Proof of concept for continuously-tunable terahertz bandpass filter based on a gradient metal-hole array

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Abstract: A continuously-tunable terahertz (THz) bandpass filter based on the resonant electromagnetic-wave transmission through a metal-hole array featuring a gradually changing period was developed and fabricated on a silicon substrate using optical lithography. A gradient geometry of the metal-hole array yields a wide tunability of the filter transmission, when operating with a focussed THz beam. The filter was studied numerically, using the finite element method, and experimentally, using the THz pulsed spectroscopy. We find that the central wavelength of the filter transmission band can be tuned in the wide range of \( \lambda_c = 400–800 \) µm with the relative bandwidth of \( \Delta \lambda / \lambda_c \approx \sim 0.4 \). Finally, Kapton-based anti-reflection coating was applied to the filter flat side, in order to suppress an interference pattern in the filter transmission spectrum. We believe that the developed filter holds strong potential for multispectral THz imaging and sensing due to its conceptual simplicity and case of operation. Moreover, the presented filter concept can be translated to other spectral ranges, where appropriate technologies are available for the fabrication of gradient sub-wavelength metal-hole arrays.

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1. Introduction

Frequency-selective optical elements and bandpass filters, with either fixed or continuously-tunable transmission spectra, are the key elements of modern multispectral imaging and sensing technologies in the visible, infrared (IR), and terahertz (THz) ranges, that have attracted significant interest due to a large number of important practical applications [1–8].

In the visible and near-IR ranges, numerous physical principles, material platforms and fabrication technologies yielded a variety of narrow- and broad-band bandpass filter designs with high optical performance. In fact, for over a century, selective spectral absorption of colored glass [9], as well as multilayer interference coatings [10] were routinely used for fabrication of the bandpass filters with fixed transmission spectra. When continuous spectral tunability is required,
a variety of monochromator designs based on the principles of interferometry [3], diffraction optics [11], or even acousto-optics [4,5] were developed.

At the same time, in the mid-IR and THz bands, there is still a lack of the frequency-selective optical elements, especially those that offer wide-band spectral tunability. Indeed, using selective spectral absorption of the natural materials or the multilayer optical media [12–14] seems to be sub-optimal for these spectral ranges due to a considerable electromagnetic-wave absorption in many common dielectrics [15,16]. One promising approach to mitigate this challenge is to use resonant electromagnetic-wave interactions with metal-based optical metasurfaces or metal-hole arrays [17–19]. Filters based on the hole array inscribed onto thin metal film were studied in-depth in the IR [20–22] and THz [23,24] spectral ranges, and recently in the visible [25–27]. Such filters usually show poor spectral tunability, with only few of them featuring the possibility of modest mechanical or electrical tunability [28,29].

Currently, an increased attention is paid to the tunable filters based on novel physical principles such as two-dimensional media, and metamaterials. For example, in Ref. [30], a tunable THz filter was proposed that uses an array of metal rings with gaps, where graphene stripes with variable conductivity are placed. In Ref. [31], a concept of the GaN-based metamaterial THz filter was developed, the transmission properties of which can be tuned by the voltage-dependent carrier density control in AlGaN/GaN heterostructures with Schottky gate configuration. In Ref. [32], a reflecting filter exploiting chirped metamaterial structures based on an array of metal and silicon bars with tunable conductivity was considered theoretically. In Ref. [33], an interesting concept of the weakly tunable THz filter was proposed that rely on bimorph microactuators, fabricated using microelectromechanical system technologies. Alternative approaches, such as the light programmable metasurfaces [34–39], the gradient dielectric metasurfaces [40,41], or the thermally stimulated reconfigurable metamaterials [42] show strong potential for advanced optical performance, but still remain quite labor intensive and expensive to fabricate.

Other options for the spectrally-selective THz imaging are based on the frequency-tunable THz-wave emitter (such as backward-wave oscillators [43] or parametric sources [44]) or broadband THz pulses followed by Fourier-domain data processing [6,7]; however, these approaches are complicated and expensive. Therefore, development of continuously-tunable THz bandpass filters for the multispectral imaging and sensing applications still remains a challenging and relevant problem for applied physics.

