3D-printed Terahertz Photonic Bandgap Bragg fiber
based resonant microfluidic sensor

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Abstract: We present a theoretical and experimental study of a 3D printed Photonic Bandgap (PBG) Bragg fiber based resonant microfluidic sensor in the terahertz (THz) frequency band. A widely used 3D printing technique (fused deposition modeling (FDM)) is employed to fabricate this sensor where the liquid analyte is filled in its microfluidic channel. A continuous-wave (CW) THz spectroscopy system is used to probe this microfluidic sensor. Its response to the filling liquid analytes presents as transmission dip and phase drop in transmitted amplitude and phase spectra respectively. These spectral responses are optimized by finely tailoring the optimal fiber length and defect layer position. Consistent with the theoretical results, the sensitivity of ~110 GHz/RIU is measured by tracking the shift of these anti-resonant features with increasing RI of analytes. Due to its low fabrication cost, capability of in-situ probing and high sensitivity, this proposed microfluidic sensor opens new perspectives in application of chemical and biological fields.

1. Introduction

THz wave (Frequency: 100GHz to 10THz) has been emerged as a promising tool for sensing due to its low photonic power and covered multiple unique spectral fingerprints [1]. For its application in biological and chemical fields, the THz microfluidic sensing for tracking the characteristic change of liquid analyte in very small proportion has been reported in recent year [2-13]. The basic principle behind most of them is resonant sensing where the sample is characterized by probing the shift of spectral transmission characteristics [14]. Compared with the amplitude based non-resonant strategy whose implementation is restricted by the limited attainable power of THz wave, the resonant sensing shows higher feasibility in THz range. It enables higher sensitivity within a broad response range. Currently, the resonant THz microfluidic sensing has been mainly realized by metamaterial and waveguide structures.

In metamaterial-based sensors, the electromagnetic response of the artificially engineered micrometer-degree inclusions on planar substrate is probed. By observing the shift of resonant frequency, the change in thickness and RI of the liquid analyte spreading on its surface can be detected [2-4]. Currently, ultrahigh sensitivities which are over 50 GHz/μm and 700 GHz/RIU have been reported by detecting the response around 3.5 THz and 1 THz respectively [5,6]. However, the feasibility of the metamaterial-based sensor for practical applications are limited due to its high structural complexity and processing cost, poor stability, and the variable sensitivity in response frequency range [15]. In contrast, the waveguide based sensors can be fabricated in much economical ways using simple structures. In [7], a parallel-plates structure is proposed for probing the RI of liquid analyte that is filled in its internal microstructural groove. The sensitivity of ~90GHz/RIU in the resonant frequency range between 0.27 THz and 0.3 THz is recorded. The same research group then
proposes a multichannel structure with similar architecture for multi-sample detection [8]. In [9], a planar sensor in which periodic grooves being slotted on thin metal plate for holding liquid analyte shows sensitivity of ~500GHz/RIU in the resonant frequency around 0.6 THz. However, its fragile structure and the requirement of scattering spectrum for signal detection make this sensor vulnerable to low environmental interference, thus limiting outdoor applications. In the pipe-shaped THz waveguides, the change in evanescent field induced by varying quantity of liquid analyte has been employed for THz microfluidic sensing [10]. Limited by their intrinsic structures, the in-situ detection is not feasible for most of the waveguide based sensors. Besides, for the reported microfluidic sensors, the thickness of liquid analyte layer needs to be intentionally maintained in order to detect the shift of the resonant frequency that is induced by RI change only, which brings difficulties in their practical applications.

Comparatively, the PBG Bragg fiber shows advantages in sensing with high reliability and stability [16]. By artificially introducing a defect inside the waveguide structure, the modal anticrossing between the core and defect modes leads to a frequency-dependent change in the transmitted spectrum, from which the characteristic of defect can be described [17,18]. Inspired by it, a THz PBG Bragg fiber based microfluidic resonant sensor is proposed. By injecting the liquid analyte into a sealed layer as defect, the RI sensing is free from the disturbance of inconstant thickness in each measurement. Additionally the response of this sensor could vary with the RI of injected liquid analyte during scanning, which enables the real time sensing. Moreover, on account of its flexible structure and simple machining process, this PBG Bragg fiber based sensor is designable for detecting liquid analytes with any desired RI range and fabricated with low cost, which allow it being widely employed in chemical and biological applications.

