

Quasiresonant Regime of Surface Plasmon for Broad Angular Responsivity of Plasmonic Diffraction

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We propose plasmonic diffraction under quasiresonant regime of surface plasmon (quasi-SPR) that exhibits broad incident-angle responsivity. Numerical simulations reveal that quasi-SPR induces efficient and large-angle diffraction toward the transmission side over a wide range of oblique incidences by tuning the metal grating period to satisfy the Rayleigh anomaly and by optimizing the grating width and height to maximize diffraction efficiency at normal incidence. In a backside-illuminated silicon image sensor integrated with metal gratings, near-infrared absorption in silicon exceeded 40% for incident angles up to $\pm 18^\circ$ within a limited thickness of 3.3 μm . The angular absorption profile reflects the inherently broad response of quasi-SPR and provides a versatile approach to enhance light-matter interaction in compact optoelectronic devices.

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Surface plasmon resonance (SPR) has been extensively explored across various nanophotonics research fields, including surface-enhanced Raman scattering, surface plasmon coupled emission, photovoltaics, thermal emission control, and related topics [1–10]. These applications are based on a common physical mechanism in which the electromagnetic field is confined and enhanced near the interface between a metal and a dielectric material, resulting from the excitation of surface plasmon polaritons. This field localization intensifies the interaction between photons and electrons at subwavelength scales. Various metal nanostructures such as gratings and nanoparticles have been utilized to enhance spectroscopic signals, improve detection sensitivity, and tailor photon emission and absorption processes in nanoscale optical systems [11–13].

At the Rayleigh anomaly corresponding to 90° diffraction, the grating period is geometrically determined by the wavelength and the refractive index of the surrounding medium [14]. The SPR is efficiently excited by adjusting the width and height of the metal grating so that Fabry-Perot resonances coincide with the Rayleigh anomaly condition [14–16]. Under normal incidence, light is diffracted along the interface and propagates laterally, forming a strongly enhanced electric field that decays evanescently into the medium. This SPR mechanism represents a

conventional plasmonic approach, in which the enhancement of optical absorption is confined to near the surface.

We have proposed and characterized a different optical behavior that emerges when the incident frequency is slightly higher than the SPR mode, where quasi-SPR is present. [Fig. 1(a)]. Under quasi-SPR, light is no longer bound as an evanescent field but is instead diffracted toward the transmission side at large angles with high efficiency. We have referred to this phenomenon as “plasmonic diffraction,” which we have identified and analyzed as a distinct optical process. When the structural parameters are tuned to satisfy this quasiresonant condition, the diffraction efficiency increases significantly. We applied the plasmonic diffraction to enhance the near-infrared (NIR) sensitivity in silicon (Si) image sensors. By extending the effective optical path length within the Si pixel, the absorption efficiency is substantially increased, leading to a marked improvement in sensitivity in the NIR regime [17,18]. The concept of plasmonic diffraction was further applied to oblique chief rays in Si image sensors, where the grating period and the width were precisely adjusted for each chief-ray angle to induce quasi-SPR, thereby improving the NIR sensitivity at sensor edges [19]. The incident-angle range was limited to approximately 8° because the grating period of 265 nm was close to the resonant period of 261 nm. By varying the grating period and width for each chief-ray angle, plasmonic diffraction was induced under oblique illumination, although it remained confined to this narrow angular range in each pixel. Recently, the plasmonic diffraction was demonstrated with silicon photodiodes incorporating gold gratings, achieving approximately 1.8-fold enhancement of responsivity in the NIR [20]. The peak of the detection

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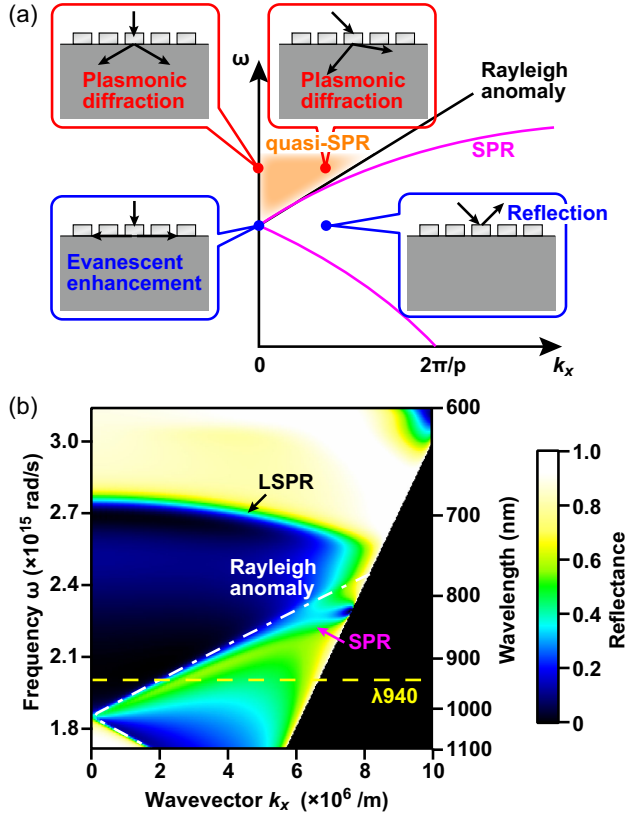


