

## Dependence of $Q$ Factor on Surface Roughness in a Plasmonic Cavity

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We investigated surface-roughness-dependent optical loss in a plasmonic cavity consisting of a semiconductor nanodisk/silver nanopan structure. Numerical simulations show that the quality factors of plasmonic resonant modes significantly depend on the surface roughness of the dielectric-metal interface in the cavity structure. In the transverse-magnetic-like whispering-gallery plasmonic mode excited in a structure with disk diameter of 1000 nm, the total quality factor decreased from 260 to 130 with increasing root-mean-square (rms) surface roughness from 0 to 5 nm. This quantitative theoretical study shows that the smooth metal surface plays a critical role in high-performance plasmonic devices.

*Keywords* : Surface plasmon polaritons, Plasmonic cavities, Surface roughness, Finite-difference time-domain simulations

*OCIS codes* : (250.5403) Plasmonics; (240.5770) Roughness; (140.3945) Microcavities; (240.6680) Surface plasmons

### I. INTRODUCTION

Plasmonic structures enable subwavelength-scale optical devices through strong confinement of surface-plasmon polaritons (SPPs) [1-11]. Further miniaturization of various nanophotonic structures such as cavities [1-4], waveguides [5-7], and nanoantennas [8-10] has been achieved by overcoming the diffraction limit of conventional optics. Plasmonic lasers are particularly promising as ultrasmall, efficient, coherent light sources in photonic/plasmonic integrated circuits [1, 2, 11]. Recent studies of plasmonic lasers/cavities show that their quality ( $Q$ ) factors can be increased further through rational cavity design, while keeping the mode volumes extremely small [1-3]. In addition, these optical properties of plasmonic structures significantly depend on the surface roughness of the dielectric-metal interface at which SPPs are excited, and thus it is very important to fabricate a metallic structure with an ultrasmooth surface [12, 13]. The typical roughness of deposited silver or gold is a few nanometers; one of the smallest roughnesses was reported as 0.59 nm [1]. However, there have been only limited studies to quantitatively investigate how optical loss in a

plasmonic structure is affected by the roughness of the metal surface. In this work, we calculate the surface-roughness-dependent  $Q$  factors of a semiconductor nanodisk/silver nanopan plasmonic cavity structure. Systematic three-dimensional (3D) finite-difference time-domain (FDTD) simulations were performed to study how the  $Q$  factors of plasmonic and optical modes depend on the surface roughness at the dielectric-metal interface. In our simulation, the roughness of the randomly patterned surface was described quantitatively using a root-mean-square (rms) height and a correlation length. In addition, to investigate the physical origin of the optical loss in a plasmonic cavity mode, the total optical loss was analyzed in terms of absorption loss and radiation loss as functions of an rms height of surface roughness. We believe that our theoretical study will be useful in designing novel, high-performance plasmonic cavities or lasers.

### II. SIMULATION METHOD

We consider surface roughness of a few nanometers at

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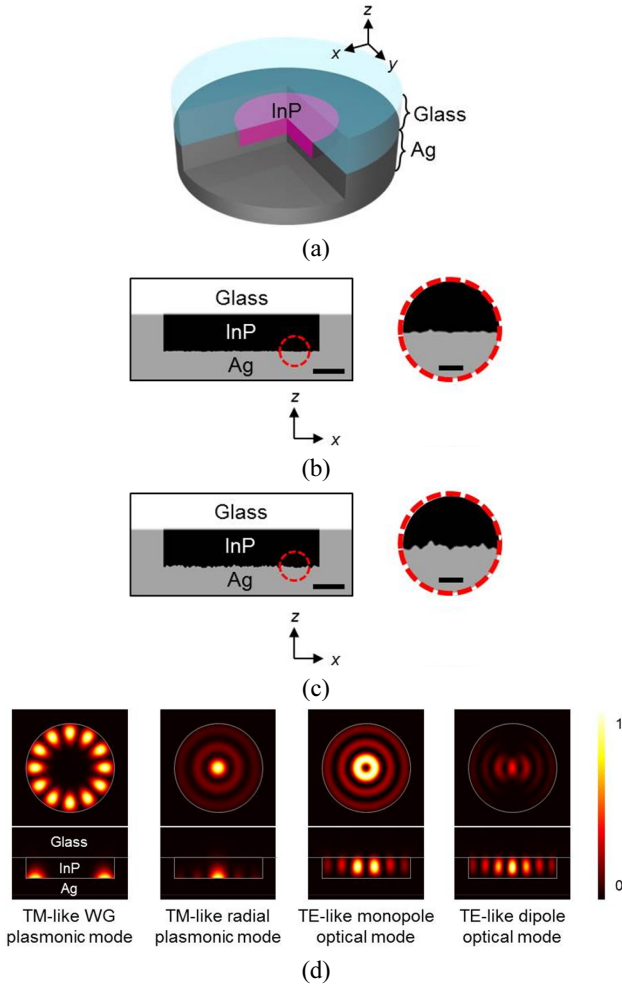


