Supplementary

Narrowband Perfect Absorber based on Dielectric-Metal Metasurface for Surface-enhanced Infrared Sensing

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Received: 18 February 2020; Accepted: 19 March 2020; Published: date

Figure S1. The cross-section view of the proposed nanostructure.

Figure S1 shows the cross-section view of the proposed metasurface sensor in COMSOL, where the period and width of metal film is 5 um and 4.3 um respectively. A linearly TM polarized plane wave light incident along the z direction, and the periodic boundary conditions are set in the x direction and the perfectly matched layers and scattering boundary conditions are applied in the z direction at two ends of computational space. In the built-in mesh parameters set of COMSOL, Free triangular feature node is applied throughout the simulation region, and the maximum element size (400 nm) is added to simulation. In addition, because the light cannot be transmitted through the aluminum film with 3.5 um thick, the choice of substrate and metal thickness is irrelevant, and the substrate only serves as a support.
Figure S2. (a) Absorptance of the metasurface absorber with different height $H$ of the dielectric grating strips when $P = 3 \, \mu m$ and $W = 2.3 \, \mu m$; (b) Corresponding absorptance and Q-factor with different $H$ of the dielectric grating strips. (c) Absorption spectra of the metasurface absorber with different groove width $W$ when $P = 3 \, \mu m$ and $H = 0.7 \, \mu m$; (d) Corresponding absorptance and Q-factor with different groove width $W$. (e) Absorption spectra of the metasurface absorber with different period $P$ when $W = 0.7 \, \mu m$ and $H = 0.7 \, \mu m$; (f) Corresponding absorptance and Q-factor with different period $P$.

Figure S2a shows the absorptance color mapped as a function of the wavelength and varying height $H$ when $P = 3 \, \mu m$ and $W = 2.3 \, \mu m$. One can see that the resonant wavelength exhibits a clear red-shift from 3.140 $\mu m$ to 3.818 $\mu m$ with increasing $H$ from 0.25 $\mu m$ to 1.5 $\mu m$, accompanied with broadening of the FWHM from 14 nm to 58 nm. Though a large Q-factor of 311 can be achieved when $H = 0.25 \, \mu m$, the absorptance of the absorber is only 0.05, as shown in Figure S2b. As $H$ gradually increases, the absorptance rapidly jumps up to 1 with Q-factor of 139 at $H = 0.7 \, \mu m$. Further increasing of $H$ has little effect on the both absorptance and Q-factor.
The absorption spectra of the metasurface with varying groove width is plotted in Figure S2c. It shows that the resonance wavelength exhibits a blueshift from 3.508 $\mu$m to 3.024 $\mu$m as $W$ increases from 0.3 $\mu$m to 2.3 $\mu$m. More importantly, nearly perfect absorption with Q-factor of 140 can be maintained for a large variation of $W$ from 0.7 $\mu$m to 1.7 $\mu$m. A smaller groove width should be chosen since the electric field is confined at the top surface of the grating strip and a larger strip width is benefit for the improvement of the sensing performance.

The effect of the period $P$ of grating groove on the absorption features was investigated for a fixed groove width of $W = 0.7$ $\mu$m. As given in Figure S2e,f, the resonance peak experiences a redshift from 2.948 $\mu$m to 3.964 $\mu$m with absorptance larger than 0.9 in a wide waveband as $P$ increases from 2.5 $\mu$m to 3.5 $\mu$m. Moreover, the Q-factor is larger for the larger period of the grating groove.

Figure S3. (a) Delta absorbance of absorber covered with molecules layer of different thickness. (b) Enhanced signal strength with different thickness.

Figure S3a shows the delta absorbance (enhanced molecular absorption) with different thickness. The corresponding enhanced signal strength are further extracted and illustrated in Figure S3b. It can be seen that the enhanced signal strength increased significantly when the thickness was smaller than 80 nm. Whereas the signal strength is hardly increased after the thickness was larger than 80 nm, indicating that the electromagnetic energy is mainly confined within 80 nm from the dielectric surface.

Table 1. The refractive index sensing performance of the proposed absorber relative to those reported in literatures.

| Structure                                      | Sensitivity (nm/RIU) | Figure of Merit (RIU)$^3$ | Resonance Mode | Wavelength Regime     | Refs. |
|------------------------------------------------|----------------------|----------------------------|----------------|-----------------------|-------|
| Semiconductor–Metal–Semiconductor (SMS)       | 404.295              | 50.3                       | Plasmonic      | Visible and Near-Infrared | [1]   |
| Metal-Insulator-Metal-Insulator-metal (MIMIM)  | 652.777              | -                          | Plasmonic      | Near Infrared         | [2]   |
| Metal-Insulator-Metal (MIM)                    | 600                  | 40                         | Plasmonic      | Visible and Near-Infrared | [3]   |
| Vertical-Square-Split-Ring (VSSR) Resonator    | 1194                 | 28.94                      | Plasmonic      | THZ                   | [4]   |
| Hybrid metasurface Dielectric-Metal metasurface| 325                  | -                          | Plasmonic      | Near-Infrared         | [5]   |
|                                                | 1800                 | 62.1                       | Guided mode    | Middle infrared       | This work |

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