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Greater than 1 THz bandwidth high sensitivity on-chip terahertz sensing achieved using spoof surface plasmon polaritons for trace substance analysis

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Abstract

Terahertz (THz) spoof surface plasmon polaritons (SSPP) can play a key role in ultra-sensitive fingerprint sensing of trace substances by the enhanced confinement of electric field they provide. However, achieving both high sensitivity and broadband detection simultaneously in such structures remains a significant challenge, owing to the necessary trade-off between field confinement and bandwidth. This study demonstrates a sensing chip based on an artificial THz SSPP slow-light waveguide that simultaneously achieves broad bandwidth (up to 1 THz) along with highly sensitive detection achieved by enhancing both field confinement strength alongside the effective light-matter interaction distance. We use α-lactose monohydrate as a model analyte, and show that our SSPP-integrated THz sensing chip detects its characteristic rotational mode at 0.53 THz at concentrations as low as 18 μg/μL, which represents a fourfold improvement in detection limit over previous sensors. Repeat measurements show reliable stability and reproducibility for the chip. In operating up to 1 THz, a frequency range of significant interest for the study of quantum excitations in condensed matter systems as well as for terahertz studies of molecular dynamics in polycrystalline materials, our scalable platform is ideal for the study of light-matter in a wide range of advanced material systems.

Keywords: terahertz time-domain spectroscopy; spoof surface plasmon polariton; trace detection; terahertz sensing chip;

Introduction

Terahertz (THz) radiation can probe a wealth of molecular fingerprint spectral information, encompassing critical physical processes such as intermolecular rotational/vibrational transitions, charge transport, intra and inter band transitions, and low-energy excitations [1]-[4]. Spectral signatures in the terahertz range show a direct dependence on material structure, and so offer a powerful tool for identifying chemical compositions, and probing biomolecular interactions, underscoring their dual importance for both fundamental research and for practical applications [5]-[9]. It is noteworthy that advancements in THz time-domain spectroscopy (THz-TDS) technology have been crucial to realizing this potential. Specifically, significant improvements in signal-to-noise ratio and spectral bandwidth have substantially enhanced the sensitivity and selectivity of molecular fingerprinting. This not only enables detailed investigation of weak biomolecular interactions in fundamental scientific research but also allows for reliable identification of trace chemicals in practical scenarios. Recent advances in THz sources and detectors, and especially in femtosecond laser-based THz-TDS, have opened up widespread applications of THz spectroscopy for medical imaging, biosensing, security, and nondestructive testing [10]-[17]. However, free-space THz-TDS is often constrained by the diffraction limit to larger lateral sample sizes and therefore larger mass samples; this limits its capability to resolve characteristic spectral features in some functional materials with a small volume, including biomacromolecules, some quantum topological materials, thin-film perovskites, and some geometries of two-dimensional(2D) materials[18],[19].

A promising strategy to address limited material response in the THz regime is the implementation of artificial resonances in device structures through on-chip THz sensing technology[20], [21]. The operating principle of such chip-based approaches is to spatially compress incident THz waves into volumes far below the diffraction limit. This spatial confinement leads to a massive increase in local electromagnetic energy density. The pronounced field confinement effectively amplifies the strength of the light-matter interaction strength, making the characteristic vibrational or rotational signatures of minute analyte volumes detectable. Qiu *et al.* for example, achieved efficient free-space-to-chip THz wave coupling via antenna coupling, which enhances the on-chip light-matter interaction for THz fingerprint spectral detection[22] while Chen *et al.* employed an on-chip coplanar strip waveguide structure in which the metal trace width and spacing were sharply reduced to the micrometer scale. This configuration compressed the transmitted THz wave mode into a very small cross-sectional area, thus enhancing the local light– matter interaction[23]. Metamaterials, first theorized by Veselago (1968) for negative permittivity and permeability materials, enable unprecedented control of electromagnetic properties via engineered structures, breaking natural material limitations and diffraction barriers[24]-[28]. The label-free and enhanced sensitivity of THz metamaterial sensors have propelled transformative progress in trace-level THz spectroscopy applications[29], [30]. The label-free nature allows for the direct detection of analytes based on their intrinsic THz vibrational fingerprints, eliminating the need for fluorescent or radioactive tags that could alter molecular structures, complicate preparation, or interfere with spectral readout. However, achieving both broadband and high sensitivity in THz sensing chips remains a significant technical challenge[31].

