# Cross Diabolo Hollow Notch Nanotweezer for Optical Trapping and Manipulation

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Abstract—Plasmonic nanotweezer manipulates nanoparticles utilizing extraordinary electric field gradients and field enhancement originated from localized surface plasmon resonance. We proposed an ingenious silver-based cross diabolo hollow notch plasmonic nanotweezer. Additional edges at the center maximize the field enhancement caused by local surface plasmon hot spots. Moreover, the bottom Ag film's screening effect significantly increases the field intensity near the trapping targets. The subsequent field gradient remarkably enhances the trapping capability of the design in comparison to conventional plasmonic tweezers. We carried out a comprehensive analysis of structural design optimization to reduce power consumption and significantly improve optical trapping properties. The proposed Ag CDHN nanotweezer can trap a polystyrene sphere of 30 nm diameter at a minimum beam intensity of 2.66 mW/ $\mu$ m<sup>2</sup> and trapping force of 2.14 nN/(W. $\mu$ m<sup>-2</sup>) towards the nanostructure. In comparison to previously reported nanotweezers, the proposed nanotweezer demonstrated a few-order increase in trapping stiffness and a few times decrease in power consumption. We also evaluated its capacity to trap polystyrene spheres of varying diameters. Our proposed design and analysis will be beneficial in realizing effective nanotweezer for nanoparticle manipulation as well as nanostructure fabrication.

Index Terms—Nanotweezer, optical trapping, plasmonics, optical force, cross diabolo hollow notch.

#### I. INTRODUCTION

N OPTICAL tweezers, the field gradient due to a highly focused laser beam exerts trapping force toward the focus of the beam on minuscule particles. This distant-controlled and non-destructive technique has paved various applications for the manipulation and characterization of dielectric nanoparticles [1]–[5] and living cells [6]–[8]. However, stable trapping of particles smaller than the incident beam wavelength is difficult due to the blunt gradient field observed by the particle. Plasmonic metallic nanostructures can be utilized for developing sufficient field gradients using low-powered sources. These structures can create localized surface plasmon resonance (LSPR) where free charges accumulate at different edges of the metal-dielectric interface for selective incident wavelengths, known as resonance wavelengths [9]. Metallic structures equipped with nano-gap can

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accumulate charges precisely at the edges of the nano-gap at one of its resonance wavelengths [10]. It amplifies the electromagnetic (EM) field at the metal edges near the gap location which is generally referred to as 'hot spots'. Some metallic structures can further amplify the hot spot field enhancement process when the lightning rod effect occurs due to structural edges of metal [11]. These hot spots originate magnified EM field over source field. Hence, generated sharp field gradient makes trapping of sub-wavelength sized particles feasible. Typically Ag and Au are the preferred metals for plasmonic tweezers due to their low plasmonic loss and superior field enhancement capability [12], [13]. There are several reports of developing hot spots in nanostructures such as nanodiscs [14], nanoholes [1], [15], and bowties [16]-[18]. However, such plasmonic nanotweezers exhibit Joule heating due to the strong absorption losses [19]. This generally elevates the temperature around the hot spots and the resultant temperature gradient can cause thermophoresis and convection. Alternatively, dielectric waveguide-based nanotweezers can mitigate this issue. A variety of dielectric nanostructures capable of producing narrow field gradients have been reported such as nanoantenna [20]-[22], artificial photonic lattices [23], [24] and cavity [15], [25]. However, they require a larger footprint to maintain resonant modes and also require a comparatively high-powered source over plasmonic ones. Research has been conducted to mitigate heating issues related to plasmonic tweezers. Wang et al. utilized metal with a high thermal conductivity as heat sink film and placed it below the plasmonic nanostructure to dissipate heat quickly from the hot spots [26].

Bowtie is one of the efficient geometries among basic plasmonic nanotweezers. Several bowtie-inspired structures were reported exceeding performance over the conventional one [9], [13], [27]-[31]. Hrtoň et al. studied EM characteristics of bowtie, diabolo (bridged bowtie) and both their aperture structures [32]. According to this report, diabolo aperture contributed dominant field enhancement due to the combination of lightning rod and nano-gap effect. Besides, Gupta and Dhawan reported that cross diabolo aperture (CDA) can furnish superior field enhancement compared to diabolo aperture because of the increased number of hot spots [9]. Lin and Lee worked on Au-based mono DHN by adding an Au film at the bottom of Au diabolo aperture [33]. The additional metal film reflected the light energy which used to get wasted due to propagating through the transparent gap region in metal film-less structures. This reflection of energy shifted major charge accumulation at the top edges of the nanotweezer. Thus, effective field enhancement