To address this challenge, we demonstrate a continuously-tunable THz bandpass filter based on a metal-hole array with gradually changing period, fabricated on a silicon substrate using optical lithography. Thanks to a slowly variable geometry of the metal-hole array, that can be considered constant over the THz beam aperture, we achieve a wide tunability of the filter transmission spectra, when working with a focussed THz beam. By combining numerical analysis and experimental study, we demonstrate that the central wavelength of the filter transmission band can be reliably tuned in the range of $\lambda_c = 400$–800 $\mu$m, while the filter relative bandwidth is $\Delta \lambda / \lambda_c \approx 0.4$. Finally, a Kapton-based Anti-Reflection (AR) coating is applied to the filter flat side, in order to suppress the interference pattern due to standing waves in the substrate. Thus disclosed broadband filter can be applied in THz multispectral imaging and sensing of various condensed matter and biological systems at room temperatures, that usually result in broad spectral absorption bands at THz frequencies [6,7]. Furthermore, this concept can be translated to other spectral ranges, where appropriate technologies are available for fabrication of the gradient sub-wavelength metal-hole arrays.

2. Fabrication of the THz bandpass filter

A schematic of the developed filter is shown in Fig. 1, with a hole geometry adopted from Ref. [26]. A 2-mm-thick 76.2-mm-diameter wafer of High-Resistivity Float-Zone Silicon (HRFZ-Si) was used as a filter substrate with the refractive index of $n_{Si} \approx 3.41$, and negligible dispersion.
and absorption at THz frequencies [15]. An array of holes with gradually changing period in the azimuthal direction is formed in a metal film – a dark band in the filter schematic (see Fig. 1(a)), with the diameter of 50.8 mm and the width of ~ 7 mm. This part of the filter contains a square array, with a period and hole sizes that change continuously in the azimuthal direction in the $p = 110–220 \mu m$, $a = 88–176 \mu m$, and $b = 53–105 \mu m$ ranges and linearly with angle $\theta$. Geometries of the metal-hole arrays at $\theta \approx 0$ and $\theta \approx 359^\circ$ are illustrated in Figs. 1(c),(d), while images of a fabricated filter are shown in Fig. 2.

Fig. 1. Schematic of the continuously-tunable THz bandpass filter. (a) An overall filter layout. (b) Geometry of the cross-shaped holes. (c),(d) Magnified sections of the hole array illustrating gradual changes in its period. The filter can operate either with or without the AR coating. A cross at the center of the filter and labels for sectors 1 to 12 are used for convenience of the filter fabrication and experimental characterization.

Fig. 2. A photo (a) and optical microscopy images (b),(c) of the fabricated filter.

Consider a ~ 7-mm-width aperture of the metal-hole array in the radial direction, and a ~ 7-mm-long sector of the circular metal-hole array in the transverse direction (see Fig. 1), which
effectively define the filter aperture as \(7 \times 7 \text{ mm}^2\). This is, in fact, close to the experimental THz beam spot size. Metal-hole array period varies independently within the tangential and radial directions of the defined aperture. In the tangential direction, a period changes linearly with the rotation angle, while its variation within the considered 7-mm-long circular sector is quite small \(\sim 2.5\%\). The period of the metal-hole array also increases linearly with radius as we fit the same number of holes along any given circumference, which results in a much larger \(\sim 25\%\) radial variation of the period across the 7-mm-width of the filter. A combination of the high radial gradient and a small transverse gradient in the filter period size impacts optical performance of the metal-hole array in several ways compared to the perfectly uniform infinite filter. Particularly, nonuniform gradient makes the filter polarization sensitive, and it also broadens the filter transmission response. The effect of the radial gradient can be reduced by increasing the filter diameter, or it can be completely eliminated using a stripe-like filter geometry, which features only one-dimensional linear gradient and which can possess much larger aperture, as compared to the circular rotary gradient filter.