The theoretical analysis and experimental research on a THz PBG Bragg fiber based resonant microfluidic sensor are carried out in this work. Its frequency range of bandgap and anti-resonance induced by defect is determined by theoretical simulation. In experiments, the preferable machining method, the optimal length, and the proper position of the artificially introduced defect of this sensor are investigated in order to achieve obvious bandgap and measurable anti-resonant response for probing analytes. Probed by CW-THz spectrometer, the response of the optimized sensor for different-RI liquid analytes in amplitude and phase spectra are found featuring as transmission dips and phase drops in the anti-resonant frequency range respectively. The sensitivity of ~110 GHz/RIU is attained by tracking the shift of these two kinds of spectral characteristics around 0.23 THz, which is in good agreement with the theoretical result. Depending on its high sensitivity and resolution, this in-situ THz microfluidic sensor fits for probing the small variation in the RI of liquid analytes.

2. **Theoretical analysis of the THz PBG Bragg fiber**

2.1 **Theoretical analysis of the PBG Bragg fiber without defect**

Mainly fabricated by extruding fiber preforms, the PBG Bragg fibers with periodic layers have been investigated systematically during recent years [19-22]. Compared with the ones for transmitting visible light with cross section at several hundred micrometer level [23,24], the PBG Bragg fiber for transmitting THz wave with millimeter-level wavelength features larger scale, which allows it to be manufactured via lower-precision machining. Currently the 3D printing technology has been proved as a competitive manufacturing method with low cost and acceptable error, thus being employed in this research [25-27]. However, restricted by its insufficient transverse resolution, the 3D printed
long-length THz PBG Bragg fiber with circular cross section, which has been mainly researched previously, performs unsatisfactory geometrical accuracy in experiment. Therefore, one with square cross section is proposed in this work, which is shown in Fig. 1(a).

![Fig. 1](image)

**Fig. 1.** (a) The sketch of the cross section of designed PBG Bragg fiber. The layers in grey and white represent the high- and low-RI material respectively. (b) The band diagram of the designed PBG Bragg fiber. The color of each dot represents the fraction of power restricted in the fiber core for each mode. The modes with more than 10% of total power confined in the core are plotted. The modal loss of the fundamental mode transmitted in the PBG Bragg fiber is shown in the upper left part.

Within the core length of 4.5 mm, the single-mode transmission of desired THz signal in PBG Bragg fiber can be guaranteed. In the cladding region surrounding this core, ten bilayer sequences act as Bragg gratings. Each period consists of one high-RI PLA and one low-RI air layer with thickness of 0.8 mm. The measurement on RI of PLA is described in the appendix. Theoretically, the wave which is capable of transmitting through this PBG Bragg fiber in experiments can be considered as the modes being confined in the core of its transversal cross section. Therefore, the complex time-consuming simulation for the 3D PBG Bragg fiber is simplified to the one based on this 2D axisymmetric cross section structure in our research.

For determining the band diagram of this structure, the commercial finite element software COMSOL is used to search the core-confined modes within a broad frequency range. According to the results shown in Fig. 1(b), the THz wave in frequency range between 205 GHz and 255 GHz can transmit through this PBG Bragg fiber. The modal loss of the supported fundamental mode in this range is around 0.1 cm⁻¹. Compared with the around 1 cm⁻¹ material loss of PLA, the THz wave can transmit through this PBG Bragg fiber for longer distance than in PLA bulk. Besides in experiments, the anti-resonant response in this range is easy to be monitored due to the high output power from THz antennas as well as the negligible disturbance induced by external environmental factors such as the water vapor absorption.