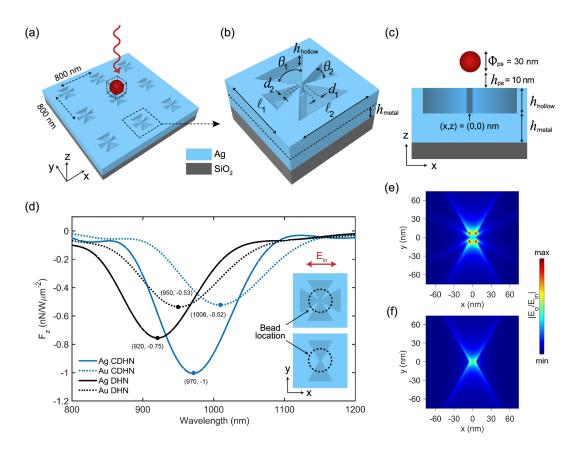


Fig. 1. Schematic representations of (a) 3x3 arrays and (b) truncated unit-cells of proposed CDHN nanotweezers. (c) Visual representation of a PS bead of 30 nm diameter placed at center of the xy-plane above the nanotweezer where  $h_{ps}=10$  nm. (d) Wavelength dependence of  $F_z$  for CDHN (blue line) and DHN (black line) nanotweezers where dotted and solid lines represented Au and Ag as selected metals, respectively. E-field intensity on xy plane at the top metal surface of (e) Ag CDHN at  $\lambda_d=970$  nm and (f) Ag DHN at  $\lambda_d=920$  nm.

positively impacted particle trapping. Moreover, Ag can provide marginally improved reflectivity at IR regime and thermal conductivity over Au which left an option to further elevate the trapping performance.

In this work, we proposed an Ag cross diabolo hollow notch (CDHN) nanotweezer by adding Ag film at the bottom of CDA. Ag CDHN can be a more efficient and cost-effective bowtie-inspired plasmonic nanotweezer design combining the benefits of CDA and bottom metal film. We theoretically analyzed the underlying physics behind the shifting of suitable trapping beam wavelength and consequent trapping performance for varying design parameters. Ag DHN nanotweezer, which we found as a very efficient tweezer design over conventional diabolo ones in our previous study [34], is outperformed by our current proposed Ag CDHN nanotweezer. For different diameters of polystyrene spherical (PS) beads, change of trapping force components and shifting of the trapping beam wavelength were also investigated which will be beneficial to implement this kind of nanotweezer for particle detection applications.

## II. STRUCTURAL DESIGN AND SIMULATION SETUP

# A. Structural Design

Our CDHN structure is composed of metal-based CDA structure on top of an analogous metal thin film. The metal structure is supported on a glass  $(SiO_2)$  substrate. The illustrations of the

3x3 array and unit cell of the CDHN nanotweezer are presented in Figs. 1(a) and Figs. 1(b), respectively. For suspended particle trapping, the whole system was considered to be immersed in water ( $n_{water}=1.33$ ). Heights of structural aperture and thin metal film were denoted by  $h_{hollow}$  and  $h_{metal}$ , respectively. In the CDHN structure, both diabolo hollow notches were perpendicular to each other and a common gap was created at the center. The central gap region of CDHN was termed as horizontal gap length,  $d_1$  and vertical gap length,  $d_2$ . Wing lengths of vertical and horizontal diabolo notches were  $l_1$  and  $l_2$ , respectfully. Hollowed bow angles of vertical and horizontal diabolo notches were  $\theta_1$  and  $\theta_2$ , respectfully. The periodicity of each cell of CDHN nano-array was considered to be 800 nm in x and y directions. Fabrication process of the proposed nanostructure is provided in Supplementary Material.

# B. Methodology

Finite difference time domain (FDTD) solver was used for analyzing properties of the proposed plasmonic nanotweezer. FDTD method provides faster convergence and better accuracy for these kind of structures compared to other methods. Perfectly matched layer (PML) boundary conditions were used in all directions during simulation. Complex dielectric constants of both Ag and Au were adopted from Johnson and Christy [35]. Material properties of glass were acquired from Palik [36]. Finite

element solver was utilized for heat transfer analysis. Thermal properties of Ag was adopted from CRC [37].

In order to mimic viruses or proteins or dielectric nanoparticles, a nanoscale PS bead of diameter,  $\Phi_{ps}=30$  nm was chosen as a trapped particle. The refractive index of PS bead,  $n_{ps}$  was 1.57. For trapping force calculation, PS was surrounded by six 2D field monitors. The resultant EM fields were post-processed into 3D optical force using the time-averaged closed surface integral of Maxwell stress tensor as shown in (1) [38].

$$F = \oint_{S} (T. n) \, \mathrm{d}s, \tag{1}$$

where F is time-averaged force, n is unit vector perpendicular to the integration surface and T is time-averaged Maxwell stress tensor which can be presented as,

$$T = \frac{1}{2} \text{Re} \left[ \varepsilon E E^* + \mu H H^* - \frac{1}{2} (\varepsilon E^2 + \mu H^2) I \right],$$
 (2)

where  $EE^*$  and  $HH^*$  denote outer products of electric field (E) and magnetic field (H), respectively. I is the identity matrix and  $\varepsilon$ ,  $\mu$  are the permittivity and the permeability of the medium, respectively. Detailed equations for force components are provided in Supplementary Material. The trapping potential along x axis was obtained by  $\int F_x \, \mathrm{d}x$ , where  $F_x$  is the x component of optical force. Similarly, trapping potential along y and z axes were calculated.

