Quantized THz Diffractive Optics Design via Automatic Differentiation

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***Abstract*—Diffractive optical elements (DOEs) in the THz range provide unparalleled, multifunctional control over radiation. Neural network-based design approaches offer significant potential in optimizing the unique phase maps of DOEs, enabling nearly arbitrary modulation of radiation. However, these neural network (NN) design methods typically require continuous values for the DOE phase profile synthesis. Often, the methods do not consider the physical quantization in DOE fabrication due to the discrete material layers produced with 3D printers. To address this, we apply automatic differentiation, a technique commonly used in neural networks, to develop a novel method for optimizing the phase profile of heavily quantized DOEs. Our simulation experiments show that this approach facilitates fast and flexible DOE design, while considering the fabrication limitations.**

I. INTRODUCTION

The use of diffractive optical elements (DOEs) in the terahertz (THz) spectrum range benefits from the extensive capability of phase modulation coupled with manufacturing simplicity. The phase modulation of DOEs is characterized by a complex transmittance function, reflecting a specific thickness profile. The complex transmittance indicates how the amplitude and phase of the incoming wave will be modified after transmitting through the structure. The structure of DOEs varies based on their functionalities, such as focusing [1], redirecting [2], and hologram imaging [3]. Various synthesis approaches for optimal DOEs functionality, such as adjoint-based optimization [1], evolutionary algorithms [4], and neural networks [2], have seen significant advancements recently.

In this work, we proposed a differentiable wave propagation model based on the angular spectrum method (ASM) to design a myriad of arbitrary THz diffractive optics with different functionalities. Moreover, taking into account the mismatch between simulated and fabricated DOEs due to manufacturing constraints, we have developed a novel method to optimize the phase profile for heavily quantized DOEs.

II. DESIGN METHOD

Our approach relies on ASM to accurately model the wave propagation in free space without any approximation. The ASM is defined as:

$$f_{\text{ASM}}(u,z) = \mathcal{F}^{-1}\big\{\mathcal{F}\{u(x,y,0)\} \cdot H(f_{\text{x}}, f_{\text{y}}, \lambda, z)\big\}. \tag{1}$$

where λ is the wavelength, z is the propagation distance, $H(f_x, f_y, \lambda, z) = e^{i\frac{2\pi}{\lambda}z\sqrt{1-(\lambda f_x)^2-(\lambda f_y)^2}}$ is the transfer function, and $\mathcal{F}$ is the Fourier transform. Suppose a source field u_{src} illuminates a DOE with a spatially-varying phase delay $\phi(x,y)$, the desired field distribution at target plane can be expressed by,

$$\begin{aligned} u_{\text{DOE}}(x,y,\lambda) &= \exp\big(i\frac{2\pi}{\lambda}\phi(x,y)\big)u_{\text{scr}}(x,y,\lambda) \\ u_z(x,y,\lambda) &= f_{\text{ASM}}(u_{\text{DOE}}(x,y,\lambda),z) \end{aligned} \tag{2}$$

Considering a differentiable framework to design a DOE, we aim to obtain an element with a specific phase map to minimize the loss function,

$$\text{Loss} = \mathcal{L}\big(|f_{\text{ASM}}(u_{\text{DOE}},z)|^2, a_{\text{target}}\big) \tag{3}$$

where a_{target} is the desired 2D intensity at the target plane. This problem can be solved by a gradient descent scheme based on the chain rule during k iterations:

$$\begin{aligned} \phi^{(k)} &\leftarrow \phi^{(k-1)} - \alpha\big(\frac{\partial \mathcal{L}}{\partial \phi}\big)^T\mathcal{L} \\ &= \phi^{(k-1)} - \alpha\big(\frac{\partial \mathcal{L}}{\partial f_{\text{ASM}}} \cdot \frac{\partial f_{\text{ASM}}}{\partial u_{\text{DOE}}} \cdot \frac{\partial u_{\text{DOE}}}{\partial \phi}\big)^T\mathcal{L} \end{aligned} \tag{4}$$

where α is the learning rate.

However, this approach is typically adopted by full-precision DOEs, but will not work for highly-quantized DOE optimization since the quantization function is not differentiable. To address this problem, the surrogate gradient methods are proposed, where the forward pass is computed using the correct quantization function q but, during the error back-propagation pass, the gradient of a differentiable proxy function $\hat{q}$ is used. Thus, the gradient-descent process can be rewritten as:

$$\phi^{(k)} \leftarrow \phi^{(k-1)} - \alpha\big(\frac{\partial \mathcal{L}}{\partial f_{\text{ASM}}} \cdot \frac{\partial f_{\text{ASM}}}{\partial u_{\text{DOE}}} \cdot \frac{\partial u_{\text{DOE}}}{\partial q} \cdot \frac{\partial \hat{q}}{\partial \phi}\big)^T\mathcal{L} \tag{5}$$