Spoof surface plasmon polariton (SSPPs) can be excited in engineered structures that mimic natural surface plasmons; such structures can be compact, and therefore highly integrable with other structures[32], [33]. On-chip THz sensing technology is a highly sensitive detection approach that can utilize SSPPs in waveguides to thereby intensifying their interaction with target substances relative to standard waveguides[34]. Engineering micro/nanostructures of metallic materials (e.g., by the use of periodic grooves[35], cylinder arrays[36], square waveguides and cylindrical rod arrays[32]) enables precise control over the

SSPP dispersion relation and field localization characteristics, offering a viable technical pathway for developing high-sensitivity THz sensing devices. Terahertz SSPP structures offer significant potential for trace substance identification through enhanced fingerprint sensing, owing to their exceptional capability in electric field localization[37]. Although SSPPs-enhanced THz sensing enables highly sensitive detection of trace substances, their practical applications still face certain limitations. Conventional SSPPs-enhanced THz sensing typically employs coupling methods such as tip scattering, prism coupling, parallel-plate waveguides, and spherical lenses. However, all these approaches suffer from poor integration, low coupling efficiency, and narrow operational bandwidth, thus significantly constraining applications. Achieving broadband spectral operation with high-sensitivity trace substance detection thus remains a critical challenge for further development of THz sensing technologies.

In our prior work, we coupled free-space THz pulses to a chip using Vivaldi antennas and slot-line waveguides, achieving broadband operation (0.2-1.15 THz) and high signal-to-noise ratio in a sensing chip[22]. The chip was capable of measuring the fingerprint spectrum of a 1 mg lactose sample. After structural optimization, the chip achieved an extended operational bandwidth (0.2-1.35 THz) with rather high sensitivity for alpha lactose (a detection limit of 72 μg/μL in 0.8 μL suspension, corresponding to 57.6 μg absolute mass) for biomolecule detection[38]. In this paper, a new design of THz sensing chip is implemented based on SSPP waveguides having a periodic metallic groove. The choice of geometric configuration of the metallic grooves enables tailoring of the cutoff frequency for sensing. Using α-lactose monohydrate as an exemplar analyte with its distinct fingerprint feature of an absorption peak at 0.53 THz[39], our experiments demonstrate that the SSPP waveguide-integrated sensing chip achieves a fourfold improvement in the detection limit for trace substances compared to previous work. It significantly enhances sensitivity while maintaining broad bandwidth, overcoming the limitation of traditional plasmonic sensors in simultaneously achieving high integration, high coupling efficiency, broad bandwidth, and high sensitivity. Consistent agreement between simulated and experimental data, supported by repeat experiments, validate the sensor chip's stability and operational reproducibility. Our highly sensitive, highly stable, frequency-tunable, and low-cost integrated sensing chip thus opens new possibilities for on-chip THz spectroscopy in trace substance detection, with potential applications ranging from pharmaceutical analysis to security screening.

Experimental Section

Sensing Chip Fabrication

The sensing chip was fabricated using a lift-off technique. A 13-μm-thick polyimide (PI) film was first laminated onto a 450-μm-thick n-type doped silicon wafer (resistivity of 1-10 Ω/cm). To enable nondestructive PI film detachment, an AR-N 4340 sacrificial adhesive layer (identical to the UV mask exposure photoresist) was applied to the silicon wafer. Then, a 1.4-μm-thick second layer of AR-N 4340 photoresist was spin-coated onto the PI film and baked at 90 °C for 60 s to remove residual solvents. The pattern was transferred onto the photoresist by the UV light exposure through a photomask using an exposure dose of 140 mJ/cm². A 10-nm-thick titanium layer, a 300-nm-thick silver layer, and then a 10-nm-thick titanium layer were each deposited sequentially on top of the partially covered PI substrate and the patterned photoresist surface by electron-beam evaporation. The initial titanium layer serves as a bonding interlayer to enhance PI-silver adhesion, while the subsequently deposited titanium layer functions as an anti-oxidation barrier for the silver layer. The highly conductive silver layer effectively minimizes Ohmic losses. Finally, the photoresist layer was dissolved in acetone, followed by rinsing with deionized water (DI-H_2O), thereby completing the fabrication of the sensing chip with a 13-μm-thick PI film as the substrate. Detailed cross section diagram can be found in Supporting Information Figure S1.