During simulation, the backscattering spectrum only provides information about LSPR wavelength while being unspecific about the location of the hot spot. At certain resonance wavelengths, LSPR mode can occur at side edges rather than the edges near the central gap which will not enhance trapping performance. Therefore, structural optimization using backscattering spectrum is defective. Typically, E-field intensity is monitored at the edges near the central gap to detect LSPR wavelength. Nevertheless, effective trapping of any nano-particle requires contributions from both electric and magnetic fields, shown in (2). Therefore, neglecting magnetic field data may deviate from accurate outcomes. For more meticulous approximation, a PS bead can be placed above the plasmonic nanotweezer at the horizontal center of the structure to observe the wavelength dependence on optical force along z direction,  $F_z$ . The spectrum of  $F_z$  has notches or dips when field enhancement peaks at the central metal gap. In our analyses, we only focused on the lowest dip of  $F_z$  when particle can be trapped effectively at that corresponding wavelength. For future discussions, the lowest dip of  $F_z$  and the corresponding trapping beam wavelength are denoted by  $F_d$  and  $\lambda_d$ , respectively.

# III. CHARACTERISTIC STUDY OF PROPOSED STRUCTURE

#### A. Mono and Cross Diabolo Hollow Notch

Trapping performance of DHN and CDHN was evaluated for Au and Ag as the metals. For CDHN nanotweezer, selected parameters were  $l_1=l_2=300$  nm,  $\theta_1=\theta_2=60^\circ$ ,  $d_1=d_2=10$  nm and  $h_{hollow}=h_{metal}=70$  nm. For DHN nanotweezer, only vertical diabolo of CDHN was considered with identical parameters i.e.,  $l_1=300$  nm,  $\theta_1=60^\circ$ ,  $d_1=10$  nm and  $h_{hollow}$ 

 $=h_{metal}=70$  nm. A PS bead of 30 nm diameter was placed at center of the xy-plane above the nanotweezer where  $h_{ps}=10$  nm (see Fig. 1(c)). The incident beam was x-polarized plane wave

For a conscientious selection of geometry and material for the nanostructure, spectra of  $F_z$  for both structures based on Au and Ag is displayed in Fig. 1(d). Moreover, E-field intensity distribution on the top surface of metal layer for Ag based DHN and CDHN nanotweezers at corresponding  $\lambda_d$  are presented in Figs. 1(e) and Figs. 1(f), respectively. When both structures were compared to associated metals, Au-built structures had a higher  $\lambda_d$  than Ag-built structures. Ag-based structures had a better screening effect which contributed to more E-field intensification at the top metal surface. Hence, nanotweezers made of Ag had a higher  $|F_d|$  than those made of Au. Furthermore, Ag provides heat sink capability comparable, if not better, than that of Au. CDHN had four hot spots on the top metal interface, whereas DHN had only two. As a result of the increased surface plasmon coupling, a redshift in  $\lambda_d$  was observed for CDHN compared to DHN, which is consistent with a previous report [9]. As fabrication of CDHN is more detailed than DHN, using Au to achieve similar performance (see dotted lines of Fig. 1(d)) is not recommended. As a result, mono diabolo or bowtie-type structures are better suited to be fabricated using Au [10], [39]. However, Ag CDHN could provide up to 33% more  $|F_d|$  than Ag DHN due to increased charge accumulation at the center for CDHN's narrow bow angles. For the reasons stated above, Ag is chosen for the proposed CDHN nanotweezer.

# B. Bottom Metal Film Induced Plasmon Coupling and Screening Effect

The color map of  $|F_z|$  spectra for Ag CDHN nanotweezer by sweeping  $h_{metal}$  from 0 to 150 nm is presented in Fig. 2(a). Other parameters were unchanged during the simulations. Fig. 2(b) presents zoomed spectra of  $|F_z|$  for sweeping  $h_{metal}$  from 0 to 6 nm for better visualization of the resonance peak in the longer wavelengths. The increase of  $h_{metal}$  blueshifted  $\lambda_d$  from 1960 nm until it saturated at 970 nm when  $h_{metal}$  exceeded 35 nm. Fig. 2(d)–(f) show E-field intensity on xz-plane along yaxis for  $h_{metal} = 0$  nm, 5 nm and 50 nm, respectively at corresponding  $\lambda_d$ . When  $h_{metal} = 0$  nm, the structure transmutes into CDA structure on a glass substrate. Free charge accumulation resulted in E-field enhancement at top and bottom edges of metal surface which is consistent with the previous reports [30], [40]. Charge density at the central metal edges which were distributed along the vertical surface, accommodated strong surface plasmon coupling resulting in  $\lambda_d$  at 1960 nm as can be seen in Fig. 2(d) [41]. Charge localization near the bottom edges of metal surface fell rapidly for minimal addition of Ag metal film ( $h_{metal} = 5$  nm) at the bottom, presented in Fig. 2(e). Due to disruption in surface plasmon coupling, blueshift of  $\lambda_d$  was observed for increasing  $h_{metal}$  up to 35 nm. After  $h_{metal}$  exceeded 35 nm, charges only localized near top edges of metal surface and plasmon coupling factor with the bottom edges became insignificant which is illustrated in Fig. 2(f) where  $h_{metal}$  was 50 nm. Therefore,  $\lambda_d$  saturated at 970 nm.