The variable geometry of cross-shaped holes was formed in a metal film using optical lithography. Namely, a 500-nm-thick metal layer comprises a 40-nm-thick Ti adhesion layer and a 460-nm-thick Au layer. Metallization was performed using an electron-beam evaporation. Then, a photoresistive mask (S1813 photoresist, and MF322 developer) was formed for the two-step metal etching. First, Au was removed using a wet chemical etching in a composition of thiosulfate Na, K-ferrosynorod, and thiourea. Second, Ti was removed using a solution of HF:HNO\(_3\):H\(_2\)O=1:1:98, followed by an inductively coupled plasma – reactive ion etching in a BCl\(_3\)/Ar environment under 1.33 Pa pressure. Finally, the filter was cleaned in the deionized water, while the photoresistive mask was removed using Dimethylformamide. In Fig. 2, a gradient geometry of the fabricated filter is shown.

As presented in Fig. 1(a), we consider two filter types, both featuring identical substrate and metal-hole array geometry. One features an unmodified HRFZ-Si substrate interface with air, while another one has a single-layer AR coating at the wafer flat side. The theoretical value of the refractive index of an ideal quarter-wave AR coating is given by \(\sqrt{n_{\text{Kapt}}^2 - n_{\text{Si}}^2} \approx 1.85\). Such coating can be conveniently realized using Kapton tape (polyimide film, coated with adhesive) [16], which closely satisfies this condition, with \(n_{\text{Kapt}} \approx 1.89\). The absorption coefficient of Kapton is \(\alpha_{\text{Kapt}}<20 \text{ cm}^{-1}\), which results in \(\approx 14\%\) loss over \(l \approx 70 \mu\text{m}\) thickness of a commercial Kapton tape. Neglecting the effect of a few-\(\mu\text{m}\)-thick layer of tape glue, the maximal efficiency of such AR coating is expected at the wavelength of \(\lambda_{\text{AR}} = 4n_{\text{Kapt}}l \approx 529.2 \mu\text{m}\) (corresponding frequency of \(\nu = 0.57 \text{THz}\)).

### 3. Numerical and experimental study of the THz filter

Thus developed filter was then studied experimentally using the transmission-mode THz Pulsed Spectrometer (TPS) described in Ref. [45] In Fig. 3(a), schematic of the filter characterization setup using focussed THz beam is shown. A pair of identical gold-coated off-axis parabolic mirrors with the diameter of 50.8 mm and the focal length of 152.4 mm are used for the THz beam focusing and collimation, while the filter transmission spectrum is varied by manual rotation. Experimentally, the filter was characterized for the tangential \(E_T\) and radial \(E_R\) polarizations, in order to study its polarization dependent performance.

In Fig. 3(b), we present results for the filter of Type I without AR coating. Presented are sample TPS waveforms \(E_s(t)\), transmitted through the filter sector \(\theta = 345^\circ\), and a reference waveform \(E_0(t)\), passed through the empty THz beam path. Here, we use the time-domain step of \(\Delta t = 0.05 \text{ ps}\), and the time-domain window size of \(T = 100 \text{ ps}\), with the corresponding frequency-domain resolution of \(\Delta \nu = 0.01 \text{THz}\). In Fig. 3(c), the transmission spectra \(T(\nu) = \left|\frac{E_s(\nu)}{E_0(\nu)}\right|^2\) are shown for the two polarizations; here, \(E_s(\nu)\) and \(E_0(\nu)\) are Fourier-spectra of the TPS waveforms. In Fig. 3(c), strong modulation of the transmission spectra
Fig. 3. The filter transmission studied experimentally using TPS and numerically using FEM. (a) Schematic of the measurement setup. (b) Sample waveforms $E_s(t)$ transmitted through the filter Type I sector 12 for polarizations $E_T$, $E_R$, as well as a reference one $E_r(t)$ acquired with an empty beam path. (c),(d) Transmission spectra $T(\nu)$ of the filter Type I sector 12, calculated either using original 100-ps-width TPS waveforms (showing a pronounced interference pattern), or using a 20 ps-width TPS waveform apodization (used to filter out satellite pulses and suppresses spectral oscillations). In (c),(d), experimental curves are overlapped with the FEM data, which is filtered using the 0.01 and 0.05-THz-width moving-average filters, respectively, for consistency with the experimental data. (e) Electric field distribution across the computation cell at the frequencies of 0.399 and 0.414 THz, that are somewhat lower or higher than the cutoff frequency of the substrate in-plane modes $\nu_c = c/(pn_{Si}) \approx 0.4$ THz. Clearly, only normally propagating modes of a substrate (with respect to the filter plane) are excited at such lower frequencies; while transversely propagating modes of a substrate are excited at such higher frequencies.

