Resolution limits of terahertz ptychography

Lorenzo Valzania^a, Erwin Hack^a, Peter Zolliker^a, Rolf Brönnimann^a, and Thomas Feurer^b

^aLaboratory for Transport at Nanoscale Interfaces, Empa, Swiss Federal Laboratories for Materials Science and Technology, 129 Überlandstrasse, CH-8600 Dübendorf, Switzerland

^bInstitute of Applied Physics, University of Bern, 5 Sidlerstrasse, CH-3012 Bern, Switzerland

ABSTRACT

We present a study on the resolution limits and resolution factors of terahertz (THz) ptychography. Simulations of a binary amplitude object show that ptychography shares the same intrinsic resolution factors with digital holography, *i.e.* it is diffraction-limited. Reconstructions of amplitude and phase objects obtained from holographic and ptychographic experiments are comparable. A lateral resolution of around one wavelength λ is achieved on an amplitude object, while a depth resolution of around $\lambda/5$ is reported on a weakly diffracting phase object. THz ptychography is expected to complement THz holography for imaging biological samples and THz transparent specimens.

Keywords: Terahertz imaging, ptychography, digital holography, phase retrieval, coherent diffraction imaging, lateral resolution, phase resolution.

1. INTRODUCTION

Sensing with terahertz (THz) radiation has been rapidly growing for three decades, supported by the continuous advancement of sources and detectors operating in the far infrared.^{1,2} Because it penetrates several optically opaque materials such as textiles, paper, wood and other building materials, and some semiconductors, THz radiation opened new paths in non-destructive testing and inspection.

Among the coherent imaging techniques, digital holography was successfully implemented at THz wavelengths, with recording and reconstruction techniques similar to the “classical” holography at visible wavelengths.^{3,4} Therefore, the intrinsic (namely, the best achievable) lateral resolution of a typical THz digital holography reconstruction is diffraction-limited, *i.e.* it depends on the wavelength and the numerical aperture set by the detector size and the object-to-detector distance.⁵ Accordingly, these factors are referred to as intrinsic resolution factors, as opposed to the extrinsic ones, *i.e.* related to the specific phase estimation approaches and experimental inaccuracies and leading to a worse resolution than the intrinsic one. In THz off-axis digital holography [sketched in Fig. 1(a)],^{6–8} the beam scattered by an object interferes with a tilted reference beam. For large enough off-axis angles, this allows the separation of the diffraction orders on the detector and thus the retrieval of the amplitude and phase of the object beam. Although the THz wavelength is long compared to the pixel pitch,⁹ which enables large off-axis angles, the numerical aperture is still limited by the requirement that the reference beam must not interact with the object. This sets a lower limit to the recording distance, and consequently to the attainable numerical aperture. The loss in resolution due to the object-to-detector distance can be compensated by an increase of the detector size with a synthetic aperture approach, consisting of acquiring holograms at shifted positions of the detector.⁶ In-line digital holography,¹⁰ while eliminating the issue with an on-axis reference beam, inherently suffers from the twin problem.

As an alternative to THz digital holography, we have recently migrated an emerging X-ray coherent imaging technique, namely ptychography,¹¹ to the THz spectrum, showing performances comparable to the holographic approach.¹² Ptychography is a non-holographic lensless solution to the phase problem, whose first concept was developed by W. Hoppe for imaging periodic (crystalline) objects with electrons.¹³ Interestingly enough,

Further author information: (Send correspondence to L.V.)

L.V.: E-mail: lorenzo.valzania@empa.ch

holography was also conceived in order to improve electron microscopy by disposing of electron objectives. The basic idea of ptychography relies on collecting a set of diffraction patterns, also called “ptychograms”, while scanning the object across an illumination function at overlapping positions [Fig. 1(b)]. Its breakthrough came when Rodenburg and Faulkner merged the ptychographic concept with the iterative phase retrieval methods employed in coherent diffraction imaging (CDI),^{14,15} leading to the so-called “ptychographic iterative engines”. Within the X-ray community, improvements on algorithms and theoretical insights have been developed for more than ten years. These include retrieving the illumination function alongside the object function,^{16–18} correcting for inaccurate knowledge of the scan positions,¹⁹ and optimizing the scanning procedure.²⁰