THz Time-Domain Spectroscopy Measurements

Our terahertz time-domain spectroscopy (THz-TDS) system utilized a 1560 nm wavelength femtosecond fiber laser (TERA K15, Menlo Systems Corp, pulse duration<90 fs) as its light source. The experimental setup comprised the following key components: (i) a fiber-coupled THz receiver, (ii) a fiber-coupled THz emitter, and (iii) a low-loss expanded polystyrene (EPS) foam sample holder specifically designed for our on-chip measurements. Between 0.2-2 THz, the refractive index of EPS foam at 10 kg/m^3 is 1.006, which is very close to the refractive index of air. Over the same frequency range, the absorption of the EPS foam is below 0.35 cm^{-1}. Thus, the EPS foam does not noticeably affect terahertz wave propagation while serving as an effective structural support without altering the transmission[38].To eliminate atmospheric moisture effects, all measurements were performed at ambient temperature in a nitrogen-filled acrylic box.

Numerical simulation of the THz sensing chip performance.

Our simulation results were obtained using CST Microwave Studio. In this numerical model, both substrate (PI) and metal (Ag) were treated as lossy materials from the CST material library, while the simulation boundary conditions were set as "open". The so-chosen permittivity of polyimide was 1 THz is $\varepsilon=\varepsilon'+i\varepsilon''$, where $\varepsilon'=3.4215$ and $\varepsilon''=0.0095$[40].while the conductivity of silver was 6.3012×10^7 S/m.

Solution titration-based sensing measurement

α-Lactose monohydrate (samples with mass of 0.0901 g, 0.1802 g, 0.3604 g, and 0.5406 g) were each individually dissolved in 5 mL of anhydrous ethanol with thorough mixing to form homogeneous suspensions at concentrations of 18 μg/μL, 36 μg/μL, 72 μg/μL, and 108 μg/μL, respectively. Droplets (0.8 μ g) of the suspension with different concentrations were then pipetted on to the SSPP waveguide surface using a micropipette. After the ethanol evaporated, THz-TDS measurements were performed using the sensing chip with the deposited sample. The acquired THz-TDS signals were processed via fast Fourier transform (FFT) to extract their characteristic spectra. To prevent cross-contamination, each concentration was measured on an independent chip, with all chips exhibiting high consistency.

Results and Discussion

Design of the SSPP Waveguide-integrated THz Sensing Chip.

Our SSPP-enhanced sensor chip architecture (Figure 1a) consisted of three functional sections: (1) coupling regions with Vivaldi antennas for free-space-to-chip THz pulse coupling (see Figure S2 for details), (2) a slotline waveguide for signal transmission, and (3) an interaction region featuring SSPP waveguides for field enhancement. The Vivaldi antenna features a structure composed of a narrow slotline that flares out exponentially into a wider aperture. This design allows the antenna to radiate or receive electromagnetic waves effectively. Due to its exponentially tapered slot line, different sections of this antenna are responsible for radiating/receiving at different frequencies. The incident THz beam is focused by a lens to achieve a favorable transverse Gaussian profile, enabling efficient reception by the input antenna and coupling onto the sensing chip. The SSPP waveguide consists of a periodic metallic groove structure sandwiched between two transition regions on both ends, as shown in Figure 1(b). The SSPP waveguides designed for this work featured periodic rectangular grooves with two depth configurations (SSPP1: 25 μm, SSPP2: 50 μm) exhibiting cutoff frequencies of 1.0 THz and 0.7 THz, respectively. The two waveguides differed only in the depth of the metal grooves, while their period length p, groove width a, and number of periods remained identical. The corresponding parameters of the two SSPP waveguides are listed in Table 1. The metallic groove structure enhances the confinement of the electromagnetic wave on the target analyte by reducing the wave propagation speed in the chip. This approach preserves the chip's transmission coefficient while resolving the momentum mismatch between the slot-line waveguide and plasmonic waveguide. Consequently, the sensing chip's detection capability is enhanced for small volume analytes.