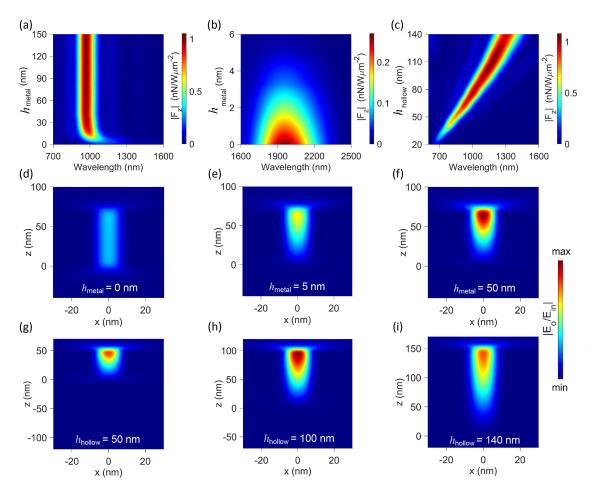


Fig. 2. Color map showing the spectra of  $|F_z|$  for (a) varying  $h_{metal}$  from 0 to 150 nm where wavelength was ranged from 700 to 1600 nm and (b) varying  $h_{metal}$  from 0 to 6 nm with wavelength variation from 1600 to 2500 nm. For both cases  $l_1 = l_2 = 300$  nm,  $\theta_1 = \theta_2 = 60^\circ$ ,  $d_1 = d_2 = 10$  nm,  $h_{hollow} = 70$  nm. (c) Color map illustrating wavelength dependence of  $|F_z|$  where  $h_{hollow}$  was varied from 20 to 140 nm,  $h_{metal} = 150$  nm and other parameters were same as previously stated. E-field intensity on xz-plane along y axis for  $h_{metal} = (d)$  0, (e) 5, and (f) 50 nm at  $\lambda_d$  equal to 1920, 1300, and 970 nm, respectively. Video 1.mp4 depicts a movie illustrating the change in E-field intensity as  $h_{metal}$  was swept from 0 to 130 nm at the corresponding  $\lambda_d$ . E-field intensity on xz-plane along y axis for  $h_{hollow} = (g)$  50, (h) 100, and (i) 140 nm at corresponding  $\lambda_d = 850$ , 1125, and 1300 nm, respectively. Video 2.mp4 demonstrates a movie showing the variation of E-field intensity for ranging  $h_{hollow}$  from 20 to 140 nm at corresponding  $\lambda_d$ .

For increasing  $h_{metal}$ ,  $|F_d|$  incremented from 0.4  ${\rm nN/W}\mu{\rm m}^{-2}$  until it saturated at  $1~{\rm nN/W}\mu{\rm m}^{-2}$  when  $h_{metal}$  exceeded 35 nm. Light reflects energy towards the upper metal edges due to screening effect when bottom metal film is present. Both screening effect and lightning rod effect accumulate more charges at the top corners and enhance E-field intensity at the top surface where a PS bead is placed and similar behavior was reported before [33]. Thus, increment in  $|F_d|$  was observed for increase in  $h_{metal}$  up to 35 nm. Due to saturation of screening effect,  $|F_d|$  saturated for  $h_{metal} \geq 35~{\rm nm}$ .

To observe heat sink capability of the proposed structure, 0.8 mW heat source was introduced at the center of the top surface and  $h_{metal}$  was varied from 40 to 150 nm. The resultant temperature profiles along y axis at xz plane can be seen in Fig. 3. Heat conduction and heat sinking capability enhanced for increasing  $h_{metal}$ . Therefore,  $h_{metal}$  height was selected to be 150 nm which can minimize thermophoresis and convection and will be beneficial for thermally-sensitive nanoparticle manipulation.

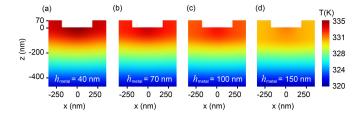


Fig. 3. Temperature profile using 0.8 mW heat source situated at the center for Ag CDHN nanotweezer with  $h_{metal}=$  (a) 40, (b) 70, (c) 100, and (d) 150 nm.

# C. Effect of Metal Hollow Height

Color map depicting the spectra of  $|F_z|$  is presented in Fig. 2(c) where  $h_{hollow}$  was varied from 20 nm to 140 nm and other design parameters were set as previously mentioned.  $\lambda_d$  was independent of plasmon coupling between top and bottom metal edges since bottom metal-film height was above the saturation height as demonstrated in Fig. 2(g)–(i), depicting