is evident, which is due to the THz standing waves in the HRFZ-Si substrate. Rapid variations in the spectral pattern can be filtered out using a Tukey time-domain apodization window [46] with the width of 20 ps and the smoothness parameter of $\alpha = 0.2$, that also reduces the resolution to $\Delta \nu \approx 0.05$ THz. After such analytical filtering, a broad transmission band is observed (see Fig. 3(d)) with the center wavelength of $\lambda_c \approx 800 \mu m$ and the full-width at the half-maximum of $\Delta \lambda \approx 0.4 \lambda_c$.

Since numerical analysis of optical performance of the entire filter seems to be a daunting task due to gradient in the filter geometry, we resort to a sector-by-sector studies. Particularly, the Finite Element Method (FEM) COMSOL Multiphysics software [47] was used to model strictly-periodic metal-hole array with geometry corresponding to the center region of the filter section 12. Next, by repeating the simulations for different values of the square lattice period $p$, we can generalize the sector-by-sector analysis to deduce performance of the entire filter. In our numerical analysis, a single unit cell of an array was used together with the periodic conditions at the transverse boundaries. The cell features a 2-mm-thick HRFZ-Si substrate ($n_{Si} = 3.41$) with a
free space at both sides ($n_{\text{air}} = 1.0$). The 1-µm-thick Au layer is placed atop of a substrate, and the Impedance Boundary Conditions (IBC) are used at the metal surface. The Au permittivity at the IBC surface was defined by the Drude model [47]: $\varepsilon = \varepsilon_\infty - \omega_{\text{pl}}^2 / (\omega^2 - i\gamma\omega)$, where $\varepsilon_\infty = 1 \times 2\pi \times 2.175 \times 10^{15}$ Hz is the plasma frequency, and $\gamma = 2\pi \times 0.648 \times 10^{13}$ Hz is the damping factor. In the vertical direction, the substrate with a patterned Au film was padded on both sides with free space of several wavelength long. Finally, the input and output periodic ports were set at the top and bottom of the computational cell to study transmission of the plane wave incident onto the filter surface.

In Figs. 3(c),(d), experimental transmission spectra are compared with the numerical curves, being smoothed using rectangular moving-average frequency-domain filters with the width of 0.01 and 0.05 THz, respectively, for consistency with the experimental data. Overall, there is a good qualitative and a moderate quantitative agreements between numerical and experimental data. We believe that the main reason for the quantitative discrepancy between the numerical and experimental results is the fact that our simulations only treat infinitely periodic ideal systems, while the actual structure of the filter features a nonuniform gradient in the period and is finite in size. That said, we also note that the value of the maximal transmission frequency, as well as position of the minima and maxima due to multi-wave interference in the substrate at lower frequencies are very well reproduced, together with the correct quantitative spectral dependence of transmission at low and higher frequencies as clearly seeing in Fig. 3. We therefore consider our simulation results to correctly capture the key governing principles behind the operation of the filter.

