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Terahertz ptychography

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We realized a phase retrieval technique using terahertz (THz) radiation as an alternative to THz digital holography, named THz ptychography. Ptychography has been used in x-ray imaging as a groundbreaking improvement of conventional coherent diffraction imaging. Here we show that ptychography can be performed at THz frequencies too. We reconstructed an amplitude and a phase object with both simulated and real data. Lateral resolution accounts to $<2\lambda$, while depth variations as low as $\lambda/30$ can be assessed. © 2018 Optical Society of America

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Terahertz (THz) radiation has been a valuable tool for imaging objects on a submillimeter scale for more than 30 years [1]. A well-established technique is digital holography, where the interference of the beam scattered by the object with a reference beam allows reconstructing the amplitude and the phase in the object plane with few- λ lateral resolution and a phase resolution on the order of a fraction of a radian.

Ptychography is a referenceless and lensless solution of the phase problem, using a set of images collected with a defined coherent beam illuminating the object in transmission at shifted positions. The idea was originally conceived by W. Hoppe in the late 1960s for crystalline objects investigated with atomic scale wavelengths [2]. However, the technique is receiving increasing attention, due to the development of the “ptychographic iterative engine” algorithm, which combines the ptychographic principle with the iterative procedure typical for coherent diffraction imaging [3]. Since then, a number of algorithms were suggested to cope with, among others, unknown illumination functions [4,5] and to account for errors in the scan position [6,7]. Owing to its lensless nature, ptychography is particularly appealing to the x-ray community, although it was also demonstrated at extreme-ultraviolet [8] and optical [4] wavelengths. Besides the transmission mode, alternative experimental configurations include reflection [9] and scattering [10] geometries as well as ptychographic computed tomography [11]. Ptychography was also implemented in the time domain to reconstruct ultrafast pulses [12].

In this Letter, we prove that ptychography can also be realized with a coherent THz source, thus providing an alternative imaging technique featuring submillimeter lateral resolution and $<10\text{ }\mu\text{m}$ depth resolution. As was shown for THz off-axis digital holography [13,14], the relatively long THz wavelengths compared to visible light and x rays make experimental requirements less stringent, thus allowing easier access to intrinsic resolution factors. However, when migrating ptychography to THz frequencies, care must be taken in checking the validity of approximations, which are usually trivial at much shorter wavelengths. In particular, the far-field approximation breaks down; i.e., diffraction patterns cannot be modeled by simply Fourier transforming the field at the object plane.

The setup of transmission ptychography is sketched in Fig. 1. An illumination function, also called “probe,” is defined by cropping a transversely and longitudinally coherent beam with an aperture. A divergent beam can be used to increase the spatial high-frequency components [15] (not shown in Fig. 1). The probe impinges on the object, and the intensity of the transmitted diffracted beam is recorded on a two-dimensional array detector at a distance d from the object. Detector coordinates are indicated as u and v in Fig. 1. The object or the probe is then shifted across the object plane xy , and another image is recorded. The procedure is repeated until the whole object is scanned. If the applied shifts are smaller than the beam diameter, common information is shared in images from neighboring positions. Such redundancy allows an iterative reconstruction of the object field at the object plane in both amplitude and phase. Therefore, a ptychographic dataset

Fig. 1. Schematic experimental setup for transmission ptychography.

consists of a set of D diffraction patterns $I_k(\mathbf{u})$, where the object is shifted by $\mathbf{x}_k$, $k = 1, \dots, D$ and where we have defined $\mathbf{x} \equiv (x, y)$ and $\mathbf{u} \equiv (u, v)$. One class of algorithms capable of finding the object transmission function $o(\mathbf{x})$ from the set of $I_k(\mathbf{u})$ and the shifts $\mathbf{x}_k$ are the so-called “ptychographic iterative engines.” Here we refer to the “extended ptychographic iterative engine” (ePIE) proposed by Maiden and Rodenburg [4] that is used when the probe is not accurately known. A multiplicative interaction between the k th estimate of the object transmission function $o_k(\mathbf{x})$ and the k th estimate of the probe $p_k(\mathbf{x})$ is considered, as follows:

$$\psi_k(\mathbf{x}) = p_k(\mathbf{x})o_k(\mathbf{x} - \mathbf{x}_k). \quad (1)$$