FIG. 1. (a) Schematic diagram of the semiconductor nanodisk/silver nanopan plasmonic cavity structure. The diameter and height of the InP nanodisk are 1000 and 235 nm respectively, and the refractive indices of the nanodisk and glass are 3.2 and 1.45 respectively. Random patterns were introduced on the bottom surface of the silver nanopan. (b), (c) Cross-sectional views of the nanodisk/nanopan plasmonic structure (left) and magnified images of the dielectric-metal interface at rms heights of (b) 2 nm and (c) 5 nm (right). The scale bars in the left and right panels are 200 nm and 50 nm long, respectively. (d) Top and side views of field intensity profiles of the TM-like WG plasmonic mode, TM-like radial plasmonic mode, TE-like monopole optical mode, and TE-like dipole optical mode (left to right), at an rms height of 0 nm.

the dielectric-metal interface of a plasmonic structure, which could be introduced necessarily in a fabrication process involving metals. Our plasmonic structure consists of a dielectric nanodisk and a silver nanopan (Fig. 1(a)), the same structure as reported by Kwon *et al.* for the experimental demonstration of plasmonic lasing [1]. The top of the nanodisk is bonded to a transparent glass substrate, and the bottom and side wall of the disk are covered with silver. 3D FDTD simulation is used to calculate the optical

properties of this nanodisk/nanopan plasmonic structure at room temperature. The diameter and height of the nanodisk are 1000 and 235 nm, respectively. In the simulation, the spatial resolution is 2 nm (10 nm) inside (outside) the cavity along each axis, and the calculation's domain size is  $3.0 \times 3.0 \times 1.5 \mu\text{m}^3$ . The refractive indices of the nanodisk and glass are set to 3.2 and 1.45, respectively. Silver is described by Drude model, which fits its experimentally determined dielectric function [14]. Random patterns to represent the surface roughness at the dielectric-metal interface are generated using a corrugation function with an rms height that varies from 0 to 5 nm, while the correlation length is fixed at 10 nm (Figs. 1(b) and (c)) [15]. The rms height and correlation length are defined respectively as the standard deviation of surface-height variation, and the peak-to-peak distance between two patterns. The correlation length of 10 nm is small enough compared to the resonant wavelength of plasmonic cavity modes, so diffraction effects can be excluded. We only consider the surface roughness at the bottom interface; the side wall is assumed to be perfectly flat. Detailed analysis of the real roughness pattern of such a plasmonic cavity will be necessary for further study. Figure 1(d) shows the field intensity profiles of four plasmonic and optical modes that are excited in the plasmonic structure at an rms height of 0 nm: the transverse-magnetic-like (TM-like) whispering-gallery (WG) plasmonic mode, the TM-like radial plasmonic mode, the transverse-electric-like (TE-like) monopole optical mode, and a TE-like dipole optical mode.

### III. SIMULATION RESULTS

To investigate the effect of surface roughness in the plasmonic cavity, first we calculate the mode profiles of two representative plasmonic and optical modes: the TM-like WG plasmonic mode (Figs. 2(a)~(c)) and the TE-like monopole optical mode (Figs. 2(d)~(f)). As shown in the calculated field intensity profile at an rms height of 0 nm, the TM-like WG plasmonic mode is well excited at the bottom surface of the silver nanopan (Fig. 2(a)). The top view of the field profile was obtained at a position 40 nm above the bottom of the silver nanopan. With increasing rms height of the surface roughness the field profiles change significantly, while the SPPs are still confined to the bottom surface of the nanopan, and the intensity antinode of the plasmonic mode is also observed. In particular, we note in Fig. 2(c) that the local excitation of SPPs at the roughened surface patterns (several bright spots at the bottom surface) leads to distortion of the field profile. Such field concentration at a metallic nanometer-sized structure can cause a qualitative deterioration of the plasmonic mode and significant optical absorption, as the rms height of the surface roughness is large [12]. In contrast, the TE-like monopole optical mode excited inside the InP nanodisk does not show significant distortion of the field profile, despite the increased rms