**2.2 The theoretical analysis in the influence of inserted defect on PBG Bragg fiber**
Fig. 2. (a) The calculated band diagram of the defected PBG Bragg fiber. The color of each dot represents the fraction of power restricted in the fiber core for each supported mode. The modes with more than 10% of total power confined in the core are plotted. The upper part is the enlarged view of the anticrossing region which is labelled by green circle in the lower part. (b) The field distribution for different mode. The axisymmetric distribution can be shown in a quarter of the cross section. Graph A and B represent the core and defect modes at the edge of anti-resonant frequency range. Graph C and D represent the core and defect mode around the center of the anti-resonant frequency range. Graph E represents the core mode which is unaffected by anticrossing phenomenon.

Then the RI of the air layer adjacent to fiber core is increased to 1.525 in simulation, which corresponds to this layer filled with liquid analyte in experiment. Influenced by the anticrossing in dispersion relation between this inserted defect and the core transmitted modes, the band diagram varies significantly, which is shown in the Fig. 2(a). Besides the bandgap covers larger frequency range, the anticrossing phenomenon acts over a specific frequency range on it, in which parts of the core-transmitting power shifts to the outer cladding region, thus resulting in the dip-shaped amplitude spectrum in experiment. The process of this power shift is revealed in Fig. 2(b). For the unaffected modes, graph E shows most power is bounded in the fiber core. As for the ones at the edge of anti-resonant frequency range, graphs A and B show part of the core confined and defect modes diffuse to the cladding and core region respectively. The resulted anticrossing phenomenon leads to part of core transmitted mode leaks out of fiber through its peripheral boundary during propagation in experiments. At the center of this frequency range, graph C and D show the intensified modal overlap. Most of the core transmitted power transfers to the cladding region, which corresponds to the maximum modal loss of core transmitted fundamental mode.
The modal loss of the core transmitted fundamental mode corresponding to different-RI defect layer is shown in Fig. 3(a). The average FWHM of loss spectrum is calculated around 10 GHz, and red shift occurs when the RI of defect layer increases. By comparing the frequencies with maximum modal loss on the calculated curves, linear shift of these signatures with increasing RI of defect can be found, which is shown in Fig. 3(b). The sensitivity of this PBG Bragg fiber based sensor is deducted as 107.3 GHz/RIU based on the slope of the fitted line.

3. Experimental implementation of the microfluidic resonant sensor

3.1 The 3D printing technology for fabricating THz PBG Bragg fiber based sensor

Currently, the lossless resin and plastic THz waveguides fabricated by stereolithography and FDM 3D printing technology have been reported [28,29]. For the former one, the photosensitive resin is cured by UV radiation and deposits on the plate layer by layer to attain the complicated architecture gradually. For the latter one, the plastic filament is melted and extruded by nozzle; then the semi-liquid continuous flow is fused with the built layer and solidified to form the designed structure. The accuracy of its printed model is mainly decided by the size of nozzle, which is larger than the beam spot of UV laser used in stereolithography. Therefore, the delicate architecture with high geometrical complexity is unavailable by this method conventionally.

Currently the small scale THz PBG Bragg fiber manufactured by stereolithography has been reported [25]. As for the FDM technology, despite of its advantages of low production cost, rapid processing speed, as well as the convenience for fabricating enveloped architecture, it hasn’t been applied in manufacturing THz PBG Bragg fiber out of concern for its inferior resolution. In this work, PBG Bragg fibers in same design have been fabricated by the Asiga Pro2 stereolithography and Makerbot Replicator FDM 3D printer in resin and PLA respectively, and their performance has been compared in experiments. The cross section of printed PBG Bragg fibers is shown in Fig. 4.
For the stereolithography 3D printed fiber, its structural stability is inferior to the PLA one due to the lower material strength of resin, thus the contour and position of printed resin layers in PBG Bragg fiber being more easily affected by external stresses during experiment. In addition, the isopropanol washing and following airflow drying, which are necessary processes to remove the uncured resin attached on the fabricated model, affect the printed structure non-negligibly. The uncontrollable surface tension effecting on the large-scale PBG Bragg fiber during these processes results in pronounced dislocation and deformation of resin layers without sufficient support frame. Observed by microscope, the thickness of resin and air layers in one processed structure is in the range between 0.7 and 1.0 mm. Compared with the uncleaned structure whose layer thickness fluctuates around 0.8 mm, the clean process leads to serious nonuniformity of resin PBG Bragg fiber. Besides for attaining the designed enveloped structure, sealing the defect layer by gluing a cover on one facet of printed PBG Bragg fiber exaggerates the dislocation of the resin and resin layers around defect. All these factors cause pronounced discrepancy between the achieved and the designed PBG Bragg fiber based sensor. The induced deformation acts as a vital geometrical defect in the periodic multilayers, which interferes the detection of anti-resonant phenomenon corresponding to the intentionally introduced defect.