Following the recent demonstration of THz ptychography, here we provide a study on its resolution limits and factors, based on theory, simulations and experiments. Emphasis is put on lateral and axial resolution, the latter being related to phase resolution, and results will be compared to the performance of THz off-axis digital holography. Section 2 provides the theoretical background of ptychographic iterative engines, and points out some peculiarities of reconstructions at THz wavelengths. The Fourier fringe demodulation technique will instead be used to calculate phase distributions in off-axis digital holography throughout this study (details can be found in Ref. 3). Section 3 investigates the factors impacting the lateral resolution by reconstructing a numerical pure amplitude object at different wavelengths, object-to-detector distances, and detector sizes. Section 4 compares experimental reconstructions and simulated ones from the previous section. Furthermore, an estimate of the axial resolution of THz off-axis digital holography and THz ptychography is provided, by reconstructing a pure phase object exhibiting features at the resolution limit of the two techniques. Finally, Sec. 5 summarizes the paper and briefly discusses the applicability of THz ptychography as an alternative to THz holography.

2. PTYCHOGRAPHIC PHASE RETRIEVAL AT TERAHERTZ FREQUENCIES

Figure 1(b) shows a schematic of ptychography in transmission. Let $\mathbf{r} \equiv (x, y)$ and $\boldsymbol{\xi} \equiv (\xi, \eta)$ describe the coordinates in the object and detector plane, respectively. A coherent incident beam, also known as “probe”, is defined by an aperture and impinges on the object. A set of J ptychograms $I_j(\boldsymbol{\xi})$, $j = 1, \dots, J$ is recorded by a two-dimensional detector, with the object moved across the object plane by $\mathbf{r}_j$ with respect to the probe. Provided that neighboring positions of the object overlap, both the probe $p(\mathbf{r})$ and the object transmission function $o(\mathbf{r})$ at the object plane can be iteratively estimated from the measured $I_j(\boldsymbol{\xi})$ and the shifts $\mathbf{r}_j$. In what follows, the steps of the “extended ptychographical iterative engine” (ePIE) conceived by Maiden and Rodenburg¹⁸ will be outlined. The algorithm is initiated by a starting estimate of the probe and the object transmission function. At each iteration $i = 1, \dots, I$, these estimates are updated J times, by using all the ptychograms. The interaction between the probe and the object at the object plane is typically approximated

Figure 1: Schematic representation of (a) synthetic aperture off-axis digital holography and (b) transmission ptychography.

by the following multiplication:

$$\psi_{i,j}(\mathbf{r}) = p_{i,j}(\mathbf{r}) o_{i,j}(\mathbf{r} - \mathbf{r}_j), \quad (1)$$

where $\psi_{i,j}(\mathbf{r})$, $p_{i,j}(\mathbf{r})$ and $o_{i,j}(\mathbf{r})$ are the j th estimates of the “exit wave”, the probe and the object transmission function at the i th iteration, respectively. Note that the multiplicative approximation in Eq. (1) will hold in our case since $t \ll \rho w/\lambda$, where t is the thickness of the object, ρ is the spatial resolution of the imaging method, w is the extent of $\psi_{i,j}(\mathbf{r})$, and λ is the wavelength.¹⁶ The estimated exit wave is then numerically propagated to the detector plane through a propagation operator $\mathcal{P}_d : \mathbf{r} \mapsto \boldsymbol{\xi}$, where d is the object-to-detector distance, thus obtaining the current estimate of the exit wave at the detector plane $\Psi_{i,j}(\boldsymbol{\xi})$, as follows:

$$\Psi_{i,j}(\boldsymbol{\xi}) = \mathcal{P}_d[\psi_{i,j}(\mathbf{r})](\boldsymbol{\xi}). \quad (2)$$