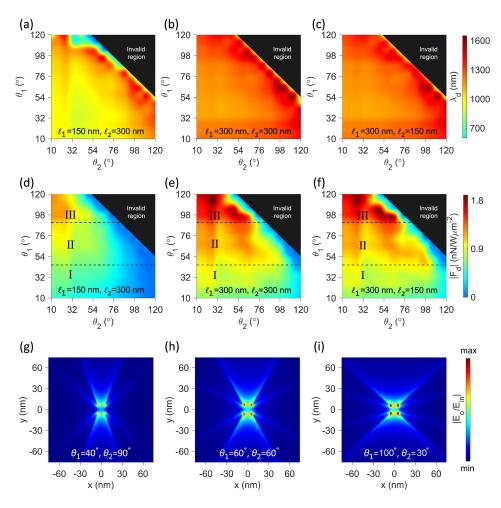


Fig. 4. Color maps showing (a-c)  $\lambda_d$  and (d-f)  $|F_d|$  for varying both  $\theta_1$  and  $\theta_2$  from 10° to 120°. Here,  $(l_1, l_2) = (150, 300)$  nm at (a,d), (300, 300) nm at (b,e) and (300, 150) nm at (c,f). Other parameters included  $d_1 = d_2 = 10$  nm,  $h_{metal} = 150$  nm and  $h_{hollow} = 110$  nm. E-field intensity on xy plane at top metal surface of Ag CDHN for  $(\theta_1 \ \theta_2) = (40^\circ, 90^\circ)$  at (g),  $(60^\circ, 60^\circ)$  at (h) and  $(100^\circ, 30^\circ)$  at (i). Corresponding  $\lambda_d$  are 1230, 1200, and 1250 nm.

E-field intensity on xz-plane along y axis for  $h_{hollow}=50$  nm, 100 nm and 140 nm at corresponding  $\lambda_d$ . For increasing  $h_{hollow}$ ,  $\lambda_d$  redshifted due to larger penetration depth of surface plasmon polariton (SPP) at longer wavelengths [42]. It was experimentally proven that E-field intensity could increase at top metal edge with the decrease of nano-aperture height, which is denoted by  $h_{hollow}$  in our design [43]. However, shorter  $h_{hollow}$  induced low concentration of charge which lead to lower E-field intensity at the top (see Fig. 2(g)). On the contrary, increasing  $h_{hollow}$  instigated charge loss at the upper edges due to charge redistribution along the vertical sidewalls of metal. This resulted in E-field intensity reduction at the top edges shown in Fig. 2(i). Therefore,  $|F_z|$  reached a peak value when  $h_{hollow}$  was between 80 to 130 nm, according to Fig. 2(c). For further analyses,  $h_{hollow}$  was considered to be 110 nm.

# D. Plasmon Coupling and Light Polarization-Dependence Due to Bow Angles

Optical trapping properties of the proposed structure depending on both vertical and horizontal hollowed bow angles ( $\theta_1$  and  $\theta_2$  respectively) were investigated to obtain the optimal

design. Figs. 4(a)–(c) and 4(d)–(e) depict color maps of  $\lambda_d$  and  $|F_d|$  respectively by sweeping  $\theta_1$  and  $\theta_2$  from 10° to 120°. To understand the effect of wing lengths on bow angles,  $|F_d|$  and  $\lambda_d$ were calculated for 3 different combinations of  $l_1$  and  $l_2$  i.e. (150, 300), (300, 300) and (300, 150) nm. Other structural parameters were kept unaltered. The black regions in the figures represented invalid structure because  $\theta_1 + \theta_2 \ge 180^\circ$ . Transitions of  $|F_d|$  and  $\lambda_d$  remained almost independent of  $l_1$  and  $l_2$  for combinations where  $l_1 \ge l_2$ . From Fig. 4(b), (c), it is apparent that  $\lambda_d$  redshifted for  $\theta_1$  or  $\theta_2$  above 90° owing to the increase in effective index of local surface plasmon polaritons (SPPs) [44]. Additional redshift can occur at these cases because of enhanced plasmon coupling at sidewalls adjacent to  $\theta_1$  and  $\theta_2$  as seen in Fig. 4(g)–(i), illustrating E-field intensity on xy plane at top metal surface of Ag CDHN for  $(\theta_1, \theta_2) = (40^\circ, 90^\circ), (60^\circ, 60^\circ)$  and  $(100^\circ, 90^\circ)$ 30°), respectively at corresponding  $\lambda_d$  (where  $l_1 = 300$  nm,  $l_2$ = 300 nm). According to these figures, sidewalls adjacent to  $\theta_1$  have significant charge accumulation compared to those of  $\theta_2$ . Therefore,  $\theta_2$  above 90° produces marginally larger red-shift over  $\theta_1$  above 90°. However, drastic drop in  $\lambda_d$  was observed for the case of  $(l_1, l_2) = (150, 300)$  nm (see Fig. 4(a)) due to reduced charge coupling for lower value of  $l_1$ .

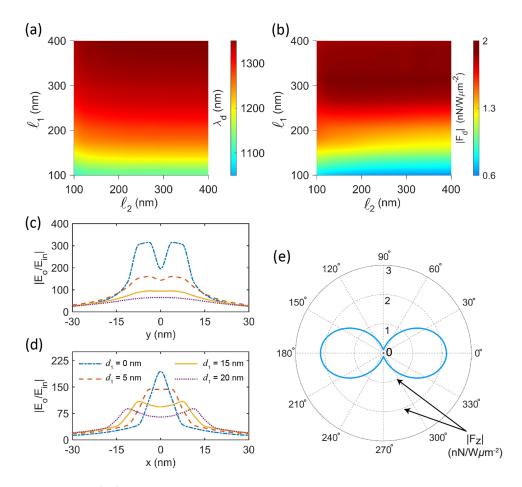


Fig. 5. Color map representations of (a)  $|F_d|$  and (b)  $\lambda_d$  where  $l_1$  and  $l_2$  were swept from 100 to 400 nm. Here,  $\theta_1=115^\circ$ ,  $\theta_2=25^\circ$ ,  $d_1=d_2=10$  nm,  $h_{metal}=150$  nm and  $h_{hollow}=110$  nm. E-field intensity (c) along y axis and (d) along x axis for  $d_2=8$  nm and  $d_1=0$ , 5, 15, 20 nm. Here,  $l_1=315$  nm and  $l_2=200$  nm and other parameters were unchanged as before. (e) Polar plot for  $|F_z|$  depending on incident beam polarization for the optimized Ag CDHN nanotweezer at 1340 nm incident wavelength. E-field intensity variation with beam polarization is illustrated in Video 3.mp4.