Compared with the stereolithography printer with longitude resolution of 1 μm, the layer resolution of FDM 3D printer is 100 μm. The printed PLA model usually features with rougher surface and higher scattering loss. However, the better material strength of PLA and the one-step printing process endow the FDM fabricated PBG Bragg fibers with higher robustness and its each layer with more uniform thickness. In experiments, one PLA PBG Bragg fiber whose thickness of layers is in the range between 0.75 mm and 0.85 mm has been manufactured. It is in better agreement with the designed architecture than the resin one. Attributed to this geometrical characteristic, its bandgap and defect-introduced anti-resonance are more obvious to be determined in transmission spectra.

Theoretically, the linewidth of the transmission dip caused by anticrossing phenomenon is decided by the degree of overlap between the transmitted core and defect modes. For achieving high-resolution PBG Bragg fiber based sensor, the artificially introduced defect should be far from the core to narrow the corresponding anti-resonant frequency range [25]. In simulation, when the defect shifts from the
first to second air layer, the FWHM of loss spectrum for core transmitted fundamental modes decreases from 10 GHz to 5 GHz accompanying with reduction in their modal loss among the anti-resonant frequency range. But in experiments, by trials and errors, it is found the insufficient geometrical accuracy and the allowable length of fabricated PBG Bragg fiber prevent the appearance of recognizable anti-resonant phenomenon when its defect is set out of the first air layer. The spectral noise induced by the slight difference in thickness of each layer interferes the observance of comparable weak anti-resonance attained by the second-air-layer-defected PBG Bragg fiber within maximum available length by the 3D printer.

In conclusion, due to the better structural robustness and qualified geometrical accuracy of its printed structure, the FDM 3D printing is a preferable processing technology over the stereolithography one for manufacturing large-scale THz PBG Bragg fiber based sensor. Although moving the defect to outer layer endows the sensor with higher resolution in RI detection theoretically, the required fiber length and uniformity of periodic multilayers are unavailable by current experimental conditions. Therefore, the PLA THz PBG Bragg fiber with first air layer as defect is investigated for resonant microfluidic sensing in this work.

For sensing the liquid analyte in defect layer, the structure of theoretical analyzed PBG Bragg fiber has been modified, which is shown in Fig. 5. The first air layer is sealed on both sides and a connected microfluidic channel in small scale is built for containing the liquid analyte flow inside. This channel also plays a role of maintaining structural stability of the PBG Bragg fiber. During experiments, the analyte is injected from the inlet in a constant flow rate, runs through the defect and outflows from the outlet as the red labeled route in Fig. 5. The level difference between the highest position of inlet and output in channel ensures the fully filling of defect layer by pressure. In contrast with the structure with only one port to inject liquid analyte in advance of measurement, the in-situ sensing can be realized by this design, which brings more application fields for this sensor.

**Fig. 5.** The profile of the PLA PBG Bragg fiber based microfluidic sensor. The red lines and arrows represent the flow direction of the injected liquid analyte.