The choice of the propagator $\mathcal{P}_d$ is affected by the wavelength and by the object-to-detector distance employed in the experiments. Owing to the much stronger diffracting nature of THz radiation compared to X-rays, one can conduct a THz ptychography experiment at Fresnel numbers N_F larger than 1. For instance, at $w = 3$ mm, $\lambda = 0.1$ mm and $d = 10$ mm, one has $N_F \equiv w^2/(\lambda d) = 9$, thus making the commonly used Fraunhofer approximation unacceptable. The Rayleigh-Sommerfeld integral without approximations but within the scalar diffraction theory²¹ is more suitable, *i.e.*,

$$\mathcal{P}_d[f(\mathbf{r})](\boldsymbol{\xi}) \equiv \frac{d}{\lambda} \iint f(\mathbf{r}) \frac{e^{-2\pi i \sqrt{|\mathbf{r}-\boldsymbol{\xi}|^2 + d^2}}}{|\mathbf{r}-\boldsymbol{\xi}|^2 + d^2} d\mathbf{r}. \quad (3)$$

Next, the calculated amplitude is replaced by the measured one, as in all CDI methods,¹⁵ leading to the corrected j th estimate of the exit wave at the i th iteration at the detector plane and at the object plane [Equations (4) and (5), respectively]:

$$\tilde{\Psi}_{i,j}(\boldsymbol{\xi}) = \sqrt{I_j(\boldsymbol{\xi})} \frac{\Psi_{i,j}(\boldsymbol{\xi})}{|\Psi_{i,j}(\boldsymbol{\xi})|}; \quad (4)$$

$$\tilde{\psi}_{i,j}(\mathbf{r}) = \mathcal{P}_d^{-1}[\tilde{\Psi}_{i,j}(\boldsymbol{\xi})](\mathbf{r}). \quad (5)$$

Finally, the object transmission function and the probe are updated based on the difference between the new and the previous estimate of the exit wave at the object plane, as follows:

$$o_{i,j+1}(\mathbf{r}) = o_{i,j}(\mathbf{r}) + \beta^{(o)} U_{i,j}^{(o)}(\mathbf{r} + \mathbf{r}_j) [\tilde{\psi}_{i,j}(\mathbf{r} + \mathbf{r}_j) - \psi_{i,j}(\mathbf{r} + \mathbf{r}_j)]; \quad (6)$$

$$p_{i,j+1}(\mathbf{r}) = p_{i,j}(\mathbf{r}) + \beta^{(p)} U_{i,j}^{(p)}(\mathbf{r} - \mathbf{r}_j) [\tilde{\psi}_{i,j}(\mathbf{r}) - \psi_{i,j}(\mathbf{r})]. \quad (7)$$

Here $\beta^{(o)}$ and $\beta^{(p)}$ are scalar, real feedback parameters weighting the update of the object transmission function and the probe function, respectively. The corresponding “update functions” $U_{i,j}^{(o)}(\mathbf{r})$ and $U_{i,j}^{(p)}(\mathbf{r})$ instead apply changes to the exit wave on a pixel-wise manner, according to the amplitudes of the probe and object transmission, respectively:

$$U_{i,j}^{(o)}(\mathbf{r}) \equiv \frac{p_{i,j}^*(\mathbf{r})}{\max |p_{i,j}(\mathbf{r})|^2}; \quad U_{i,j}^{(p)}(\mathbf{r}) \equiv \frac{o_{i,j}^*(\mathbf{r})}{\max |o_{i,j}(\mathbf{r})|^2}, \quad (8)$$

where $*$ stands for complex conjugate. The calculated estimates in Eqs. (6) and (7) are then used again in Eq. (1), where a different position of the object is considered. The above steps are iterated I times, where at each iteration the ptychograms are used in a randomly shuffled order.