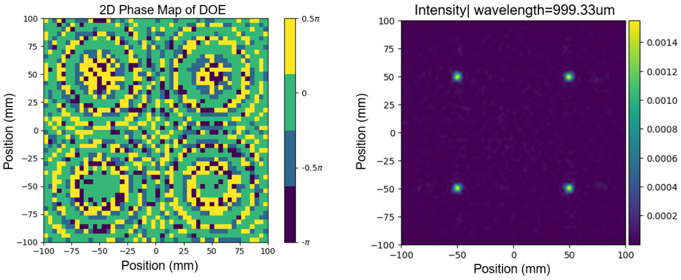
where q is the quantization operator that projects the full-precision phase map $R^{M\times N}$ to the closest discrete phase in the predefined feasible set Q. The differentiable proxy function $\hat{q}$ based on the gumbel-softmax method [5] can be formally expressed as:

$$\begin{aligned} \hat{q}(\phi) &= \sum_{l=1}^{L} \mathcal{Q}_l \cdot \mathcal{G}_l(\mathbf{score}(\phi,\mathcal{Q})) \\ \mathcal{G}_l(z) &= \frac{\exp\left((z_l+g_l)/\tau\right)}{\sum_{l=1}^{L}\exp\left((z_l+g_l)/\tau\right)} \\ \mathbf{score}_l(\phi,\mathcal{Q}) &= \sigma(w\cdot\delta(\phi,\mathcal{Q}_l))(1-\sigma(w\cdot\delta(\phi,\mathcal{Q}_l))) \end{aligned} \tag{6}$$

here $g_{\text{l}} \backsim$ Gumbel(0, 1) denotes Gumbel noise for each category $l = 1,\dots,L$, which correspond to quantized phase levels. σ is a sigmoid function, δ signifies the signed value difference, and w is a scale factor.

III. Simulation Results

To evaluate our method's effectiveness,we conducted synthetic simulations for designing DOEs with various functionalities. To benchmark our focusing and redirecting capabilities against prior work, we designed a DOE with four discrete phase levels that produce four focal spots at 0.3 THz, shown in Fig. 1. This DOE features 200 mm length on each side with 4 mm $\times$ 4 mm pixels, making it suitable for fabrication via 3D printing. We utilized Rexolite 1422 for this design, with relative dielectric permittivity of $\epsilon_r \approx 2.52 - j0.0005$. From the phase distribution in Fig. 1, we can observe four similar patterns with periodic arrangement and each pattern exhibits a phase distribution similar to that of Fresnel zones.



a) b)

Fig. 1. a) The designed DOE's phase map with 4 discrete level in $[-\pi, \pi)$. b) The intensity distribution at 500 mm target plane.

To assess our method's capability in generating complex field distributions, we designed dual-plane holograms for 'A!' and 'A?' images at $D_1 = 100$ mm and $D_2 = 300$ mm. For a fair comparison, we designed a DOE with 50×50 square pixels, matching simulation specifications from a previous dual-plane THz hologram study [3]. The imaging results, presented in Fig. 2, demonstrate that our approach yields more detailed distributions across a larger field-of-view and with fewer discrete levels (8 discrete levels compared to the 25 levels mentioned in [3]).

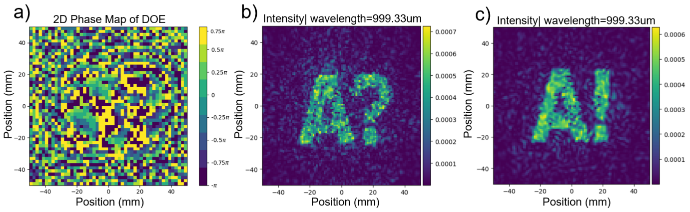


Fig. 2. a) Phase distribution of designed DOE. b) The intensity distribution of at 100 mm and c) 300 mm imaging planes.

DOEs have shown significant promise in multi-frequency modulation in [6]. We developed DOEs for spatial frequency-division (de)multiplexing for frequencies from 0.3 to 0.7 THz, in 0.1 THz increments. Fig. 3a) displays the DOE's phase distribution, showing dual functionalities of focusing and spectrum splitting. Fig. 3b) illustrates the 1D intensity distribution for these frequencies at different position. Comparing with the phase map in Fig. 1 which produced four focal-spots at single frequency, the phase distribution in this design is more varied. As frequency increases, the local phase zone displays increasingly intricate patterns with pixel-level discontinuities. This occurs because the optimized phase distribution, designed for the lowest frequency, may not span the full $[-\pi, \pi]$ range at higher frequencies as the more rapid phase change leads to modulo jumps 2π jumps thus requiring more efficient pixel utilization.

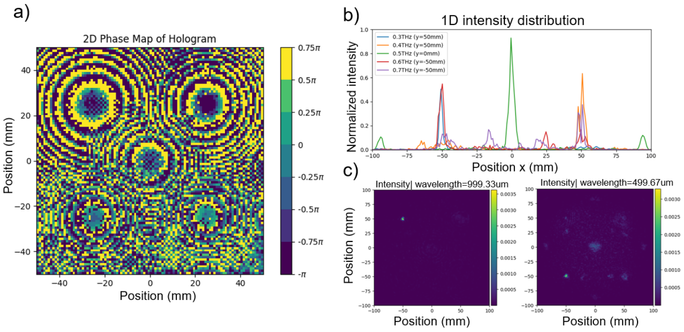


Fig. 3. a) Phase distribution of spatial frequency-division multiplexing DOE. b) The 1D intensity distribution of multiple frequencies along x-axis while different y postion. c) 2D intensity distribution at 0.3THz and 0.6THz.

IV. Summary

In summary, we present a new THz diffractive optics design framework. This framework includes a differentiable wave propagation model for precise gradient calculation by a defined loss function, and a surrogate gradient method for optimizing the heavily quantized phase pattern of DOEs. Our simulations have explored the efficacy of the proposed method in modulating both spatial and spectral domains.

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