### 3.2 The CW-THz spectrometer for measuring transmitted spectrum

For monitoring transmission spectrum, the THz PBG Bragg fiber based sensor is placed in the CW-THz spectrometer whose working principle has been detailed in Ref [30,31]. As shown in Fig. 6, the combined output power of two distributed feedback (DFB) lasers with slight difference in operational wavelength is split equally into two THz photomixers, which play roles as THz signal emitter and detector. Under bias modulation, the emitter generates THz radiation in beat frequency of
the combined waves. After propagating in the guide of free space components, the transmitted signal is re-collimated into the detector and modulated for lock-in detection. For generating and detecting THz signal within a broad linewidth, the frequency difference of DFB lasers is modulated rapidly by adjusting temperature of the fiber Bragg grating in each cavity during scanning. Besides, two fiber stretchers in structure of long length polarized single fiber surrounding a piezoelectric actuator have been employed as delay lines to modulate the optical path length of the split laser for THz signal collection [32].

![Schematic of CW-THz spectrometer](image)

Fig. 6. The schematic of CW-THz spectrometer for characterizing the THz PBG Bragg fiber based sensor

One thing needs to be noticed is the noise induced by standing waves. By the optimized arrangement of free space components as shown in Fig. 6, the standing waves caused by parabolic and planar mirrors have been suppressed to a large extent. However, the transmitted spectrum is still influenced by the one induced by the silicon lens integrated in THz emitter and detector, which results in fluctuation on the measured amplitude spectrum. This irremovable noise and the one introduced by the facets of inserted waveguide sample obstruct the accurate sensing based on transmission dip shift severely, which is detailed in Chapter 4.

In this work, the amplitude and phase change introduced by the inserted PBG Bragg fiber on the transmitted THz signal is measured by the CW-THz spectroscopy in following processes. Firstly after coinciding focal points of the two neighboring parabolic mirrors and placing a metal barrier with window in the same size of PBG Bragg fiber core at the middle position, the transmitting THz signal is measured as the reference spectrum. Then the distance between these two parabolic mirrors is enlarged by adjusting the position of movable section in order to make their focal points to coincide with the core center on both facets of the inserted PBG Bragg fiber. Two metal barriers are placed adjacent to each side for restricting the input power as the reference one and avoiding the influence of output from cladding region. The scanned transmitted THz signal under this condition is recorded as the sample information. The comparison between these reference and sample results has been used for contrasting the performance of PLA PBG Bragg fibers with defect in different layers as well as determining the optimal length of PLA PBG Bragg fiber for THz microfluidic sensing.

3.3 The optimal length of PLA PBG Bragg fiber for sensing
Although the simulation result indicated in Character 2 shows the desired bandgap and anticrossing phenomenon are attainable by the designed cross section theoretically, the transmission spectra for PBG Bragg fibers with same cross section varies with different fiber lengths in experiments. By dividing the measured amplitude of sample spectrum to the reference one, the transmission loss for PBG Bragg fibers with length of 5cm, 7.5cm, 10cm and 12.5cm is shown in Fig. 7(a). The difference in measured loss between the frequency in bandgap and out of this range is not distinguishable enough until the length is over 10cm. Below this critical length, owing to the insufficient times of Fourier reflection, non-negligible part of wave which should leak into the periodic multilayers theoretically keeps transmitting through the core of PBG Bragg fiber. The resulted blurred edge of bandgap could lead to the invalid data and errors for sensing specific analyte with anti-resonant response around this range.

Fig. 7. (a) The transmission spectra of PLA PBG Bragg fibers with different lengths. (b) The intensity of the anti-resonance induced by filling the first air layer of PBG Bragg fibers with same kind of liquid analyte.