Field Confinement and Propagation Characteristics.

To validate the strong field confinement effect of our SSPP waveguides, the electric field intensity was numerically simulated and compared with that of a slotline waveguide, as shown in Figure 2. The denser electric field vector arrows on the SSPP waveguide compared to those on the slotline waveguide indicate stronger electromagnetic field intensity during propagation. While both SSPP1 and SSPP2 demonstrate comparable densities of electric field vector arrows, SSPP2 exhibits a significantly stronger electric field intensity, as confirmed by the absolute electric field magnitude results in Figure 2. Simulation results demonstrate that the SSPP waveguide with metallic grooves demonstrates significantly stronger electromagnetic field confinement than the slotline waveguide, resulting in an enhanced light-matter interaction. This intense field directly amplifies the interaction with the vibrational dipoles of analyte molecules. A stronger interaction force leads to a more pronounced perturbation of the THz wave, resulting in a deeper and more distinct characteristic absorption peak, which is crucial for detecting trace amounts. Furthermore, deeper grooves provide stronger localized field enhancement (see Figure S3), which leads to more pronounced confinement effects in SSPP waveguides with lower cutoff frequencies.

Dispersion curves, transmission, and reflection coefficients were also simulated for the two transmission modes of the SSPP waveguides, with the results presented in Figure 3. The dispersion curves for the two modes show a considerable separation. This aspect is particularly pronounced for SSPP2. The resulting momentum mismatch effectively prevents intermodal crosstalk, enabling pure SSPP propagation and reliable sensing chip performance. Figure 3(c) shows the SSPP1 waveguide transmission remains above -2 dB across 0.4-1.0 THz while reflection stays below -10 dB across this bandwidth. Similarly, SSPP2 demonstrates transmission remains above -2.5 dB from 0.3-0.6 THz, with corresponding reflection stays below -10 dB (Figure 3d). These results indicate that both waveguide designs achieve low reflection loss and effectively support SSPP propagation modes. Additionally, an increase in the depth of the metal groove is accompanied by a decrease in the wave propagation velocity. This reduction in propagation speed increases the interaction time between the THz wave and the analyte molecules in the sensing region, thereby enhancing the signal strength. This temporal enhancement, combined with the spatial field enhancement, synergistically boosts the total energy exchange, making the fingerprint signal more detectable above the noise floor.

Structural Optimization of the metallic groove.

To further optimize the transmission performance of the SSPP waveguides, we designed three kinds of groove structures with different configurations and simulated each numerically, as illustrated in Figure 4. Three structures are compared: a bilaterally symmetric structure with grooves, a bilateral asymmetric structure with offset grooves, and a unilateral structure with grooves. Figure 4(d) shows that the simulated dispersion curves of fundamental mode (FM) and high-order mode (HOM) in bilateral groove structures (including both symmetric and asymmetric offset configurations) are closely spaced. This indicates that the phase velocity between the two transmission modes is small, which makes interference between transmissions likely to occur. In comparison, the unilateral metal groove structure ensures that the dispersion curves of fundamental mode and high-order mode remain sufficiently separated. As a result, the SSPP waveguides supported by this structure can effectively suppress inter-mode crosstalk, maintain mode singularity, and thereby improve the spectral smoothness and broadband characteristics.

To investigate the effect of metal groove depth on the SSPPs, we simulated the dispersion curves for periodic metal grooves with depths ranging from 20 to 60 μm, while maintaining a fixed groove period (p = 90 μ m) and width (a = 60 μ m), as shown in Figure 5(a). The experimental data demonstrate a clear inverse correlation between the cutoff frequency of SSPP waveguides and groove depth. At small groove depths, the waveguide exhibits relatively high cutoff frequencies, indicating weaker confinement of the electromagnetic field within the metallic grooves. Simulation results of the maximum electric field under different groove depths also demonstrate this (see Figure S3). The weaker confinement consequently reduces the transmission efficiency of SSPPs. As the groove depth increases, the cutoff frequency decreases monotonically and drops to approximately 0.6 THz at a depth of 60 μ m. This phenomenon demonstrates that deeper groove structures can significantly enhance the confinement capability for SSPP waveguides, thereby effectively reducing their cutoff frequency. These results conclusively establish the groove depth as a critical structural parameter for controlling the cutoff frequency of sensing chip.