Here, $\psi_k(\mathbf{x})$ is the “exit wave” when the object is at position $\mathbf{x}_k$. A sufficient condition for the validity of Eq. (1) was given by Thibault *et al.* [5] and suggests $t \ll R w / \lambda$, where t is the thickness of the object, R is the resolution of the imaging system, w is the size of $\psi_k(\mathbf{x})$, and λ is the wavelength. The exit wave propagated to the detector plane is

$$\Psi_k(\mathbf{u}) = \mathcal{P}_d[\psi_k(\mathbf{x})](\mathbf{u}), \quad (2)$$

where $\mathcal{P}_d: \mathbf{x} \mapsto \mathbf{u}$ is a suitable operator propagating a two-dimensional complex field to a parallel plane located at a distance d . We used the Fresnel–Kirchhoff integral without approximations [16]. The intensity constraint at the detector plane is then applied, leading to the corrected exit wave at the detector plane,

$$\Psi'_k(\mathbf{u}) = \sqrt{I_k(\mathbf{u})} \exp\{i\angle[\Psi_k(\mathbf{u})]\}, \quad (3)$$

where $\angle$ denotes the phase, and at the object plane,

$$\psi'_k(\mathbf{x}) = \mathcal{P}_d^{-1}[\Psi'_k(\mathbf{u})](\mathbf{x}). \quad (4)$$

The estimates of the object transmission function and the probe are, respectively, given by

$$\begin{aligned} o_{k+1}(\mathbf{x}) &= o_k(\mathbf{x}) + \alpha U_k^o(\mathbf{x} - \mathbf{x}_k)[\psi'_k(\mathbf{x} + \mathbf{x}_k) - \psi_k(\mathbf{x} + \mathbf{x}_k)], \\ p_{k+1}(\mathbf{x}) &= p_k(\mathbf{x}) + \beta U_k^p(\mathbf{x} - \mathbf{x}_k)[\psi'_k(\mathbf{x}) - \psi_k(\mathbf{x})], \end{aligned} \quad (5)$$

where α and β are scalar values controlling the amount of feedback when updating the object transmission function and the probe function, respectively. The corresponding “update functions” $U_k^o(\mathbf{x})$ and $U_k^p(\mathbf{x})$ read

$$U_k^o(\mathbf{x}) \equiv \frac{p_k^*(\mathbf{x})}{\max |p_k(\mathbf{x})|^2}; \quad U_k^p(\mathbf{x}) \equiv \frac{o_k^*(\mathbf{x})}{\max |o_k(\mathbf{x})|^2}, \quad (6)$$

where $*$ indicates complex conjugation. Such update functions are meant to weight the change in the exit wave more when the probe and the object amplitudes are high. The following mean square error [4] was chosen as the convergence metric, as follows:

$$E \equiv \sum_{k=1}^D \sum_{\mathbf{u}} \left| \sqrt{I_k(\mathbf{u})} - |\Psi_k(\mathbf{u})| \right|^2 / \sum_{k=1}^D \sum_{\mathbf{u}} I_k(\mathbf{u}). \quad (7)$$

The procedure is repeated N times with permuted images, where N is the number of iterations, until the error E reaches a stationary value.

Our THz source was a CO₂-laser-pumped, CW far-infrared gas laser (FIRL100, Edinburgh Instruments, Livingston, Scotland), delivering narrow emission lines between 60 and 500 μm . We used the line at $\lambda = 96.5 \mu\text{m}$ (corresponding to 3.1 THz, with a linewidth ~ 10 MHz) caused by a rotational