Note that the strongest discrepancy between the theory and experiments is observed at higher frequencies (see Fig. 3), while at lower frequencies multi-wave interference in the substrate is well reproduced both qualitatively (spectral positions of the transmission peaks) and quantitatively (absolute value of transmission). This is because at low frequencies we only excite normally propagating modes (perpendicular to the filter plane) in the substrate, while at higher frequencies we also excite substrate modes that propagate along the filter plane with non-zero in-plane (of the filter) wavevectors $G = \pm 2\pi/p$ (solutions satisfy Block theorem in the direction of periodicity). This is clearly seeing when plotting the field distribution in the substrate at frequencies somewhat lower or higher than the cutoff frequency of the substrate transverse modes $\nu_c = c/(pm_{\text{Si}}) \approx 0.4$ THz; $c$ is the speed of light in free space; see Fig. 3(e). These sideway propagating modes in the substrate carry energy along the substrate to its periphery. To model the contribution of such modes properly, we need to model the whole filter including its edge, which is currently impossible to due large filter size.

As a result, numerical data overestimates transmission efficiency of the filter especially at higher frequencies. Moreover, such mechanisms as scattering and diffraction, or THz-wave absorption by real materials and finite conductivity of metals can additionally lower the filter transmission. More investigations are, therefore, in order to improve qualitative agreement between simulations and experiments.

In Fig. 4, a measured evolution of the filter transmission $T(\nu)$ is shown for the $E_R$ polarization, where: (a) corresponds to the filter Type I without AR coating, and it shows a pronounced interference pattern; (b) shows transmission spectra of the filter Type I, smoothed by a 20-ps-width TPS waveform apodization; finally, (c) features transmission of the filter Type II, with a 70-µm-thick AR coating and with significantly suppressed spectral oscillations. Figure 4 also demonstrates wide tunability of the filter transmission band. The center transmission wavelength $\lambda_c$ can be varied linearly with the filter rotation angle in the 400–800 µm range, while the filter relative bandwidth remains $\Delta\lambda/\lambda_c \approx 0.4$. In fact, as confirmed by simulations, filter center wavelength is given by $\lambda_c = pm_{\text{Si}}$. At shorter wavelength ($\lambda<\lambda_c$), higher-order transverse harmonics in the substrate with in-plane wavevectors $\pm 2\pi m/p$ (here, $m \in N$) are excited, thus, leading to transmission drop due to transverse energy transfer in a substrate.
Fig. 4. Experimental filter transmission $T(\nu)$ as a function of the filter rotation angle $\theta$. (a) Filter Type I (see Fig. 1) without AR coating, 100-ps-long time traces, no filtering. (b) Filter Type I, no AR coating, smoothed using a 20 ps-width apodization of TPS waveforms. (c) Filter Type II (see Fig. 1) with AR coating (~70-µm-thick Kapton film) showing a significantly suppressed standing wave interference / reduced spectral oscillations.
4. Discussions

While the gradient-based periodic hole-array filter demonstrated in this work has many practical advantages over other reported THz filters such as wide spectral tunability, simplicity and robustness, technological reliability, flexibility of the design, and scalability to other spectral ranges [23,24,28–33], there is still a room for improvements of its optical performance.

First, the demonstrated filter possesses quite a low maximal transmission of $\sim 30\%–40\%$. The transmission efficiency can be significantly enhanced (by tens of percent) when using alternative low refractive index substrates for the filter fabrication. While in this work we used technologically robust low THz-absorption-loss HRFZ-Si substrate, it also features very high refractive index at THz frequencies \(n_{Si} \approx 3.41\). This leads to high Fresnel reflection losses \(~(n_{Si} - 1.0)^2 / (n_{Si} + 1.0)^2 \approx 0.3\), and strong oscillations in the transmission spectrum due to standing wave excitation in the substrate.

Typically, for narrow-band applications antireflection coatings are employed very successfully to alleviate many challenges associated with using high refractive index substrates. Thus, as evident from Fig. 4, even a simple one-layer AR coating is quite effective in suppressing the standing wave interference pattern, however some frequency-dependent modulations in the filter transmission is still present beyond the optimal operational frequencies for which AR coating is designed. Furthermore, the AR coating leads to additional THz-wave power loss, thus, reducing optical performance of the filter even further. In principle, broadband antireflection coatings using multilayer deposition techniques can be designed to somewhat alleviate these effects, but this will dramatically increase the fabrication complexity.