3. SIMULATIONS

Simulations were performed in order to identify the factors impacting the lateral resolution of THz ptychographic reconstructions, and to evaluate how they compare to those of THz off-axis digital holography. A binary amplitude mask in the shape of a nine-spoked Siemens Star with an inner diameter of 4 mm (shown in Fig. 1) was reconstructed at different THz wavelengths, object-to-detector distances, and detector sizes. The simulation values reflect typical parameters of our THz imaging experiment. The wavelengths correspond to two of the

most intense emission lines delivered by far-infrared gas lasers, namely $\lambda = 96.5 \mu\text{m}$ and $\lambda = 118.8 \mu\text{m}$ (CO₂-laser-pumped methanol lines²²). The object-to-detector distance d spans the range 1 to 35 mm, and detectors featuring $N_\xi \times N_\eta = 480 \times 640$ pixels on pixel pitches of $\Delta\xi = \Delta\eta = 17 \mu\text{m}$ and $\Delta\xi = \Delta\eta = 25 \mu\text{m}$ are considered, according to the specifications of two popular microbolometer arrays which proved to image THz radiation.⁹

For each combination of values, three reconstruction approaches were used. The first approach consisted of propagating a plane wave normally impinging on the Siemens Star to the detector plane, cropping the complex field distribution according to the detector size, convolving it with the pixel pitch, and back-propagating it to the object plane. Note that this approach does not replicate a phase retrieval experiment, since the phase is known at the object plane. However, it proves useful because it allows separating the intrinsic resolution factors from the extrinsic ones. We will refer to this approach as the “Forth-and-back propagation” method. The second approach, referred to as the “FFT holography” method, reproduced a THz off-axis digital holography experiment. The hologram obtained from the superposition of the field transmitted through the Siemens Star and a tilted plane reference wave was simulated. The angle between the propagation directions of the object and reference beam was set to 45°. The phase of the object beam at the detector plane was retrieved from the cropped and re-sampled interference pattern with a Fourier fringe demodulation algorithm.³ The third approach reproduced a THz ptychography experiment. A collimated flat-top beam with a diameter of 3 mm was assumed to impinge on the Siemens Star. The object was moved across a square grid of 7×7 points with steps of 0.75 mm, resulting in a relative overlap of 75%, as defined by Bunk *et al.*²³ The simulated, cropped and re-sampled ptychograms were used in a ptychographic algorithm without probe updating [$\beta^{(p)} = 0$ in Eq. (7)] with 5 iterations. For all the methods, the Rayleigh-Sommerfeld integral [Equation (3)] was used as a propagation operator.

The lateral resolution for each reconstruction was calculated by evaluating the modulation of the intensity of the reconstructed wave at the object plane along concentric rings with decreasing radii (modulation transfer function). The noise-equivalent modulation was determined in such a way that the estimated resolution is the same as half the width of the reconstruction of an on-axis point object at its first zero using the “Forth-and-back propagation” method.

Figure 2 shows the calculated lateral resolution ρ , normalized to the wavelength, as a function of $d/(N\Delta\xi) = 1/\tan\theta$, where θ is half the acceptance angle of an equivalent, square detector with $N^2 \equiv N_\xi N_\eta$ pixels seen by an on-axis point a distance d apart. Each point represents the average resolution obtained at the two wavelengths $\lambda = 96.5 \mu\text{m}$ and $\lambda = 118.8 \mu\text{m}$ and at the two pixel pitches $\Delta\xi = \Delta\eta = 17 \mu\text{m}$ and $\Delta\xi = \Delta\eta = 25 \mu\text{m}$, where different reconstruction approaches are encoded with different marker types (o for “Forth-and-back propagation”, • for “FFT holography”, and × for ptychography). Any difference of the resolutions of the “FFT holography” and ptychographic methods from the ones of the “Forth-and-back propagation” method is ascribed to different extrinsic resolution factors. For the “FFT holography” method, these include residual errors in the elimination of the carrier fringes, and in the optimization of the window used to isolate the first diffraction order from the DC component.³ For the ptychographic method, we mention the influence of the overlap parameter²³ and the number of iterations. Plotted with a solid line is the resolution function

$$\frac{\rho}{\lambda} = \frac{1}{2 \sin \theta} = \frac{1}{2} \sqrt{1 + \left(\frac{2d}{N \Delta\xi} \right)^2}, \quad (9)$$

corresponding to the diffraction limit, with a numerical aperture determined by the acceptance angle of the detector. Therefore the lateral resolution cannot be pushed below Abbe’s limit $\rho \rightarrow \lambda/2$, which is reached at distances $d \ll N\Delta\xi$. At distances $d \gg N\Delta\xi$ within the Fresnel diffraction regime, the resolution function approaches the intrinsic resolution limit derived by Picart and Leval⁵ for an on-axis object reconstructed with digital Fresnel holography, *i.e.*, $\rho/\lambda = d/(N\Delta\xi)$.