transition in CH₃OH molecules. The output power was several tens of mW. To define the probe function, the beam was cropped with a circular aperture with a diameter of 3 mm before it impinged on the sample. Pure amplitude and phase objects were imaged. The former was a 100- μm -thick metallic nine-spoked Siemens Star with an inner diameter of 4 mm [see Fig. 2(a1)]. The latter was a 2-mm-thick polypropylene (PP) slab into which three intersecting rings of 2.1 mm outer diameter and 1.5 mm inner diameter were engraved using laser ablation. The depths of the rings ranged from 37 to 234 μm [see Fig. 2(a2), where the corresponding wrapped phase map calculated at $\lambda = 96.5 \mu\text{m}$ is color coded]. Diffraction patterns were acquired with an uncooled microbolometer array based on amorphous silicon and featuring 480×640 pixels on a 17 μm pixel pitch (Gobi-640-GigE, Xenics, Leuven, Belgium). The incoherent infrared radiation from the environment at room temperature was subtracted by chopping the incident THz beam.

Figures 2(a1)–2(k1) summarize the experiment on the amplitude object. Being totally reflective at THz frequencies, the validity of the multiplicative approximation [Eq. (1)] is trivial. The object was scanned across a square grid of 7×7 points with a period of 0.75 mm. This resulted in a relative overlap parameter (approximating the beam diameter with the aperture diameter [17]) of 75%. In addition, the diffraction pattern of the aperture without the object was taken. The distance from the aperture to the detector was estimated by fitting a simulated diffraction pattern of a circular aperture to the experimental one. In a similar way, the distance from the aperture to the object and from the object to the detector can be estimated by comparing experimental diffraction patterns and simulated ones. We obtained an average object-detector distance of 12.2(7) mm and a distance from the aperture to the object of 3.8(7) mm (standard deviations are given in parentheses). Figures 2(b1)–2(g1) compare simulated and experimental diffraction patterns at the detector plane when the probe illuminated the three positions highlighted in Fig. 2(a1). Experimental patterns were denoised by setting the pixels below a suitable threshold to zero. The threshold was determined by a statistical calculation performed in regions with low signal [18]. Ptychographic reconstructions are shown in Figs. 2(h1)–2(k1). Simulated reconstructions [amplitude in Fig. 2(h1) and phase in Fig. 2(j1)] were obtained with $N = 100$. The used probe, shown in the nearby insets (amplitude in the top left inset image, phase in the bottom left inset image), was the diffraction pattern of a 3 mm aperture calculated at the retrieved aperture-to-object distance. Reconstructions from real data were performed with an ePIE algorithm ($N = 200$), which was initialized by the probe used in the simulation. A flat distribution in both amplitude and phase was used as a first estimate of the object. Figures 2(i1), 2(k1), and the corresponding probe insets show the obtained reconstructions. Note that phase reconstructions are not meaningful in regions where the amplitude of the transmitted beam is lower than the noise level. In those regions they can be modeled as a uniform distribution in the range $[-\pi, \pi]$ rad. For both simulated and experimental reconstructions, the lateral resolution was calculated by averaging the amplitude along concentric circles of decreasing radius and evaluating the signal modulation at each step (modulation transfer function [19]). Lateral resolutions of 190 and 300 μm at 10% noise-equivalent modulation were estimated for

Fig. 2. Ptychographic reconstruction of an amplitude object (label 1) and a phase object (label 2). (a) Simulated object transmission function, with the relative position of the probe in three examples of the scan. Corresponding diffraction patterns obtained from the (b), (d), (f) simulated and (c), (e), (g) real object. Simulated reconstructed (h) amplitude and (j) phase. Experimentally reconstructed (i) amplitude and (k) phase. Insets show the probe (top, amplitude; bottom, phase; left, simulation; right, experiment). All phase distributions share the same phase scale, shown in (a2).

simulated and experimental reconstructions, respectively, i.e., 16 and 10 times smaller than the beam diameter.