FIG. 1. (a) Concept of plasmonic diffraction under quasi-SPR. Incident light plasmonically diffracts toward the transmission side. (b) Simulated dispersion relation of reflectance in silver grating with period of 285 nm, line width of 215 nm, and height of 95 nm. Low reflectance near zero was observed in broad area above the SPR dispersion.

efficiency improvement was observed at a higher frequency than the Rayleigh anomaly resonance, which supports the physical feasibility of quasi-SPR. However, these studies were designed at slightly higher frequencies than SPR and focused only on normal incidence or a specific incident angle, thus retaining the angular limitation inherent to conventional SPR [19].

In this Letter, we focused on the broad incident-angle responsivity of quasisonant plasmonic diffraction up to the Rayleigh anomaly for 90° diffraction. We designed a metal grating for plasmonic diffraction with broad angular response, where the period was defined by the Rayleigh anomaly at the desired maximum incident angle, and the width and height were optimized for peak diffraction efficiency under normal incidence. We expected that this broad angular response contributed to enhanced near-infrared sensitivity in Si image sensors by maintaining high diffraction efficiency over a wide range of incident angles. Conventional SPR exhibits strong angular selectivity due to the wave vector matching condition, and oblique incident light is predominantly reflected. Therefore, the Si absorption efficiency due to the SPR-based electric field enhancement

is limited to normal incidence. In contrast, quasi-SPR sustains the diffraction under oblique incidence, extending the optical path length in the Si absorption layer and increasing the absorption efficiency across a wide angular range.

To investigate the angular responsivity of the quasisonant condition at a wavelength of 940 nm, the grating period was set to 285 nm to satisfy the Rayleigh anomaly for 90° diffraction at an incident angle of 18° . The wavelength of 940 nm is widely used in NIR sensing because the solar irradiance at ground level is relatively low [21]. Incident angle range of $\pm 18^\circ$ corresponds to an f number of approximately 1.5, which is typical of practical illumination angles in Si image sensors [22]. As the design concept in this Letter, the grating width and height were optimized to maximize diffraction efficiency under normal incidence while maintaining operation in the quasisonance. Figure 1(b) shows the simulated reflectance dispersion of an Ag grating on Si, using the optimized structural parameters of period = 285 nm, width = 215 nm, and height = 95 nm. A 2 nm-thick Al_2O_3 passivation layer, which suppresses dark current by introducing negative fixed charges, was placed between the Ag grating and the Si absorption layer. The grating was encapsulated by an SiO_2 overlayer, 235 nm thick on the Si surface to prevent chemical degradation of Ag such as sulfidation. The simulation was carried out using rigorous coupled-wave analysis with the commercial software DiffractMOD by RSoft. The wave vector k_x is defined along the grating period. The Rayleigh anomaly in Si for a period of 285 nm appears at a frequency of 1.85×10^{15} rad/s under normal incidence, corresponding to a wavelength of 1020 nm. The SPR coincided with the Rayleigh anomaly at this frequency. In the higher frequency region above the SPR dispersion curve, the reflectance remained low until the upper frequency limit defined by the localized surface plasmon resonance. At the target wavelength of 940 nm within the quasi-SPR region, a broad angular response extending up to 18° was achieved. Over this wide range of incident angles, the reflectance dropped to nearly zero, corresponding to the wave vector range from $k_x = 0$ to $1.9 \times 10^6 \text{ m}^{-1}$.