Alternatively, in order to enhance the filter transmission and reduce standing wave effects, lower-refractive index THz materials such as polymers [16,48] or crystalline quartz [15] can be used as substrates. Other option is to use optically thin substrates or even free-standing gradient metal-hole arrays, made of a metal foil using, for example, a laser pen [49]. Such filters should provide the highest-possible THz-wave transmission; however, in our opinion, such structures tend to be less robust than those fabricated using photolithography on standard mechanically stable substrates.

Beyond transmission efficiency, the filter spectral signature (bandwidth of the central peak, intensity of sidelobes, etc.) is also of great importance. Here we argue that the observed tunability range of the filter transmission, its shape and relatively large bandwidth of the main transmission peak appear to be well-suited for the THz applications in biology, medicine and security. First, in THz biophotonics, the content and state (free or bound) of water serve as the main marker of pathological processes in biological tissues, while sensitivity of THz waves to the water-related features of tissues is much higher at sub-THz frequencies [7,50]. Second, Mie scattering of THz-waves on tissue inhomogeneities is less pronounced at low frequencies, which simplifies description of the THz-wave tissue interactions in the frameworks of the effective medium theory [50]. Third, biological tissues do not possess any resonant spectral features in the THz range, which do not require using narrow-bandwidth filter for tissue sensing and imaging [7]. Finally, the developed filter can find its applications in security systems, where sub-THz radiation is used to detect concealed objects on a human body [51], while the high-frequency THz radiation is strongly scattering in cloths [52].

Another advantage of the developed filter is a high degree of its design tunability for operation in largely distinct parts of the electromagnetic spectrum. This can be achieved by simply changing the metal-hole geometry and the metal-hole array gradient. Moreover, by reducing the rotational symmetry of a metal hole, the filter can be made strongly polarization sensitive [53]. The considered photolithographic approach for the filter fabrication has a potential to reduce the gradient metal-hole array dimensions and, thus, to enable the filter operation at high THz frequencies. For example, our photolithographic equipment allows for fabrication of metal-hole arrays on a circular dielectric substrate with the diameter as large as 76.8 mm, and the typical
lateral dimensions of elements (holes or stripes) as small as \( \sim 5 \mu m \). The described principle can be even translated to other spectral ranges, such as the practically-important mid-IR range, given availability of optically transparent dielectric substrates, as well as available technologies for the metal-hole array fabrication. For example, the electron beam lithography yields production of metal nanostructures on a 76.8-mm-diameter substrate with elements as small as \( \sim 100 \) nm [54], while the plasmonic nanoparticle lithography allows to produce large area arrays of holes with the diameter of >50 nm [55].

Among the limitations of our filter we also mention its rather low optical aperture – namely, the width of the gradient metal-hole array in a radial direction is limited by \( \sim 7 \) mm, which is comparable with the THz beam spot size; see Figs. 1,2. Thus, the current filter application is limited to single point sensing, raster-scan or coded aperture imaging [6,56–58]. In order to make possible its use in a wide-field multipixel imaging, the filter aperture should be increased. To this end, a stripe-like filter with linear gradient of the metal-hole array, which features a wider aperture and which is tuned by a linear mechanical translation, can be used instead of the circular geometry.

Finally, in our experiments, the filter transmission was tuned by mechanical rotation of the filter disc placed in the path of the focused THz beam. In this respect, the mechanical nature of the filter would bring the well-known limitations of the mechanical micro-positioning systems (accuracy, repeatability, activation time, etc.) when compared to alternative electrically, microelectromechanically or optically tunable THz filters [30–42].

5. Conclusions

In summary, in this work, a continuously-tunable THz bandpass filter based on a gradient metal-hole array was developed, fabricated and studied numerically and experimentally. A wide tunability of the filter transmission properties was demonstrated. We believe that such filters hold strong potential in the THz imaging and sensing technologies. Furthermore, the developed design and fabrication principles can be translated to other spectral ranges, where appropriate microfabrication technologies are available.

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