E-field enhancement of the nanotweezer can be explained by dividing Fig. 4(d)-(f) into 3 regions. For increasing horizontal bow angle  $\theta_2$ , peak E-field at the center dropped for all cases due to the increased perpendicular relation with x-polarized source beam which was consistent with previous reports [17], [45]. When  $\theta_1$  was around 10° to 45° (Region I), sidewalls adjacent to  $\theta_1$  were perpendicular to the light polarization. Hence, low E-field intensity occurred at the center as can be seen in Fig. 4(g). When  $\theta_1$  was around 45° to 90° (Region II), sidewalls adjacent to  $\theta_1$  were less perpendicular to light polarization compared to the structures for Region I. Consequently higher E-field intensity was observed as shown in Fig. 4(h). While  $\theta_1$  was above 90° (Region III), sidewalls adjacent to  $\theta_1$  were almost parallel to light polarization and generate maximum E-filed intensity as shown in Fig. 4(i). Thus, maximum  $|F_d|$  could be observed in this region. To avoid complexity during fabrication process, we considered  $(\theta_1, \theta_2) = (115^{\circ}, 25^{\circ}).$ 

# E. Redistribution of Accumulated Charge With Variation in Vertical Wing Length

Optical trapping characteristics of the proposed structure were monitored by varying vertical wing length,  $l_1$  and horizontal

wing length,  $l_2$ . Fig. 5(a) and (b) represent colour maps of  $\lambda_d$  and  $|F_d|$  respectively for varying  $l_1$  and  $l_2$  from 100 to 400 nm while setting other parameters as mentioned before. Increasing  $l_1$  engaged more charge coupling at the sidewalls adjacent to  $\theta_1$  (see Fig. S3 of Supplementary Material). Thus, red-shift was observed for increasing  $l_1$ . However, resonance wavelength remained mostly unaltered for the increment of  $l_2$ due to less dominance of charge localization at the sidewalls adjacent to  $\theta_2$ . Consequently,  $|F_d|$  was also mostly independent of  $l_2$ . Screening effect provided less impact for lower values of  $l_1$  [33]. Thus, decline in  $|F_d|$  was noticed for  $l_1$  decreasing from 250 to 100 nm. Moreover, charges redistributed more along the sidewalls while dropping at the central edges for increased values of  $l_1$ . Therefore,  $|F_d|$  started to drop for  $l_1$  over 330 nm. Both these effects were minimized when  $l_1$  was ranging from 250 to 330 nm. According to simulation results, maximum  $|F_d|$ was detected at  $l_1 = 315$  nm and  $l_2 = 200$  nm which were considered for further analyses.

# F. Charge Coupling and Overlapping Factor for Gap Distance

 $\lambda_d$  and  $|F_d|$  were calculated by varying horizontal gap,  $d_1$  and vertical gap,  $d_2$  from 0 to 20 nm as can be seen in the

color maps of Fig. S4 in Supplementary Material. Increment of  $d_1$  resulted in reduced charge coupling between adjacent corners related to  $\theta_1$  where major charge accumulation occurred. Hence,  $\lambda_d$  blueshifted. Increment of  $d_2$  had insignificant impact on  $\lambda_d$  because of low charge accumulation from adjacent sidewalls related to  $\theta_2$ .

However,  $|F_d|$  had inconsistent dependence on  $d_1$  and  $d_2$ . It can be explained by combining effects of target-field overlapping factor and E-field intensity applied over the PS bead. For better understanding, E-field intensity was observed along y axis (see Fig. 5(c)) and along x axis (see Fig. 5(d)) for  $d_2 = 8$  nm and  $d_1 = 0$ , 5, 15, 20 nm. Peak E-field intensity along x and y axis attenuated more with the increase of  $d_1$ . Simultaneously, peak E-field shift followed central edges creating dual modes and increased E-field spreading which lead to amplified target-field overlapping factor. Combined contribution of target-field overlapping factor and E-field intensity over a 30 nm diameter PS bead resulted in maximum  $|F_d|$  for  $(d_1, d_2) = (5, 8)$  nm which was considered for further analyses.

# G. Polarization Sensitive Optical Trapping

Spectra of EM-field at the central location is illustrated at Fig. S5 in Supplementary Material. According to these analyses, the required incident wavelength for efficient trapping was 1340 nm. Incident beam polarization dependence on  $|F_z|$  of the optimized Ag CDHN is illustrated at the polar plot in Fig. 5(e). The nanotweezer exerted maximum  $|F_z|$  for x polarized incident beam as the design was optimized considering this condition.  $|F_z|$  dropped due to low charge accumulation at the central edges when incident light polarization was rotated towards y axis.