Figures 2(a)–2(c) show the electric field intensity distributions of Ag gratings on Si under quasi-SPR at incident angles of 0° , 9° , and 18° , respectively. The simulations were performed using the finite-difference time-domain method implemented in the commercial software FullWAVE by RSoft. Plasmonic diffraction into the Si transmission side was observed at each angle. Under normal incidence, the diffracted light was split symmetrically into ± 1 st diffraction orders. For oblique incidence, diffraction was primarily directed into the ± 1 st order, with the angle approaching 90° (see Movie 1 in Supplemental Material [23]).

To quantitatively evaluate the angular characteristics of plasmonic diffraction, the diffraction efficiency as a function of the diffraction angle was calculated. A fast Fourier

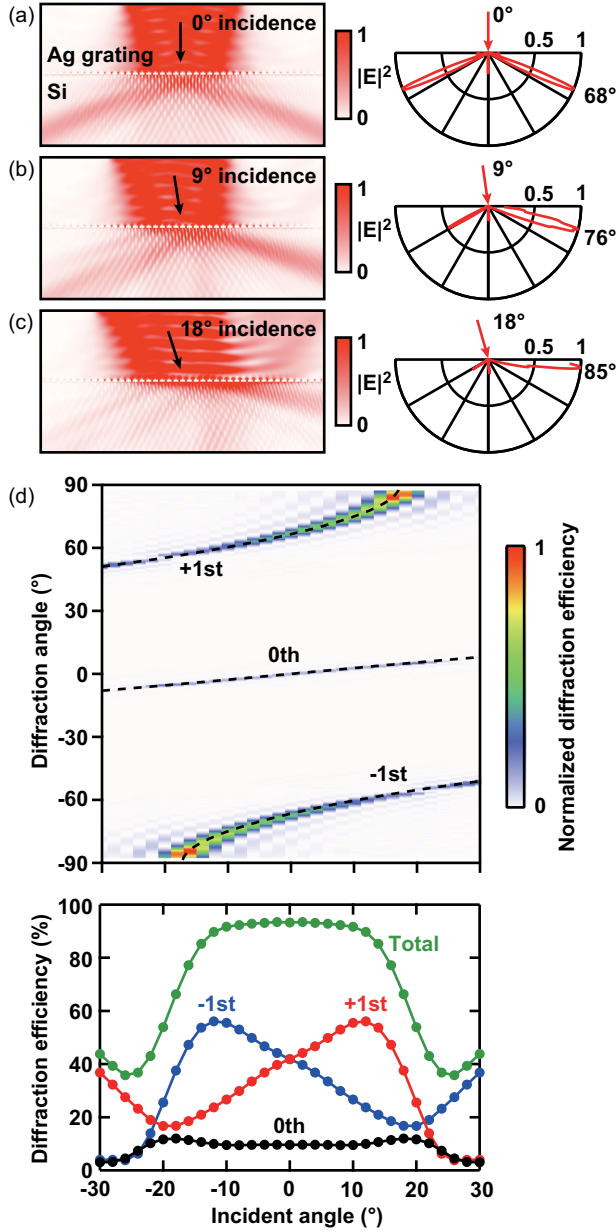


FIG. 2. (a)–(c) Simulation results of electric-field intensity distributions and polar graph of normalized diffraction efficiencies in Ag grating on Si at incident angle of 0°, 9°, and 18°. The first order diffraction was dominantly observed in plasmonic diffraction. (d) 2D normalized diffraction efficiency map dependence on incident angle, overlaid with theoretical diffraction (± 1 st) and refraction (0th) angles (top). Diffraction efficiency dependence on incident angle (bottom).

transform algorithm was applied to the simulated complex electric field amplitude and phase at a depth of 1 μm inside Si. The resulting polar plots shown alongside Figs. 2(a)–2(c) were normalized to their respective peak values. The diffraction angles corresponding to the peak intensities for incident angles of 0°, 9°, and 16° were found to be 68°, 76°, and 85°, respectively.

While conventional gratings typically exhibit dominant zeroth-order transmission, the gratings tuned for quasi-SPR reduced the zeroth-order transmission to negligible levels, as shown in polar plots of Figs. 2(a)–2(c). Quasi-SPR led to both a large diffraction angle and high diffraction efficiency owing to tilted quadrupole oscillation [18]. These calculated diffraction profiles show good agreement with the corresponding electric field intensity distributions.