A transition region was designed at the junction between the slotline and groove. To verify the necessity of the transition region, simulations were conducted for two plasmon waveguides (matched and mismatched) to compare their transmission and reflection coefficients in Figure 5. Although transmission coefficients of the two waveguides are comparable, the curve of the mismatched waveguide exhibits significant fluctuations. These fluctuations arise from the momentum mismatch between the regions of SSPP waveguide and the slotline waveguide. Compared with the mismatched waveguide, the matched design achieves significantly better momentum matching, which manifests as smoother transmission coefficient curves and improved transmission performance. This behavior is similarly observed in the reflection spectra. The mismatched SSPP waveguide exhibits reflection coefficients consistently above -5 dB (blue curve), whereas the matched SSPP waveguide demonstrates significantly improved performance with reflection coefficients above -10 dB (red line) across the measured frequency range. These results confirm that the transition region effectively facilitates momentum matching between the regions of SSPP waveguide and the slotline waveguide. The transition region consists of metallic grooves with progressively increasing depths, which simultaneously supports SSPP and slotline waveguide propagation modes. The shallow-groove region predominantly supports slotline waveguide modes, while increasing groove depth induces a gradual transition to SSPP waveguide propagation modes.

The enhanced sensing performance is the result of an optimized signal path. The THz waves are coupled on-chip by Vivaldi antennas and are transferred to the SSPP waveguide via a transition region. The core enhancement occurs within the SSPP waveguide, where the periodic metallic grooves simultaneously confine the electromagnetic field and decrease the wave propagation velocity. This combination of enhanced field confinement and prolonged interaction time dramatically boosts the light-matter interaction, ultimately resulting in a substantial increase in the chip's sensitivity.

Manufacturing and Characterization of THz Sensing Chips.

Based on the above design principles, the fabrication of the plasmonic waveguide-based sensing chip was achieved through micro/nanofabrication processes including spin coating, soft baking, UV exposure, post-exposure baking, development, and electron-beam evaporation deposition. Figure 6 shows optical microscopy images of the sensing chip integrated with SSPP waveguides, where (a) and (b) display the full waveguide characterization of SSPP1 and SSPP2, respectively. The SSPP waveguide exhibits a high degree of fabrication integrity and demonstrates excellent interconnection with curved groove waveguides, with no observable wrinkling for the regions of bend. Figure 6 shows the localized characterization images of metallic grooves in SSPP1 and SSPP2 waveguides. As demonstrated, all fabricated metallic grooves exhibit excellent quality with well-defined edges and consistent uniformity. The as-fabricated SSPP1 and SSPP2 sensing chips were first characterized under unloaded conditions using a THz-TDS system. The corresponding spectra obtained by a Fast Fourier Transform (FFT) are displayed in Figures 6. The pronounced dip at 1.0 THz in the spectral curve of the SSPP1 sensing chip (Figure 6e) shows a cutoff frequency at 1.0 THz, which agrees well with simulation results. The measured spectral curve exhibits a smooth profile across the 0.1 – 1.0 THz frequency range, thereby demonstrating excellent momentum matching between the SSPP waveguide and the slotline waveguide. Moreover, the spectral curves measured by three different sensor chips show excellent agreement, indicating that the sensor chip with SSPP waveguide exhibits high testing repeatability and stability. The spectral curve of the SSPP2 sensing chip in Figure 6(f) exhibits a distinct dip at 0.7 THz, matching the simulated cutoff frequency. Furthermore, the spectral curves of the three sensing chips in the figure show excellent consistency, demonstrating that the SSPP2 chip also achieves high reliability and repeatability. We note that the spectral curve of SSPP2 sensing chip in the 0.1-0.7 THz range exhibited slight fluctuations, which we assume arise because the metallic grooves of SSPP2 have a greater depth, meaning the (length-constrained) transition region in this chip cannot achieve ideal momentum matching between the SSPP and slot-line waveguides, resulting in some residual momentum mismatch. Nevertheless, this issue did not affect its performance in subsequent application testing.

