshold gain is minimized. Figure 6(b) shows the minimum threshold gain as a function of core layer thickness with \( h_d = 3 \) and 5 nm, respectively. As expected, an optimal value of the core thickness (8 and 13 nm, respectively) exists for each case, depending on the thickness of the insulating layer.

![Fig. 6. (a) Minimum threshold gain as a function of the insulating layer thickness with a fixed total thickness of insulating and core layers of 20 nm. The |E| profile of a slot mode mixed with a SPP mode along the x axis in a MISIM cavity is shown in the inset. (b) Minimum threshold gain as a function of the core layer thickness with two values of the insulating layer thickness: 3 and 5 nm.](image-url)
3. AlGaAs/GaAs quantum well nanolaser: a design example

Using the design and optimization procedures for the MSM cavity discussed above, we now consider a specific example: an Al$_{0.3}$Ga$_{0.7}$As/GaAs/Al$_{0.3}$Ga$_{0.7}$As single quantum well structure sandwiched between two Ag layers, as shown in Fig. 7(a). The thickness of Al$_{0.3}$Ga$_{0.7}$As, GaAs and Ag layers is optimized to be 1.5 nm, 5 nm and 15 nm, respectively, and the length and width of the cavity is 100 nm. With the separation of 1.5nm-thick AlGaAs layer, dipole quenching due to pair excitations can be well suppressed. For the electrical injection operation, the whole cavity is usually coated by silicon nitride (SiN$_x$) in the device fabrication for electric isolation and mechanical support [3, 4, 10]. We use the dielectric constant of silicon nitride in the near infrared range as the ambient dielectric constant (~4). The dielectric constant of Al$_x$Ga$_{1-x}$As and GaAs can be found in Ref [32]. Since the material gain is available within a limited frequency range above the bandgap of the active semiconductor, we only study the modes within the gain bandwidth of AlGaAs/GaAs single quantum well (from 1.45 to 1.7 eV according to Ref [25]). Our simulation results showed that two modes, TM$_{014}$ and TM$_{015}$ exist in this range, as shown in Fig. 7(b). The peak wavelength of TM$_{014}$ mode is $\lambda_0 = 813$ nm (1.525 eV) and the lasing threshold gain is 3859 cm$^{-1}$, achievable at room temperature according to a theoretical calculation [33]. Since the plasmonic modes have two strong electric field components in the $x$ and $z$ direction, respectively, material gain due to the in-plane (TE) and off-plane (TM) dipole transitions in the quantum well contributes to the mode. The quality factor for this mode without material gain is about 52. TM$_{015}$ mode is at $\lambda_0 = 740$ nm (1.677 eV) whose quality factor and lasing threshold gain is 66 and 3641 cm$^{-1}$. Although the threshold gain is slightly smaller than that of TM$_{014}$ mode, it can hardly be achieved since the TM gain provided to TM$_{015}$ mode is from the transition between the first excited state in the conduction band and the first excited state in the light-hole band, which is too small to satisfy the requirement of the threshold gain [25]. The cavity hence works as a single-mode device. The physical volume of the Al$_{0.3}$Ga$_{0.7}$As/GaAs/Al$_{0.3}$Ga$_{0.7}$As cavity is only $8 \times 10^{-5}$ µm$^3$ ($~1.5 \times 10^{-3} \lambda_0^3$), which is the smallest nano-laser cavity reported so far. The total volume of the structure, including metal layers, is $3.8 \times 10^{-4}$ µm$^3$ ($~7.1 \times 10^{-3} \lambda_0^3$).

Figure 7(c) shows the near field energy density pattern of TM$_{014}$ mode at the lasing threshold in the $x$-$z$ plane. We can see most energy is confined in the cavity, as shown by the deep red color. The far-field pattern, shown in Fig. 7(d), is an important characteristic of any laser. As can be seen, the full-width at the half-maximum of the far-field angle is $~92^\circ$.

Fig. 7. (a) Schematic structure of an optimized MISIM nanolaser. (b) Intensity spectrum of the nanolaser within the gain bandwidth of AlGaAs/GaAs/AlGaAs quantum well showing two possible modes. (c) Near field energy density pattern of the TM$_{014}$ mode at lasing threshold in the $x$-$z$ plane. (d) Angular dependence of the far field $|E|^2$ radiation pattern of the TM$_{014}$ mode at the lasing threshold in the $z$-$x$ plane.
4. Summary

In summary, we studied a prototype of a surface plasmon polariton nanolaser with a finite MSM rectangular cavity, where the cavity modes are pure SPP modes. To find the smallest cavity with practically achievable threshold material gain for lasing, we performed a systematic study of the dependence of threshold gain on structure parameters. We found that there is an interesting interplay between the facet loss and the SPP modal loss and that such interplay leads to the existence of a minimum-threshold mode. The threshold gain decreases continuously when shrinking the thickness of the semiconductor core from 30 nm to 5 nm and maintains a minimum value if the length and width is over 200 nm. The smallest core thickness is eventually limited by pair-excitation loss occurring in the gain material within 2 nm of the interface with metal layer. The red-shift of the minimum-threshold mode as the thickness of the device decreases further leads to the reduction of the threshold gain, making the SPP nanolaser threshold achievable for many semiconductors, even at room temperature. Such new understanding and comprehensive optimization lead to the predication of the smallest nanolaser with practically achievable threshold gain. In addition, we found that the threshold can be further reduced by using thinner metal cladding without much exacerbated mode leakage. The threshold gain can be reduced by reducing the thickness of the metal cladding layer from 20 nm to 10 nm, still maintaining less than 0.5% leakage through the metal layers. We also showed that the existence of an insulating layer between the semiconductor core and the metal layer always increases the threshold due to the poor overlap of the mode and gain region, but the threshold gain can be minimized by adjusting the thickness of the core layer if the thickness of the insulating layer is fixed. We finally proposed a more realistic design example consisting of an Al$_{0.3}$Ga$_{0.7}$As/GaAs/Al$_{0.3}$Ga$_{0.7}$As single quantum well sandwiched by Ag layers with optimized parameters. Single mode lasing in a SPP mode can be achieved in the cavity at room temperature, and the physical volume of the cavity, including insulating and semiconductor core layers, is as small as $8 \times 10^{-5} \mu m^3$ ($\sim 1.5 \times 10^{-4} \lambda_0$), the smallest semiconductor nanolaser designed or demonstrated so far.

We point out that many of the quantitative results of this paper depend on the values of metal losses we use for Ag. The values in [24] which were used for our simulation are known to overestimate the metal loss, most likely because they were obtained with metals of low quality available at the time. According to the more recent dielectric function data [34] for Ag, the threshold gain could be smaller since the Ag material loss (given by Eq. (1) with a positive sign) is 5% to 10% smaller than that calculated by using Ag dielectric function data from Ref [24], within the wavelength range studied here. Therefore, the threshold gain required here is likely larger and thus our design and feasibility study represent a more conservative upper limit. We believe that with the improvement of deposition techniques of metals, metal loss can be further reduced, increasing the likelihood of observing the SPP mode lasing studied here. Our results and conclusions can serve as the guideline of the design and optimization of SPP nanolasers.

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