One can observe that simulations of the ptychographic method also follow the trend described by the resolution function in Eq. (9), thus suggesting that ptychography and digital holography share the same intrinsic lateral resolution factors. As a consequence, part of the analyses in Ref. 5 can be migrated to ptychography. For example, ptychograms can be zero padded prior to back-propagation to the object plane, leading to a denser sampling of the resolution function. Furthermore, the influence of the finite size of the pixels can be derived in an analogous manner.

Figure 2: Lateral resolution (normalized to the wavelength) calculated for a simulated amplitude object reconstructed with the “Forth-and-back propagation” (○), “FFT holography” (●), and ptychography (×) methods as a function of the reconstruction distance normalized to the detector size. The intrinsic resolution function from Eq. (9) is plotted with a solid black line. The blue filled circle and the red cross indicate the experimental resolution reached by synthetic aperture THz off-axis digital holography and THz ptychography, respectively. The insets show the corresponding reconstructed amplitudes. Scale bar: 2 mm.

4. EXPERIMENTS

In order to experimentally verify the conclusions drawn in Sec. 3, synthetic aperture THz off-axis digital holography and THz ptychography experiments were carried out on a real binary amplitude object, a 100 μm -thick metallic nine-spoked Siemens Star with an inner diameter of 4 mm and fabricated by laser ablation. We used the emission line at $\lambda = 96.5 \mu\text{m}$ from a far-infrared gas laser delivering continuous wave powers of several tens of mW (FIRL100, Edinburgh Instruments, Livingston, Scotland). Holograms and ptychograms were recorded with an uncooled microbolometer array detector with $N_\xi \times N_\eta = 480 \times 640$ pixels on a $\Delta\xi = \Delta\eta = 17 \mu\text{m}$ pitch (Gobi-640-GigE, Xenics, Leuven, Belgium).

In the synthetic aperture holographic experiments, holograms were acquired by shifting the detector across the ξ -plane as far as interference fringes could be distinguished. This resulted in an increase of the physical size of the detector by a factor 3 and 2.5 along ξ and η , respectively. A 11×11 grid with steps of 1.6 mm along both ξ and η was chosen. The detector was placed at the minimum distance from the object ensuring no interaction between the object and the reference beam, *i.e.* $d = 15.4$ mm. The object was then reconstructed with a Fourier fringe demodulation algorithm followed by a stitching of the holograms and back propagation to the object plane. In the ptychographic experiments, an aperture with a diameter of 3 mm clipped a diverging (divergence angle of 4.5°), lowest order transverse electro-magnetic (TEM_{00}) Gaussian laser beam at distance of 7.3 mm from the object. The latter was placed at a distance $d = 6$ mm from the detector, which is a factor of 2.6 closer than the distance employed in the holographic experiments, resulting in a comparable numerical aperture. The recorded ptychograms were then fed in an ePIE algorithm to reconstruct the object. For the sake of a fair comparison between the two approaches, the same number of images was used: the object was scanned across a 11×11 grid with steps of 0.7 mm along both x and y , resulting in relative overlaps of 77%. Furthermore, identical integration time and procedure for the correction of the incoherent infrared background were employed. The average THz power incident on the object plane differed by less than 10% in the two experiments.

