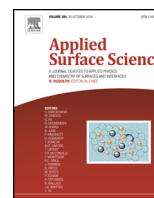




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## Excitation of surface phonon polariton modes in gold gratings with silicon carbide substrate and their potential sensing applications

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### ABSTRACT

We demonstrate the excitation of surface phonon polaritons (SPhPs) in the mid-infrared (mid-IR) Reststrahlen band (10.288  $\mu\text{m}$ –12.563  $\mu\text{m}$ ) on patterned surfaces with silicon carbide (SiC) substrate and gold (Au) gratings. The very large negative permittivity of Au limits its applications in the mid-IR range, and to couple incident light to SPhPs modes, their momentum mismatch can be compensated by patterning Au grating onto the surface of SiC substrate. Samples were fabricated and characterized experimentally by Fourier transform infrared reflection (FTIR) spectroscopy. The optical properties were also simulated by the rigorous coupled wave analysis (RCWA) method. Reflection dips are observed for light polarized vertical to the grating lines (TM-polarized), which are attributed to the coupling of electromagnetic (EM) waves into the SPhP modes. In addition, we present small-volume index sensing with analyte specificity based on mid-IR SPhPs in the fabricated configuration.

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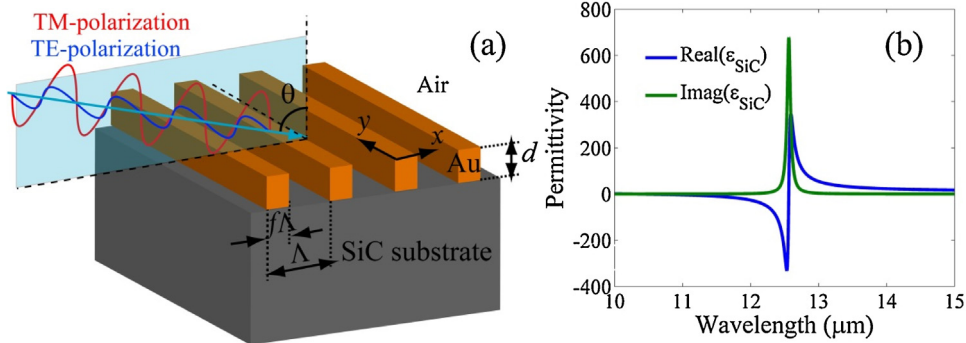
### 1. Introduction

Strong enhancement of the electromagnetic (EM) field, sub-wavelength scale confinement, sensitive to changes in the environment and optical non-linearity are among the remarkable effects related to surface plasmons (SPs) [1,2]. These remarkable effects bring many advancements, such as subwavelength waveguiding and modulating, light trapping in solar cells, superlensing, near-field optical microscopy, tip and surface-enhanced Raman scattering, analysis for the label-free detection, as well as enhanced quantum efficiency for detectors in the ultraviolet (UV), visible (VIS) and near-infrared (NIR) spectral ranges [3–15]. Surface plasmon polaritons (SPPs), evanescently confined in the perpendicular direction, are EM excitations propagating at the interface between a dielectric and a conductor. These EM surface waves arise via the coupling of the EM fields to oscillations of the conductor's electron plasma. SPPs can be excited by illuminating the surface under

the conditions that provide momentum-matching, called surface plasmon resonance (SPR) conditions, which is shown as a dip in the reflectance spectrum [3]. When the surface mode is excited, the EM energy comes to be strongly confined in the proximity of the surface, with the fields evanescently probing to the surrounding environment. Any change in the refractive index (RI) of outer medium has an effect on varying the propagation constant of SPPs, making it naturally to be exploited as probes for surface analysis and sensing devices. The metal-based plasmonics has been successfully demonstrated in the sensing application with high performance from UV to NIR, however, their very large negative permittivities at longer wavelengths limit their usefulness beyond the NIR [16–18].

Fortunately, polar dielectrics offer an opportunity to simultaneously achieve sub-diffraction confinement, low optical losses and operation in the mid-IR to THz spectral ranges through the stimulation of SPhP mode, which is the coupling between the EM fields and optical phonons (lattice vibrations) of the polar crystal [19–25]. A high reflectivity and negative real part of permittivity are also observed for polar dielectric crystals within a spectral range referred to as the Reststrahlen band which gives rise to the SPhP phenomenon [26–30]. Within this spectral band, the reflec-

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**Fig. 1.** (a) The schematic image of the Au grating patterned on the SiC substrate. The angle  $\theta$  denotes the incident angle to the sample surface. (b) Real (blue) and imaginary (green) parts of the permittivity of SiC around its Reststrahlen band. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

tion of incident light approaches to 100%, but unlike that in metals, this is realized without free carriers. SPhPs are studied less extensively than metal-based SPPs due to the fact that few materials can support SPhPs [31].

Due to the low intrinsic loss, SPhPs, especially on silicon carbide (SiC) based structures, examples of various applications including enhanced near-field light-matter interaction [32], high-sensitivity mid-infrared index sensing [23,33,34], mid-IR perfect absorption [35], extraordinary optical transmission and absorption in perforated membranes [36] have been reported. Similar to the case of SPPs, there exists a momentum mismatch between the incident photons and the SPhP modes, which can be overcome by using the coupling of the incident field to surface modes through the diffraction gratings [20,24] and high-index prism [21,37]. The existence of magnetic polariton within the phonon absorption band in SiC-based slit array and deep gratings has been revealed by Zhang et al. [38], and the corresponding applications as an IR filter and a coherent thermal emission source were considered.