As for probing the anti-resonance brought by liquid analyte, another frequency scan is conducted when it flows through the microfluidic channel after the above mentioned procedures in experiments. Comparing this measured spectrum with the reference one attained by scanning the waveguide only, the change in amplitude and phase introduced by the filled analyte can be detected. Apart from determining the optimal length of PBG Bragg fiber based sensor, this strategy has also been adopted for sensing different liquid analytes in Character 4. For comparing the anti-resonant intensity achieved by different lengths, Fig. 7(b) shows the transmitted amplitude ratio between the PBG Bragg fibers filling with and without same kind of analyte. The positive value for the higher frequency is attributed to the enlarged bandgap for defected PBG Bragg fiber as theoretical analysis. For the 5 cm fiber, the transmission dip induced by anticrossing phenomenon is too weak to be observed in experiments. Although the extinction ratio seems apparently when fiber length is increased to 7.5 cm, it is mainly caused by the ambiguous edge of bandgap not the desired overlap between core and defect modes. The measured dip deviates from its actual position, thus leading to errors in sensing. As for the length beyond 10 cm, the anti-resonant frequency range is stabilized. Despite of the noticeable anti-resonant phenomenon it induces, the over long length fiber is difficult to be fabricated with tolerable defect. Therefore, the PBG Bragg fiber with length of 10 cm is employed for microfluidic sensing in experiments.

4. The performance of the THz PBG Bragg fiber based microfluidic sensor
For investigating the performance of this microfluidic sensor, the oil mixtures with RI in the range between 1.465 and 1.545 have been employed as liquid analytes. At first, the RIs of two kinds of oil are measured as 1.455 and 1.555 by a terahertz time-domain spectroscopy (THz-TDS) using cutback method in an independent experiment. According to the Arago-Biot relation, the employed nine sets of liquid analytes with RI of 1.465, 1.475, 1.485, 1.495, 1.505, 1.515, 1.525, 1.535, and 1.545 are achieved by mixing these two kinds of oil with volume ratio of 1:9, 2:8, 3:7, 4:6, 5:5, 6:4, 7:3, 8:2, and 9:1 respectively. Before injected into the microfluidic channel for probing their anti-resonant responses in transmission spectra in experiments, these analytes are agitated sufficiently to guarantee the uniform RI distribution.

4.1 The microfluidic sensing based on the transmission dip shift in amplitude spectrum

![Image](image.png)

Fig. 8. (a) The measured transmission loss corresponding to different-RI liquid analyte. (b) The fitted Lorentzian curves for the measured transmission dips. They are in the form of $y = Y_0 + \frac{\Delta}{\pi} \frac{w}{4(x-x_c)^2+w^2}$, in which $x$ and $y$ represent the frequency and fitted transmission loss respectively. The $X_c$ in each equation is regarded as the frequency signature of transmission dip and listed in the lower left corner with the corresponding RI of analyte.

By dividing the amplitude of THz wave transmitting through the PBG Bragg fiber with and without analyte filling in its microfluidic channel, Fig. 8(a) plots the measured dip-shaped transmission loss induced by anticrossing phenomenon on bandgaps. Within scan resolution of 100 MHz, it is found the frequency range of transmission dips features a red shift with the increasing RI of liquid analyte. However, due to the disturbance of the irremovable standing waves and the external noise on the measured spectrum from CW-THz spectrometer, the central frequencies of these broad-linewidth dips are hard to be determined accurately. For recognizing their relationship with RIs of analytes, these measured data in transmission loss has been fitted into Lorentz equations, which are shown in Fig. 8(b). The average FWDM of dips is calculated as 12 GHz, which is larger than the theoretical one due to the geometrical discrepancy between the printed and designed structures. The frequency corresponding to the highest transmission loss on each curve is regarded as the frequency signature for the anticrossing phenomenon in amplitude spectrum.
Fig. 9. (a) The comparison between the measured and the Lorentzian-fitted transmission dips corresponding to the liquid analytes with RI of 1.525, 1.495, and 1.465. The signature $X_c$ determined by Lorentzian equation and the frequency with maximum measured transmission loss for each analyte is indicated in the left lower part. The error in frequency signature for each fitted Lorentzian curve is labeled as black line. (b) The shift of frequency signatures for different-RI liquid analytes in amplitude spectrum. The $R^2$ (coefficient of determination) for each fitted Lorentzian curve is indicated. The red line is the linear fit for the shift of frequency signature. The sensitivity of the PBG Bragg fiber based sensor is detected as 113.7 GHz/RIU by the slope of this equation.