Performance Evaluation of Trace Analysis

To validate the sensing capability of the chip for trace-level detection, α-lactose monohydrate was employed as a model analyte for sensing tests. The α-Lactose monohydrate is ideal for verifying the chip's trace-detection capability because of its high stability, non-toxicity, distinct low-frequency terahertz fingerprints, and its narrow 0.53 THz absorption peak that we note slightly exceeds the SSPP waveguide's cutoff frequency. Figure 7 displays the spectral responses of different types of sensing chips to α -lactose monohydrate at varying concentrations. The black, red, and blue curves show the sensing results for chips with a slot waveguide, a 1.0-THz-cutoff plasmonic waveguide, and a 0.7-THz-cutoff plasmonic waveguide, respectively. All three sensor chips demonstrate increasingly sharper characteristic lactose absorption peaks with higher masses of added lactose powder. Figure 7 shows the sensing results for α-lactose monohydrate at concentrations of 108 μg/μL and 72 μg/μL. When lactose powder of the same mass/concentration is added, the image shows that the absorption peak intensity measured by the sensing chip with an SSPP waveguide is stronger than that with only a slot waveguide. Moreover, the lactose absorption peak intensity measured with the SSPP2 sensing chip is stronger than that of SSPP1. This result indicates that the SSPP's field confinement effect further enhances the interaction between THz waves and lactose, which in turn improves the sensitivity of the sensing chip. Furthermore, the broadband measurements (Fig. 7) captured a broad spectral profile. The observed spectrum of the lactose sample matches the known fingerprint of pure lactose, with characteristic peaks appearing at expected positions (e.g., 0.53 THz). Moreover, no extraneous absorption signals were detected, indicating high sample purity. This result demonstrates the advantage of a wider bandwidth for detecting trace substances.

Figure 7(c) presents the frequency response spectra obtained from three different sensing chips after depositing 28.8 μg of lactose powder (0.8 μL of a 36 μg/μL lactose suspension) on the sensor surface. The figure shows that the absorption peak intensity of lactose measured by the slot waveguide sensing chip is notably weak, whereas the SSPP waveguide-based chip detects a significantly stronger characteristic absorption peak. Figure 7(d) displays the spectral curves measured by three different sensing chips after adding 14.4 μ g lactose powder. Under these conditions, the groove waveguide sensing chip fails to detect lactose's characteristic absorption peak. The SSPP1 sensing chip shows relatively weak absorption peaks, whereas the SSPP2 chip still exhibits significantly stronger characteristic peaks for lactose. These results demonstrate both that: (i) SSPPs enhance the chip's sensing capability, enabling fingerprint-spectrum detection of small-mass powder samples, and (ii) a lower cutoff frequency of the SSPP waveguide reduces the detectable mass limit, thereby improving sensing performance. The lower the cutoff frequency of a SSPP waveguide, the deeper its metallic grooves. This increased groove depth improves the confinement of SPP modes, thereby enhancing the interaction between electromagnetic waves and matter.

Table 2 compares broadband THz spectroscopy studies on a-lactose monohydrate, including free-space and on-chip THz-TDS methods. Compared with other studies, the proposed THz sensing chip has quadrupled the sensitivity and reduced the lactose concentration required for detection.

Conclusions

In summary, a broadband THz sensing chip exhibiting high sensitivity was implemented using engineered SSPP waveguides with periodic metallic grooves, demonstrating enhanced spectral resolution in trace substance detection. Simulations and experiments results demonstrate that the field-confined SSPP waveguides enable impedance matching with slot-line waveguides, significantly enhancing terahertz wave-matter interaction to enable highly sensitive trace substance detection. The cutoff frequency of SSPP sensing chip can be precisely tailored by engineering periodic metallic groove geometries, thereby facilitating substance-specific fingerprint detection. The field confinement effect exhibits a positive correlation with metallic groove depth in SSPP waveguides, leading to progressively lower detection threshold. Using solution titration, we applied 14.4 μg of α-lactose mono-hydrate and detected its characteristic absorption features at concentration as low as 18 μg/μL. The SSPP sensing chip with distinct cutoff frequencies demonstrated consistent reproducibility and measurement stability across multiple samples from the same batch. This work proposes an innovative design strategy for the THz sensing chips, providing critical insights for advancing THz spectroscopy applications in trace substance detection.