In this paper, we theoretically describe and experimentally demonstrate the coupling of free-space radiation to SPhPs on Au gratings with SiC substrate. The TM-polarized infrared attenuated total reflection measurements are performed by using transform infrared (FTIR) spectroscopy. Based on the RCWA calculations, the mechanisms of the observed modes are revealed, which offers insights into the anomalous response of the variation of the geometrical parameters. Furthermore, a reflection-type sensor based on an angle scanning method was achieved. The proposed concept can be extended to different wavelength region by using other polar dielectrics that support SPhPs, e.g., AlN (11.2–16.4  $\mu\text{m}$ ), GaP (24.8–27.4  $\mu\text{m}$ ), GaAs (34.2–37.2  $\mu\text{m}$ ), CdTe (59.1–70.9  $\mu\text{m}$ ), and PbSe (49.2–256.5  $\mu\text{m}$ ) [24].

## 2. Structure and theoretical calculation

The majority of SPhP-based phenomena have been investigated on SiC surfaces because the high-energy phonons of SiC lie in the mid-IR and are thus accessible using standard IR sources and detectors [19,21,22]. In the absence of free carriers, the frequency-dependent dielectric permittivity of SiC is given by [39,40]:

$$\epsilon_{\text{SiC}}(\omega) = \epsilon'_{\text{SiC}} + i\epsilon''_{\text{SiC}} = \epsilon_{\infty} \frac{\omega^2 - \omega_{\text{LO}}^2 + i\gamma\omega}{\omega^2 - \omega_{\text{TO}}^2 + i\gamma\omega} \quad (1)$$

where the longitudinal optical phonon frequency  $\omega_{\text{LO}} = 972 \text{ cm}^{-1}$  at  $\lambda_{\text{LO}} = 10.288 \mu\text{m}$ , the transverse optical phonon frequency  $\omega_{\text{TO}} = 796 \text{ cm}^{-1}$  at  $\lambda_{\text{TO}} = 12.563 \mu\text{m}$ , the damping rate due to vibrational anharmonicity  $\gamma = 3.75 \text{ cm}^{-1}$ , and  $\epsilon_{\infty} = 6.5$ . The Reststrahlen band defined by  $\epsilon'_{\text{SiC}} < 0$  corresponds to  $\omega_{\text{TO}} < \omega < \omega_{\text{LO}}$ , within which SPhPs can be excited. In order to couple the incident light to SPhP

modes, their momentum mismatch can be bridged by patterning a grating onto the materials' interface [20,24,38].

The structure used and coordinates system in the calculations are shown in Fig. 1(a), where the  $x$ -direction is parallel to the surface and perpendicular to the ridges of the grating. The  $y$ -direction is assumed to be infinite along the grating grooves in this study, the  $z$ -direction is set along the surface normal, and  $\theta$  represents the angle of incidence (from normal). The permittivity of SiC was modeled using the equation developed in Ref. 40 and is shown in Fig. 1(b). The simulation of optical phonons within the Reststrahlen band of SiC induces a negative permittivity which is similar to the plasmonic materials below their plasma frequency. Outside of this band, SiC behaves as a typical and transparent dielectric material mainly defined by its index of refraction.

Two-dimensional rigorous coupled-wave analysis (RCWA) algorithm [41–43], a frequency domain technique which utilizes the Floquet theorem to calculate the amplitudes of a large number of spectral orders of diffraction is employed to study the spectral property of the proposed structure with a plane wave incident on the grating. Although no approximations to Maxwell's equations are made in the RCWA method, the number of spatial harmonics retained in calculations must be truncated in order to obtain a solution. For 2D grating problems, the number of equations to be solved increases with the square of the number of orders retained, and the tradeoff between speed and accuracy becomes much severer. To ensure the numerical accuracy of the calculation with reasonable computational time, all the calculations have been tested for convergence and calculated with the number of diffracted orders equal to 203.

The frequency-dependent dielectric constant of Au is expressed by Lorentz-Drude model [44]:

$$\epsilon_{\text{Au}}(\omega) = \epsilon_{\infty} - \frac{\omega_{\text{p}}^2}{\omega^2 + i\Gamma_{\text{p}}\omega} - \frac{f_1 \omega_1^2}{\omega^2 - \omega_1^2 + i\Gamma_1 \omega} \quad (2)$$

where  $\omega_{\text{p}}$  and  $\omega$  are the frequencies of the plasma and interest respectively,  $\Gamma_{\text{p}}$  is the damping (or relaxation) rate,  $i$  denotes the complex number ( $i = \sqrt{-1}$ ), and the contribution from interband transitions at infinite frequency is  $\epsilon_{\infty}$ . The Lorentz term includes the Lorentz oscillator damping rate  $\Gamma_1$ , the Lorentz resonance width  $\omega_1$  and the weighting factor  $f_1$ . The values of different parameters for Au are given in Table 1.

Reflectance of the designed sample as a function of grating period and incident wavelength is shown in Fig. 2(a), where only the zero order mode is propagating and the other modes are evanescent. The parameters are chosen as  $f = 0.22$ ,  $d = 0.28 \mu\text{m}$ , and  $\theta = 45^\circ$ . It is understood that the dark area is caused by propagating SPhP which is generated by different diffracted orders from the grating. Or in other words, the  $k$ -vector of a diffracted order for normal inci-

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