The amplitudes of the object wave reconstructed with off-axis digital holography and ptychography are shown in the top left inset of Fig. 2, and the corresponding resolutions are plotted in colors (blue filled circle for synthetic aperture THz off-axis digital holography, and red cross for THz ptychography). It can be noted that

the larger reconstruction distance needed to perform off-axis digital holography was compensated by increasing the synthetic detector size by the same amount, so to yield the same resolution as ptychography. This conclusion supports the trend predicted with simulations and using Eq. (9). The fact that the experimental resolution does not meet the theoretical value is mainly due to defocus aberrations, caused by residual errors in the estimation of the reconstruction distances with both approaches. It should also be noted that such low values of ρ/λ , *i.e.* ≈ 1 , are obtainable thanks to the strong diffraction properties of THz radiation for this type of sample structures. This in turn allows recording diffraction patterns with a much lower $d/(N\Delta\xi)$ ratio compared to X-ray diffraction-based imaging techniques.²⁴

A similar type of comparison was done with a pure phase object, to provide an estimate of the axial resolution. Unlike lateral resolution, axial resolution is not diffraction-limited, thus any resolution limit must be ascribed to the finite signal-to-noise ratio in the measurement data²⁵ and to limitations of the experimental setup. The pure phase object was a 4 mm-thick Teflon (polytetrafluoroethylene, PTFE) slab where 9 squares with a side of 3 mm each and depths ranging from 11 to 473 μm were engraved by laser ablation. As a reference, the same object was measured with projection moiré profilometry, and the retrieved profile is plotted with black symbols in Fig. 3. Holographic and ptychographic reconstructions of the wrapped phase are shown in the insets (a) and (b), respectively. For each square, the average phase within an adjacent flat surface region was subtracted from the average phase within the square, in order to compensate for tilts of the object with respect to the detector plane. The unwrapped phases were then translated into depths according to $\Delta d = \lambda \Delta\phi / [2\pi(n-1)]$, where Δd is the profile variation induced by a phase difference $\Delta\phi$ in a medium with a refractive index n at the wavelength λ . In our case, $n = 1.45$ at $\lambda = 96.5 \mu\text{m}$. The obtained depths are plotted in Fig. 3 (blue filled circles for synthetic aperture THz off-axis digital holography, and red crosses for THz ptychography). The results from the two approaches are comparable. After tilt compensation, both techniques can resolve depth variations as small as $\approx 20 \mu\text{m}$ ($\approx \lambda/5$), while the standard deviation of the depth within each square, where it is assumed to be homogeneous, is $\approx 10 \mu\text{m}$. However, for more strongly diffracting phase objects, flat regions could be successfully reconstructed with a standard deviation as low as $3 \mu\text{m}$ ($\approx \lambda/30$).¹²

Figure 3: Reconstructed profile of a pure phase object consisting of 9 squares with different depths. Black symbols show the result of a reference measurement by projection moiré profilometry; blue [red] symbols indicate the depths retrieved by synthetic aperture THz off-axis digital holography [THz ptychography], while the corresponding reconstructed wrapped phase is shown in the inset (a) [(b)]. Wrapped phases share the same colorbar, shown at the bottom. The total length of each errorbar is twice the standard deviation of the retrieved depth within the corresponding square.

5. CONCLUSIONS

In conclusion, we have discussed the theoretical and experimental resolution limits of THz ptychography, and compared them to the performance of THz off-axis digital holography. Simulated reconstructions show that the two approaches share the same intrinsic resolution factors determining the lateral resolution, which is limited by the diffraction limit. A lateral resolution $\rho \approx \lambda$ could be experimentally reached with both techniques, 20% higher than the diffraction limit because of defocus aberrations. In the holographic measurement this was achieved by a synthetic aperture approach, which compensated the long object-to-detector distance needed for the recording of the off-axis reference beam. Furthermore, details as low as $\approx \lambda/5$ could be distinguished along the axial direction of a flat and weakly diffracting phase object. Therefore, THz ptychography is a valid alternative to THz digital holography for imaging objects with sub-mm lateral resolution and $\approx 10\ \mu\text{m}$ depth resolution. It may be preferred to off-axis digital holography in case of extended objects covering the detector field of view, where the increase in the object-to-detector distance in order to access the reference wave cannot be efficiently compensated by synthetic aperture recording schemes. On the other hand, holography is a direct, non-iterative solution to the phase problem, which makes it less computationally complex than ptychography. We expect THz ptychography to complement already reported THz holographic reconstructions of biological specimens and THz transparent samples.¹⁰

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