Results for the phase object are displayed in an analogous way in Figs. 2(a2)–2(k2). The object was moved across a two-dimensional, rectangular grid of 21×7 points with steps of 0.4 and 0.6 mm, resulting in relative overlaps of 87% and

80% along x and y , respectively, ensuring a correct reconstruction of all the features of the object. The intensity of the probe after propagation through the PP slab was also measured in a region far from the three rings [Fig. 2(c2)] to account for refraction of the beam through the slab. The multiplicative approximation is valid in this case too, because the

Table 1. Depth and Reconstructed Phase of the Phase Object Measured with an Optical Microscope (Second and Third Columns, Respectively) and Measured with THz Ptychography (Fourth Column)^a

Region	Depth [μm]	THz Phase from Optical Measurement [rad]	THz Phase from Ptychography [rad]	
			Experiment	Simulated Object
Left ring	157(3)	5.2(1)	4.7(2)	5.2(2)
Crossing left/middle ring	234(3)	7.8(1)	7.8(2)	8.1(1)
Middle ring	77(3)	2.6(1)	2.4(3)	2.4(2)
Crossing middle/right ring	117(3)	3.9(1)	3.8(3)	3.7(1)
Right ring	37(3)	1.2(1)	1.2(1)	1.2(1)

^aThe reconstructed phase of the simulated object is given in the fifth column. Standard deviations are given in parentheses in units of the least significant digit.

maximum ring depth satisfies the sufficient condition mentioned above. The object was at 9.6(6) mm from the detector and 12.0(6) mm from the aperture. Owing to the low scattering and absorption properties of the object (real part of the refractive index $n_{\text{pp}}(3.1 \text{ THz}) = 1.51$, absorption coefficient $\alpha_{\text{pp}}(3.1 \text{ THz}) = 1.5 \text{ cm}^{-1}$ [20,21]), diffraction patterns in Figs. 2(b2)–2(g2) are shown with a logarithmic scale. Visualization 1 shows an excerpt from the ptychographic reconstruction with real data. One can appreciate how acceptable lateral and phase resolutions can be obtained already after five iterations of the ePIE algorithm. The higher noise at the top left corner of the reconstructed phase and amplitude was due to a drop of the laser power toward the end of the scan. Here the lateral resolution was calculated from the 10%–90% width of the experimentally reconstructed phase edges at the borders of the rings. A conservative estimate accounts to 170 μm , i.e., 1.8λ . Phase reconstructions along the three rings and in the regions where they cross are summarized in Table 1. The profiles of the rings were measured with an optical microscope (2nd column in Table 1), translated into phase differences at the THz wavelength of $\lambda = 96.5 \mu\text{m}$ through the refractive index n_{pp} (3rd column), and compared to ptychographic reconstructions (4th column). The reconstructed phase differences from the simulated object are listed in the 5th column. The same approach was used by Hack and Zolliker [13] to evaluate the reconstruction performance of THz off-axis digital holography. Note that *a priori* knowledge of the general nature of the profile of the object is needed to retrieve its absolute phase. The phase resolution is estimated by the standard deviation of the reconstructed phase in the regions of interest. A phase resolution as low as $\Delta\phi = 0.1 \text{ rad}$ was estimated, corresponding to a depth variation of $\Delta d = \lambda\Delta\phi/[2\pi(n_{\text{pp}} - 1)] = 3 \mu\text{m}$ in PP at $\lambda = 96.5 \mu\text{m}$.

In conclusion, we have shown that ptychography can be performed in the THz regime. It allows reconstruction of both amplitude and phase objects with $<2\lambda$ lateral resolution and $\sim\lambda/30$ depth resolution. Although the optimum experimental conditions for THz ptychography still need to be elucidated, we can already claim that THz ptychography is a promising alternative to THz digital holography. A ptychographic experiment takes much longer than a holographic experiment, which needs only one hologram to be acquired. This may pose a problem when laser stability is an issue. Unlike in-line [22,23] and off-axis [14,24] holography, ptychography requires no reference beam, making it possible to move a larger object closer to the detector and thus improving the lateral resolution. Moreover, ptychography can reconstruct objects larger than the beam diameter due to its moving field of view. Besides these preliminary considerations, further investigations are needed

to quantitatively compare their performances. We expect that THz ptychography will be used in particular for imaging biological specimens, thus complementing already reported in-line holographic reconstructions [23].

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