The incident angle dependence of the diffraction angle and normalized diffraction efficiency is mapped in Fig. 2(d), which summarizes the far-field characteristics derived from the fast Fourier transform analysis of electric field distributions in the near field. The broken line represents the Rayleigh diffraction corresponding to zeroth and plus or minus first orders, based on Eq. (1),

$$\theta_d = \arcsin\left(\frac{n_1 \sin \theta_i + m \frac{\lambda_0}{p}}{n_{Si}}\right), \quad (1)$$

and aligns well with simulation results.

The diffraction efficiency for each order was evaluated as a function of incident angle by integrating the angularly resolved power as shown in the bottom of Fig. 2(d). Within the designed angular range of 0° to 18°, the plus-first-order diffraction was dominant. Beyond 18°, the plus-first-order mode became evanescent, and the minus-first-order component progressively increased. The zeroth-order transmission was consistently suppressed throughout the entire angular range. While the optimization of the grating width and height at the resonant angle tends to exhibit a sharp efficiency peak confined to a narrow angular range, tuning these parameters for normal incidence achieved a diffraction efficiency of 40% for plus or minus first-order modes at an incident angle of 0° and exceeded 50% with increasing incident angle toward the Rayleigh anomaly. Quasi-SPR sustained high efficiency over a broad incident-angle range, resulting in a total diffraction efficiency surpassing 90% within $\pm 12^\circ$. In typical diffraction gratings, transmission is mainly concentrated in the zeroth order. Plasmonic gratings designed for SPR exhibit strong angular dependence, where efficient coupling is limited to a narrow angular range. In contrast, quasiresonant plasmonic gratings support high efficiency diffraction into plus or minus first-order modes over a broad range of incidence angles.

We applied broad angular plasmonic diffraction to enhance the NIR sensitivity of backside-illuminated Si image sensors and investigated the optical absorption characteristics in Si pixels. The backside-illuminated Si image sensor incorporates an Ag grating on the incident side and Ag-based deep trench isolations (DTIs) surrounding each pixel as illustrated in Fig. 3. The diffracted light is confined within the Si pixel through multiple reflections from the metal DTIs and the bottom interface of the Si pixel. Additionally, Cu wiring layers are employed as reflective plates to further enhance optical confinement.

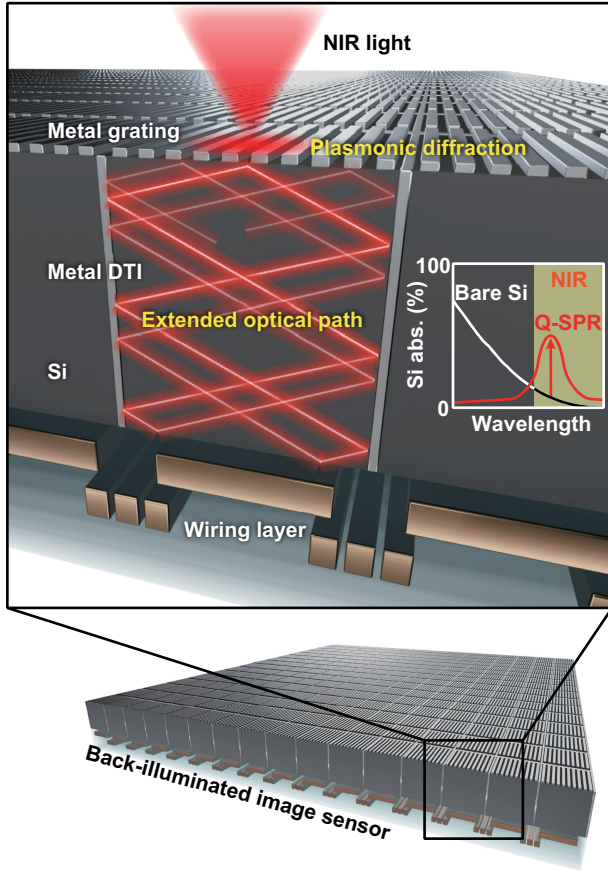


FIG. 3. Schematic diagram of back-illuminated image sensor incorporating metal gratings and metal DTIs. Enlarged diagram shows light confinement pixel. Optical path length is effectively extended in Si absorption pixel by multiply reflecting diffracted light at metal DTIs and silicon bottom interface.