#### IV. ANALYSIS ON NANOPARTICLE TRAPPING

Trapping forces and potentials were investigated considering x-polarized plane wave illumination for a unit cell of nanotweezer. Due to structural symmetry, only certain force components were required to visualize the trapping incident. Therefore,  $F_x$ ,  $F_y$  and  $F_z$  were calculated for a PS bead moving along x, y and z axis, respectively. When the bead was moved along x and y axis, it was considered to be positioned at  $h_{ps} =$ 10 nm along z axis. Corresponding potentials  $(U_x, U_y, U_z)$  were normalized in  $k_B T/W \mu m^{-2}$  unit, where  $k_B$  is the Boltzmann constant and T is the ambient temperature (300 K). Vital trapping force components and corresponding potentials of optimized Ag CDHN and Ag DHN are displayed in Fig. 6(a)–(c) for  $\Phi_{ps}$  = 30 nm. Both nanotweezers had lower  $F_x$  compared to  $F_y$  because of reduced resultant E-field contribution. Thus, a small potential depth was observed in  $U_x$  compared to  $U_y$  in both nanotweezers. While comparing both nanotweezers, proposed CDHN have 100%, 43% and 84.2% improved peak to peak trapping forces (of  $F_x$ ,  $F_y$ ,  $F_z$  respectively) over DHN. Furthermore, potential wells of  $U_x$ ,  $U_y$  and  $U_z$  raised by 83.5%, 20% and 122%, respectively. Hence, a significant improvement of optical trapping can be achieved using Ag CDHN. Moreover, the proposed CDHN nanotweezer will require a low-powered light source to achieve identical trapping performance. For stable trapping, the requirement of minimum potential depth is  $-10 \text{ k}_{\text{B}}\text{T}$ . The

TABLE I
THE TRAPPING STIFFNESS ALONG DIFFERENT DIRECTION

Nanotweezer	$k_x$	$k_y$	$k_z$	
	(pN/(nm.W))	(pN/(nm.W))	(pN/(nm.W))	
Ag CDHN	29.4	20.5	227.35	
Ag DHN	14.68	39.5	119.37	

proposed nanotweezer can trap a PS bead of 30 nm diameter at x = y = 0 for illumination intensity above 2.66 mW/ $\mu$ m² while DHN will require intensity above 4.85 mW/ $\mu$ m². Additionally, inward force of 2.14 nN/(W. $\mu$ m²) and 1.14 nN/(W. $\mu$ m²) was observed for the above cases, respectively. The proposed nanotweezer provided enhanced trapping stiffness ( $k_x$ ,  $k_z$ ) over DHN nanotweezer as can be seen in Table I. Stiffness parameters were approximated considering tangential forces at (x, y, z) = (0, 0, 110) nm.

Spectrum of  $|F_z|$  for different values of  $\Phi_{ps}$  on optimized Ag CDHN nanotweezer is presented at Fig. 6(d). For increasing  $\Phi_{ps}$ ,  $\lambda_d$  red-shifted and  $|F_d|$  increased. Effects of  $\lambda_d$  for changing  $\Phi_{ps}$  was monitored as can be seen in Fig. 6(e).  $\lambda_d$  can be expressed using following equation with respect to  $\Phi_{ps}$ ,

$$\lambda_d = 0.5\Phi_{ps} + 1329. \tag{3}$$

Fig. 6(f)–(h) display force and potential components at corresponding  $\lambda_d$  for  $\Phi_{ps}=30$ , 50 and 100 nm. Stable trapping can be achieved for all the above cases. Increasing the diameter of the bead exerted higher trapping force and deeper potential well. Therefore, larger beads will require low intensity beam to trap. Similar minor drop in  $F_x$  compared to  $F_y$  was observed in these cases.

In Table II, the parameters of the proposed design are compared to those of previous theoretical studies using MST method that trapped PS beads with diameters near 30 nm. According to a recent report, Si dimer with ring geometry provided better thermal performance but lacked in trapping performance, as evidenced by the threshold intensity requirement [15]. A similar performance trait was observed with slotted photonic crystal cavity and slot waveguide based optical nanotweezer designs [46], [47]. On the other hand, Au nanostructures on glass substrates or on Si waveguides demonstrated enhanced trapping stiffness and reduced source power requirement [16], [48]-[50]. An analysis on Ag coaxial plasmonic aperture revealed a trapping stiffness of 1.05 pN/(nm.W) on a 10 nm sized PS bead with source beam power requirement of less than 7 mW [51]. In comparison to these reports, the proposed Ag CDHN design requires several times less threshold power and had better trapping stiffness when trapping a PS bead with a diameter of 30 nm. Ag CDHN also focuses on improving heat sink capability, which was missing from the other reports. A heat sink capable nanotweezer using Au DHN nanostructure demonstrated a 0.64 mW threshold power requirement for trapping a 100 nm sized bead [33]. Our proposed CDHN design is more efficient than the previous report due to it's improved geometry increased field intensity at the center. As a result, the beam power requirement is reduced by 45% while trapping a 100 nm sized bead.