For investigating the conformity of the measured data and the fitted Lorentzian equation with the actual respond of the PBG Bragg fiber based sensor, Fig. 9(a) shows the results for liquid analyte with RI of 1.525, 1.495, and 1.465. As analysis in Character 2, the anticrossing phenomenon can induce a peak-shaped modal loss of the core transmitted fundamental mode on the bandgap. The obtained frequency signature corresponding to the actual maximum loss can be observed easily. For the experimental results, influenced by the irregular oscillation of measured data around the dip of each curve, the frequency with maximum transmission loss deviates from this value. While for the fitted results, with the suppressed interference of the intrinsic noise of CW-THz spectrometer, the frequency signatures which can be identified from the curves accurately are close to the simulation results. As shown in Fig. 9(b), they are found to shift linearly with the increasing RI of analytes injected into the microfluidic channel. According to the slope of fitted line, the calculated sensitivity of this PBG Bragg fiber based microfluidic sensor is 113.7 GHz/RIU. Considering its 50 GHz-linewidth bandgap and 12 GHz-linewidth anti-resonant response, this PBG Bragg fiber based sensor shows potential in detecting liquid analyte with RI in the range between 1.4 and 1.8, which covers most of the common organic solvents for chemical and biological applications [33,34]. However, the irremovable standing waves acting on the measured broad-linewidth amplitude spectrum lead to the low $R^2$ of fitting, thus resulting in the high uncertainty of the frequency signatures. The error bars indicated in Fig. 9(b) is achieved by analyzing the conformity of fitted Lorentzian curves with the measured data. According to their average value of 0.89 GHz, the resolution of this sensor in RI detection is around 0.016 RIU. This high value reflects non-negligible sensing errors and restricts this transmission dip shift based sensing being used for accurate RI probing.

4.2 The microfluidic sensing based on the phase drop shift in phase spectrum
The phase drops corresponding to different-RI liquid analytes

Fig. 10. (a) The measured phase drop corresponding to different-RI liquid analytes. (b) The fitted Boltzmann curves for the measured phase drops, which are in the form of $y=A_2 + (A_1 - A_2) / (1 + \exp((x - X_0) / \text{SLOPE}))$. The x and y represent the frequency and fitted phase drop respectively. The slope center $X_0$ in each equation is regarded as the frequency signature of phase drop and indicated in the left lower corner with the corresponding RI of analyte.

Compared with the transmitted amplitude spectrum, the measured phase spectrum reflects the actual response of the PBG Bragg fiber better because it is free from the influence of standing waves. By subtracting the phase of transmitted THz wave of the PBG Bragg fiber without and with analyte filling its microfluidic channel, a phase drop occurs in the anti-resonant frequency range, which can be employed for higher-resolution microfluidic sensing. The measured phase drops for different-RI liquid analytes are plotted in Fig. 10(a). For establishing an explicit relationship between them and the RIs of analytes, these phase results are fitted into Boltzmann curves, which are shown in Fig. 10(b). The central frequency of each slope is adopted as the frequency signature in phase spectrum. Consistent with results got from amplitude spectrum, these signatures linearly shift with the increasing RI of analytes, which are shown in Fig. 11(b). The obtained sensitivity of 111.1 GHz/RIU matches the result achieved by tracking the transmission dip in amplitude spectrum with acceptable tolerance. Therefore, the predicted sensitivity of 107.3 GHz/RIU in simulation has been confirmed in experiments.

The shift of frequency signatures for different-RI liquid analytes detected by the PBG Bragg fiber based sensor

Fig. 11. (a) The comparison between the measured and the Boltzmann-fitted phase drops corresponding to the liquid analytes with RI of 1.525, 1.495, and 1.465. The frequency signature $X_0$ determined by Boltzmann equation is indicated in the left lower part. The error in frequency signature for each fitted Boltzmann curve is labeled as black line. (b) The shift of frequency
signature in phase spectrum, which is induced by injecting different-RI analytes into sensor. The dots represent the frequency signature for each analyte. The $R^2$ (coefficient of determination) for each fitted Boltzmann curve is indicated. The red line is linear fit for the shift of frequency signature. The sensitivity of the PBG Bragg fiber based sensor is detected as 111.1 GHz/RIU by the slope of this equation.