Supporting Information

Detailed cross section diagram (Figure S1), function curve of the Vivaldi antenna (Figure S2), and maximum field versus groove depth (Figure S3).

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Notes

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Figure 1. Schematic of the SSPP waveguide-integrated THz sensing chip. (a) THz pulses are coupled into and out of the sensing chip via Vivaldi antennas. A transition region facilitates gradual transmission mode conversion from slotline waveguide modes to a SSPP waveguide mode. (b) Detail diagrams of two kind of SSPP waveguide grooves. Detailed parameters are listed in Table 1.

Figure 2. Simulation results for the slotline and SSPP waveguide. The instantaneous electric field vector diagrams of the slotline(a), SSPP1(b), and SSPP2 (c) waveguide. The electric field of the slotline(d), SSPP1(e), and SSPP2(f) waveguide at 0.5 THz. (Electric field strength≥ 1e+06 is shown in red for contrast.)

Figure 3. Simulation results for the SSPP1 and SSPP2 waveguide. The dispersion curves of the two transmission modes in the SSPP1(a) and SSPP2(b) waveguide. Simulated S-parameters for the SSPP1(c) and SSPP2(d) waveguide.

Figure 4. Schematic diagrams and simulated curves of metal groove units with different structures. Three structural units: (a) bilaterally symmetric grooves, (b) bilaterally asymmetric grooves, and (c) unilateral grooves. (d) Simulated dispersion curves of the three structures under fundamental mode (FM) and high-order mode (HOM).

Figure 5. Simulated results of SSPP waveguide with different depths of metal grooves. (a) Simulation results of periodic groove structures at different depths. Transmission (b) and reflection (c) coefficients of the matched and mismatched waveguide.

Figure 6. Full view and locally magnified optical microscope images of the SSPP1 (a, c) and SSPP2 (b, d) waveguide sensing chips. The black spots are dust particles on the polyimide film, and they have no significant impact on the performance of the sensing chip. Frequency-domain signals of SSPP1 (e) and SSPP2 (f) sensing chips in zero loading conditions (without analyte).

Figure 7. The detected absorption fingerprints of α-lactose monohydrate at 108 μg/μL (a), 72 μg/μL (b), 36 μg/μL (c), and 18 μg/μL (d) concentrations for different sensing chips.

Table 1. Geometric parameters of the SSPP waveguide's metallic groove structure.

	h_1/H_1	h_2/H_2	h_3/H_3	h_4/H_4	h_5/H_5	h/H	p	a
SSPP1	5	10	15	20	25	30	40	20
SSPP2	10	20	30	40	50	60	40	20

P: period length; *a*: groove width; *h*/*H*: depth of periodic metallic grooves; *hn*/*Hn*: depth of transition region (n=1,2,3,4,5).

Table 2. Comparison of trace substance detection capabilities in the THz spectroscopy studies.

ID	**Coupling mode**	**Frequency range**	**Detection limit**	**Sample (form)**	**Year**	**Study**
1	free-space	0～2.0 THz	10 mg	α-lactose	2022	[41]
2	scattering edge coupling	0.4-1.4 THz	Not specified	α-lactose (powder)	2014	[39]
3	parallel-plate waveguide	0.1-1.0 THz	5.5 mg	acetone, methanol, ethanol (solution titration)	2017	[42]
4	prism coupling	0.2-1.0 THz	Not specified	water, gasoline	2019	[43]
5	on-chip (vivaldi antenna)	0.2-1.15THz	1.0 mg	α-lactose (powder)	2023	[22]
6	on-chip (extended circular)	0.2-1.35THz	57.6 μg	α-lactose (solution titration)	2024	[38]
7	on-chip (metallic groove)	0.3-0.7 THz	14.4 μg	α-lactose (solution titration)	2025	this study