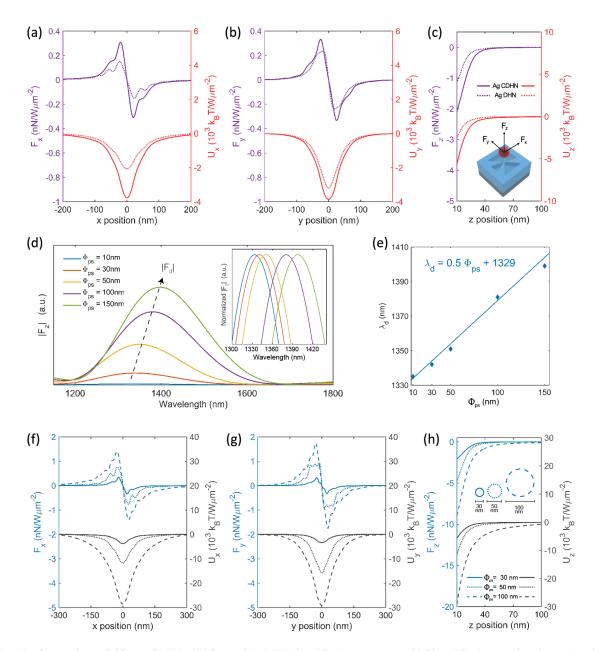


Fig. 6. Trapping force and potential for Ag CDHN (solid line) and Ag DHN (dotted line) nanotweezers with 30 nm PS sphere moving along (a) x axis  $(F_x, U_x)$ , (b) y axis  $(F_y, U_y)$  and (c) z axis  $(F_z, U_z)$ . (d) Wavelength spectrum of  $|F_z|$  at the central location of Ag CDHN nanotweezer for PS bead diameter,  $\Phi_{ps}=10$ , 30, 50, 100, and 150 nm. Inset shows normalized  $|F_z|$  for better visualization of shifting of  $\lambda_d$ . (e) Variation of  $\lambda_d$  with respect to  $\Phi_{ps}$ . (f-h) Trapping force and potential for Ag CDHN with  $\Phi_{ps}=30$  (solid line), 50 (dotted line), and 100 nm (dashed line) at  $\lambda_d$  equalling 1340, 1350, and 1380 nm, respectively.

TABLE II
PERFORMANCE COMPARISON WITH REPORTED GENERATORS

Geometry	$n_{ps}$	Bead diameter	Wavelength	Threshold	Threshold intensity	Maximum horizontal	Ref
		(nm)	(nm)	power (mW)	$(\mathrm{mW}/\mu\mathrm{m}^2)$	Stiffness	
Si dimer with ring	1.6	20	1064	-	9.5	0.1 fN/nm	[15]
Slotted photonic crystal cavity	1.45	30	1400	10	-	3.49 pN/(nm.W)	[46]
Slot waveguide	1.55	35	1550	8.19	-	0.118 pN/(nm.W)	[47]
Waveguide coupled Au bowtie	1.59	20	1620	10.2	-	-	[16]
Au dual nanohole	1.6	25	1064	-	6.67	0.26 fN/nm	[48]
Au nanohole	1.575	50	1064	-	1.6	6.6 fN/nm	[49]
Modified Au nanohole	-	30	980	-	55	0.48 fN/nm	[50]
Ag coaxial plasmonic aperture	2	10	818	<7	-	1.05 pN/(nm.W)	[51]
Au DHN	1.59	100	1154	0.64	-	-	[33]
		30	1340	1.7	2.66	29.4 pN/(nm.W)	
Ag CDHN	1.57	50	1350	0.54	0.85	91.67 pN/(nm.W)	This work
		100	1380	0.22	0.35	116.82 pN/(nm.W)	

# V. CONCLUSION

We proposed a nanotweezer consisting of an Ag cross diabolo aperture structure on a bottom Ag metal film. Superior reflectivity of Ag enhanced the screening effect which resulted in amplified field enhancement at the upper surface of the metal. The resultant effect of four hot spots can be far more impacting than mono diabolo type nanostructures. We comprehensively studied the dependence of structural parameters on trapping wavelength and trapping forces. Charge density at the top and bottom edges of Ag, SPPs, screening, and lightning rod effect impacted trapping properties for variation of Ag thin film height and structural hollow height. Charge density, consequent LSPR coupling at the central edges, and the top sidewalls affected trapping characteristics when hollow bow angles and wing lengths were varied. Theoretical analysis shows that the optimized Ag CDHN nanotweezer can trap a 30 nm diameter PS bead for minimum incident beam intensity of 2.66 mW/ $\mu$ m<sup>2</sup> while generating 2.14 nN/(W. $\mu$ m<sup>-2</sup>) inward force. Maximum horizontal trapping stiffness of 29.4 pN/(nm.W) was found for our tweezer which is few-order larger than previous studies. Further analyses showed low-powered light source is required for larger beads. Shifting of resonance wavelength due to bead size can be beneficial for nanoparticle sensing applications. Additionally, the proposed nanostructure offers superior heat sink capability similar to previously reported bottom metal film-based nanostructures. This work opens up opportunities for the study of further research on diabolo aperture or notch-based nanotweezers. We believe our optimized CDHN nanotweezer can be a useful tool for the fabrication of nanomaterials, manipulating and assembly of nanoparticles and bioparticles, analyzing the interaction between nanoparticles, and sensing and characterization of nanoparticles.

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