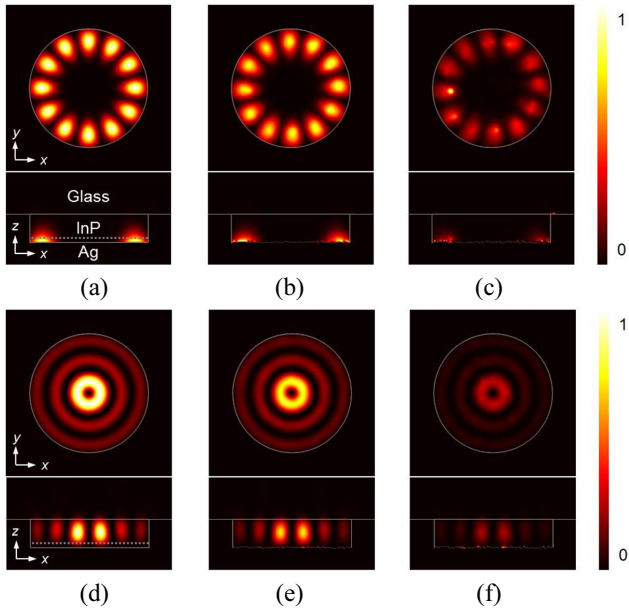


FIG. 2. Top and side views of electric-field intensity profiles of (a-c) the TM-like WG plasmonic mode and (d-f) the TE-like monopole optical mode, with varying rms height of the bottom surface from 0 to 5 nm. The rms heights are (a, d) 0 nm, (b, e) 3 nm, and (c, f) 5 nm. The correlation length is fixed at 10 nm. The top view of the field profile was obtained at a position 40 nm above the bottom surface of the nanopan, as indicated by a gray dotted line in the side view. All images are normalized to the maximum intensity at an rms height of 0 nm. In (f), the intensity was tripled after normalization.

height of the bottom surface roughness in the nanopan. Strong field concentration at each rough feature is not observed in Figs. 2(e) and (f). These results indicate that the TM-like WG plasmonic mode confined to the bottom surface of the nanopan is more affected by metal surface roughness than is the conventional optical mode.

To examine quantitatively the optical losses of the plasmonic and optical modes excited in the nanodisk/nanopan structure, we calculate each of their  $Q$  factors as a function of the rms height of the metal surface roughness (Fig. 3). Five different surface roughnesses are tried, and each rms height varied from 0 to 5 nm. In Fig. 3 the  $Q$  factors are plotted, with errorbars denoting one standard deviation from the average of five simulations (different random structures but same rms height of roughness). As expected from the mode profiles of Fig. 2, the  $Q$  factors of the plasmonic modes decrease quickly with increasing rms height of the metal surface roughness. The  $Q$  factors of the TM-like WG and the TM-like radial plasmonic modes change from 260 to 140 and 180 to 110 respectively, as the rms height increases from 0 to 5 nm. On the other hand, the  $Q$  factors of the optical modes are higher than those of the plasmonic modes, even with the introduction of roughness, because the optical modes are less affected by the absorption loss of the metal.

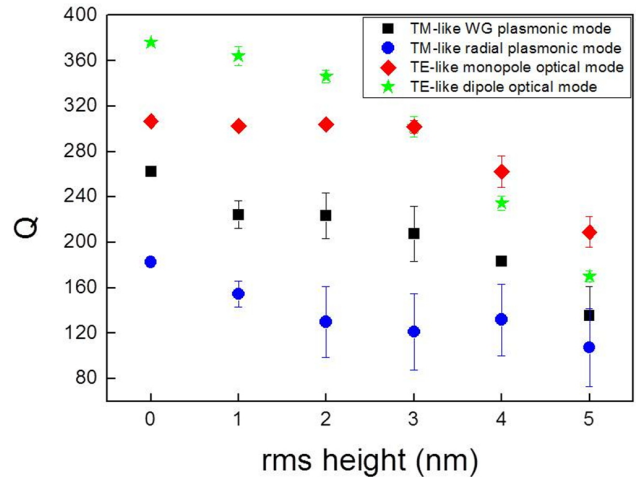


FIG. 3.  $Q$  factors of the TM-like WG plasmonic mode (black squares), TM-like radial plasmonic mode (blue circles), TE-like monopole optical mode (red diamonds), and TE-like dipole optical mode (green stars) are calculated as a function of rms height of the metal surface roughness. Error bars denote one standard deviation from the average of five simulations.