Compared with the fitted Lorentzian curves for the measured noisy transmission dips with average $R^2$ of 0.9145, the conformity of the fitted Boltzmann curves with the measured phase drops is higher. As examples shown in Fig. 11(a), in the anti-resonant frequency range for the liquid analytes with RI of 1.525, 1.495, and 1.465, the fitted curves match the measured data with smaller deviation than the amplitude spectrum one. The average $R^2$ of 0.984 of all the fitted curves allows smaller error of frequency signature, thus endowing the phase drop shift based sensing with finer RI resolution. The error bars for each analyte are indicated in Fig. 11(b). With their average value of 0.53 GHz, the resolution in RI detection is below 0.01 RIU, which is smaller than the one for transmission dip shift based sensing. In addition, this phase drop shift based sensing fits for the analyte RI probe depending on the anti-resonant response occurring at higher-order bandgaps, which performs higher sensitivity conventionally. Limited by the low available reference power from THz antennas, the amplitude change induced by anticrossing phenomenon at higher frequency is hard to be detected; while the measured phase spectrum is irrelevant to the attainable magnitude of transmitted THz radiation, thus allowing the phase drop shift based sensing being implemented under such conditions.

5. Conclusion

In this work, a THz PBG Bragg fiber based resonant microfluidic sensor has been investigated theoretically and experimentally. Adding a sealed microfluidic channel in the designed PBG Bragg fiber, this sensor is fabricated in PLA by a low-cost commercial FDM 3D printer with adequate geometrical accuracy. Through trial and error method, the optimum fiber length of 10 cm and the proper defect position in the air layer adjacent to fiber core are adopted by this sensor. Probed by a CW-THz spectrometer, its transmitted amplitude and phase spectra with and without analyte in its microfluidic channel are compared. The transmission dips and phase drops in the bandgap, which represent the anti-resonant phenomenon, are found to be linearly red shift with increasing RI of liquid analyte. The sensitivity of this THz PBG Bragg fiber based resonant microfluidic sensor is measured as $\sim$110 GHz/RIU, which is consistent with the theoretical simulation. Due to its high sensitivity and resolution, this proposed microfluidic sensor can find its applications in in-situ chemical and biological liquid detection.

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Appendix: The RI of PLA used in FDM 3D printing

The RI and absorption loss of the PLA which is used in PBG Bragg fiber based sensor is identified by CW-THz spectrometer using cutback method. As shown in Fig. 12(a), the printed PLA plates with thickness around 4 mm are closely touched between a flat mirror and a parabolic one for measurement. During experiments, the plates are removed successively, by which the transmission spectra corresponding to different thicknesses can be detected by THz planar waves. By comparing them with the reference one that no plate inserts, their transmission efficiencies and the induced phase change are calculated, which are shown in Fig. 12(b) and (c). Based on these results, the RI and absorption loss of PLA can be attained via equations (1) [35],

\[
T(\omega, L) = \frac{E_{sam}}{E_{ref}} = C_1 \cdot C_2 \cdot \exp[-\frac{\alpha(\omega)}{2} \cdot L] \cdot \exp[i\varphi(\omega, L)];
\]

\[
\varphi(\omega, L) = -\frac{\omega}{c} (n_{\text{real}}(\omega) - 1) L
\]

\[
\alpha(\omega) = \frac{2\omega}{c} n_{\text{imag}}
\]

In the equations, the \( E_{sam} \) and \( E_{ref} \) are the complex transmission spectra of the PLA with length of L and the reference one. \( C_1 \) and \( C_2 \) represent the coupling efficiency between the PLA and air, which are fixed for different-length samples. The refractive index and absorption coefficient of the PLA plates are deducted as,
\begin{align}
    n_{\text{real}}(\omega) &= 1.636 - 0.0331 \cdot \omega \text{[THz]} \\
    \alpha(\omega) \text{[cm}^{-1}] &= 0.16482 + 0.19395 \cdot (\omega \text{[THz]})^2
\end{align}