The simulation results of the Si absorption in this configuration for various incident angles are shown in Fig. 4. Detailed parameters of the simulation model provided in Supplemental Material, Fig. S1 [23]. As shown in Fig. 4(a), the maximum absorption of 54% was achieved at normal incidence, representing a substantial enhancement compared to the 5% absorption of Si without the grating (see Fig. S2 [23]). This improvement is caused by multiple reflections of plasmonically diffracted light confined within the Si pixel. Moreover, due to the broad angular efficiency of quasisresonant plasmonic diffraction as shown in Fig. 2, the enhanced absorption persists over a wide angular range. Within the designed incident-angle range of $\pm 18^\circ$, the absorption maintained above 40%. The angular width at half-maximum extended to 22° , corresponding to an f number of approximately 1.24. Periodic modulations observed in the angular absorption curve are considered to result from optical interference within the Si pixel. The angular characteristics of the enhanced absorption are consistent with the broad angular plasmonic diffraction

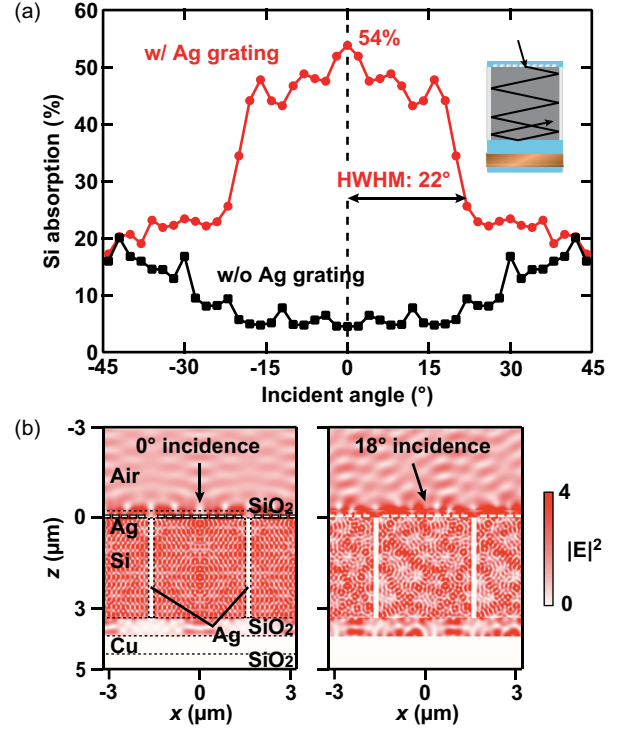


FIG. 4. Simulation results of angular responsivity with light confinement pixel. (a) Silicon absorption efficiency dependence on incident angle with or without Ag grating. (b) Electric-field intensity distributions with light confinement pixel at incident angle of 0° and 18° .

response governed by the quasi-SPR, suggesting that the diffracted light is effectively guided within the Si pixel.

The electric field intensity distribution at normal incidence in Fig. 4(b) revealed fine interference patterns along both the lateral and depth directions inside the Si pixel, indicating multiple internal reflections of diffracted light and confirming effective optical confinement. A similar interference was observed at an incident angle of 18° , as shown in the right-hand side of Fig. 4(b), further validating the robustness of the confinement under oblique illumination.

Optical crosstalk induced by the diffracted light was suppressed to below 1% (see Fig. S3 [23]). The suppression is due to the presence of metal-filled deep trench isolations, which block lateral propagation between pixels. In addition, large diffraction angles satisfy total internal reflection at the bottom Si/SiO₂ interface, guiding the light back into the Si pixel.

In conclusion, broad angular plasmonic diffraction induced by quasi-SPR was proposed and numerically investigated to enhance NIR absorption in thin Si image sensors. By designing a grating period to satisfy Rayleigh anomaly at the largest incident angle, the diffraction condition for oblique illumination was satisfied. The grating width and height were then optimized to maximize the diffraction efficiency for normal incidence at the target wavelength. This design strategy led to angularly large and

efficient first-order diffraction across a wide range of incident angles. In contrast to conventional SPR, quasi-SPR supports efficient large-angle diffraction without severe angular restrictions. Optical simulations of backside-illuminated Si image sensor incorporating Ag gratings and metal-filled DTIs revealed strong light confinement within the Si pixel. Multiple internal reflections of plasmonically diffracted light contributed to the enhanced absorption. The simulated absorption reached 54% at normal incidence and maintained above 40% across incident angles of $\pm 18^\circ$, corresponding to a f number of 1.5. Quasi-SPR-based diffraction offers a practical light-trapping approach for improving the NIR sensitivity of Si optoelectronic devices without increasing absorber thickness or sacrificing pixel resolution.

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Data availability—The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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