We observe two unique features when we compare the  $Q$  factors of the plasmonic and optical modes: (1) the error bars for the plasmonic modes are much larger than those for the optical modes, and (2) the rate of decrease of the plasmonic modes is faster than that of the optical modes at an rms height  $\leq 3$  nm, but slower at an rms height  $> 4$  nm. First, the plasmonic modes strongly confined to the bottom surface of the silver nanopan are highly sensitive to how the random patterns at that surface are dispersed, and thus a slight change of the metal's properties such as surface roughness can lead to a significant change in  $Q$  factor. Therefore, even in the case of identical rms height of the surface roughness, the deviation of  $Q$  factor can be larger in the plasmonic modes. Second, regarding the fast decrease of  $Q$  factor in the optical modes at an rms height  $> 4$  nm, we can understand that such a large rms height starts to affect the properties of the optical modes, and thus their  $Q$  factors also decrease, although the intensity antinodes of the optical modes are relatively distant from the rough metal surface.

To further investigate the physical origin of optical losses due to surface roughness, we calculate separately the absorption loss and radiation loss of the TM-like WG plasmonic mode by accumulating electromagnetic power dissipated into the silver nanopan and scattered out of the cavity, respectively. The absorption  $Q$  factor ( $Q_{\text{abs}}$ ) and radiation  $Q$  factor ( $Q_{\text{rad}}$ ) calculated from these optical losses are plotted as a function of rms height of the bottom surface roughness (Fig. 4, left and right axes).  $Q_{\text{abs}}$  and  $Q_{\text{rad}}$  decreased from 270 to 140 and 6400 to 2200 respectively, with increasing rms height from 0 to 5 nm. As mentioned above, the decrease of  $Q_{\text{abs}}$  can be understood by the local

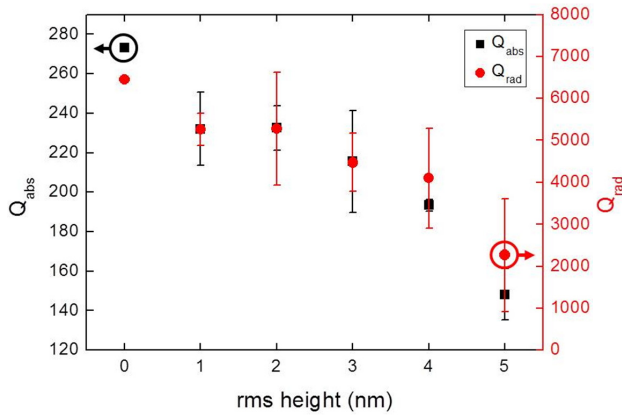


FIG. 4. Absorption  $Q$  ( $Q_{\text{abs}}$ , black squares; left axis) and radiation  $Q$  ( $Q_{\text{rad}}$ , red circles; right axis) of the TM-like WG plasmonic mode are calculated as a function of rms height of the metal surface roughness. Error bars denote one standard deviation from the average of five simulations.

excitation of SPPs at rough surface features. On the other hand, it is noted that  $Q_{\text{rad}}$  decreases more rapidly with increasing rms height. The ratio radiation loss to absorption losses  $Q_{\text{rad}}/Q_{\text{abs}}$  decreases from 23.6 to 15.0 with increasing rms height from 0 to 5 nm. This shows that the absorption loss is dominant at a small rms height, whereas both absorption and radiation losses are critical at a large rms height. Since the absorption loss is always dominant and difficult to decrease, even in the case of the smooth metal surface, to obtain a higher  $Q$  factor in the plasmonic cavity we can conclude that it is more efficient to reduce the radiation loss.

#### IV. CONCLUSION

In summary, we have performed systematic 3D FDTD simulations to examine the surface-roughness-dependent  $Q$  factors in a nanodisk/nanopan plasmonic structure. The simulation results show that a surface roughness of even a few nanometers can cause deterioration of the optical properties of the plasmonic cavity. The  $Q$  factors of plasmonic modes tend to significantly decrease at an rms height  $\geq$  just 1 nm, whereas those of optical modes decrease more slowly, until an rms height of  $\leq$  3 nm. In addition, absorption loss is dominant in the optical loss at a smooth surface, but radiation loss also becomes important with increasing rms height. We can therefore conclude that it is important to fabricate a metallic structure with ultrasmooth surfaces to yield a high- $Q$  plasmonic cavity.

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