

Phase-and-amplitude computer tomography

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A tomographic technique is proposed for reconstruction under specified conditions of the three-dimensional distribution of complex refractive index in a sample from a single projection image per view angle, where the images display both absorption contrast and propagation-induced phase contrast. The algorithm achieves high numerical stability as a consequence of the complementary nature of the absorption and phase contrast transfer functions. The method is pertinent to biomedical imaging and nondestructive testing of samples exhibiting weak absorption contrast. © 2006 American Institute of Physics. [DOI: 10.1063/1.2226794]

X-ray computer tomography (CT) is a well-established technique for three-dimensional (3D) imaging of internal structure of samples.^{1,2} Conventional CT imaging is based on the differential attenuation of transmitted x rays by constituents of the sample. This contrast mechanism is effective for distinguishing between elemental components with significant differences in atomic number or density, e.g., between flesh and bones in the case of medical CT. However, the difference in x-ray attenuation by different types of soft tissues (e.g., healthy and malignant ones) is typically rather weak, which results in poor image contrast, hampering diagnostics. It has been suggested that x-ray phase contrast can be utilized for improvement of the contrast in transmission images of noncrystalline samples consisting predominantly of light chemical elements.^{3–5} Subsequently, phase-contrast x-ray CT (PCT) has been implemented in several forms, including x-ray interferometry,^{6,7} analyzer-based^{8,9} and propagation-based phase contrast,^{10–12} and others. The subject of this letter is closely related to the propagation-based PCT.

It has been recognized early in its development that the PCT reconstruction of a 3D distribution of the refractive index in the sample can be performed as a two-stage process.^{11,12} In the first stage, the projected distribution of the refractive index is reconstructed for each angle of view by using a suitable method of phase retrieval. The second stage then coincides with a conventional CT reconstruction, typically using a filtered backprojection. An alternative strategy is to integrate the phase-retrieval step into a modified CT reconstruction algorithm.^{13,14} Bronnikov^{15,16} has demonstrated that in the case of nonabsorbing objects or objects with almost homogeneous weak absorption the latter (integrated) strategy may be preferable, as it involves a beneficial partial cancellation of singularities associated with the inverse Radon transform and phase retrieval. Both the inverse Radon transform and phase retrieval are examples of inverse problems, and as such are numerically unstable operations. This fact presents a challenge for practical implementation of PCT reconstruction algorithms. The instabilities of inverse problems can usually be traced back to the suppression of

certain information channels in the corresponding direct problems. In the case of propagation-based PCT, the information transfer from the object to individual projection images can be conveniently described in terms of the amplitude and phase contrast transfer functions (CTFs).¹⁷ Importantly, at low spatial frequencies when the phase CTF is close to zero in magnitude, i.e., when the information related to the corresponding spatial frequency is not reflected in the phase contrast, the amplitude CTF is close to its maximum, i.e., the absorption information corresponding to the same spatial frequency is encoded in the image with the highest possible contrast. This complementary nature of the two CTFs has been exploited in Refs. 18 and 19 resulting in a very robust method for phase retrieval. In this letter we use a similar approach to derive a numerically stable CT algorithm which utilizes the complementarity of the amplitude and phase CTFs in propagation-based imaging to achieve optimal information extraction from a set of projection images. The proposed algorithm is directly applicable to x-ray CT with projections acquired at sufficient sample-to-detector distance to register propagation-induced phase contrast, however, other forms of tomography utilizing different types of radiation or matter waves may also benefit from the application of similar reconstruction strategies.

Let an object be illuminated by a plane monochromatic x-ray wave with wavelength λ and intensity I_{in} and let the transmitted wave be registered by a position-sensitive detector. We use Cartesian coordinates $\mathbf{r}=(x, y, z)$ to describe the spatial distribution of the complex refractive index in the object, $n(\mathbf{r}) \equiv 1 - \Delta(\mathbf{r}) + i\beta(\mathbf{r})$. The direction of the incident x-ray wave makes an angle θ' with the z axis, $-\pi/2 \leq \theta' < \pi/2$ and $\theta = \theta' + \pi/2$. We assume as usual that the projection approximation can be applied to calculate the phase $\varphi_{\theta}(x', y) = -k(\mathbf{P}_{\theta}\Delta)(x', y)$ and intensity $I_{\theta}(x', y) = I_{\text{in}} \exp[-2k(\mathbf{P}_{\theta}\beta)(x', y)]$, of the wave after transmission through the object, where

$$(\mathbf{P}_{\theta}f)(x', y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z) \delta(x' - x \sin \theta - z \cos \theta) dx dz \quad (1)$$

is the projection operator, $k=2\pi/\lambda$ and $\mathbf{r}'=(x', y, z')$ are

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Cartesian coordinates rotated by angle θ' around the y axis with respect to coordinate system \mathbf{r} (the object plane is located at $z'=0$ and the image plane is $z'=R$).

Taking the two-dimensional (2D) Fourier transform, $(\mathbf{F}g)(\xi', \eta) = \iint \exp[i2\pi(x'\xi' + y\eta)]g(x', y)dx'dy$, of Eq. (1) and using the Fourier slice theorem one can easily obtain¹ that

$$f(x, y, z) = \int_0^\pi \int_{-\infty}^\infty \int_{-\infty}^\infty \exp\{-i2\pi[\xi'(x \sin \theta + z \cos \theta) + \eta y]\}(\mathbf{F}\mathbf{P}_\theta f)(\xi', \eta)|\xi'|d\xi'd\eta d\theta. \quad (2)$$

Therefore, if projections $(\mathbf{P}_\theta f)(x', y)$ can be measured for all view angles θ from the interval $(0, \pi)$, Eq. (2) can be used to reconstruct the 3D distribution $f(x, y, z)$.

We are interested in the reconstruction of the 3D distribution of the complex refractive index in the sample $n(\mathbf{r})$. As this implies the reconstruction of two different real-valued 3D distributions, $\Delta(\mathbf{r})$ and $\beta(\mathbf{r})$, such reconstruction generally requires acquisition of at least two different 2D projections at each view angle θ .² However, in some cases, it can be shown *a priori* that the distributions of the real and imaginary parts of the refractive index are proportional to each other, i.e.,

$$\beta(\mathbf{r}) = \varepsilon \Delta(\mathbf{r}), \quad (3)$$

where the proportionality constant ε does not depend on \mathbf{r} . If Eq. (3) holds, then a single projection per each view angle is sufficient for reconstruction of the 3D distribution of the complex refractive index (which is the basis for the reconstruction algorithm presented below). Such proportionality can be easily shown to exist in the case of objects consisting of a single material.¹⁸ The proportionality constant ε for chemical elements and compound materials can be found, e.g., at the NIST website.²⁰ With possible medical applica-

tions in mind, the values of ε for representative chemical elements and x-ray energies are 3.7×10^{-4} , 4.4×10^{-4} , 5.5×10^{-4} , 2.5×10^{-3} , and 5.7×10^{-3} for carbon, nitrogen, oxygen, phosphorus, and calcium, respectively, at $E=30$ keV, and 5.1×10^{-4} , 5.4×10^{-4} , 5.7×10^{-4} , 1.1×10^{-3} , and 1.9×10^{-3} for the same elements at $E=60$ keV. One can see that the variation in the value of ε is not particularly large, especially for higher energies and low- Z elements. For x-ray energies between approximately 60 and 500 keV the value of ε is almost the same for all chemical elements with $Z < 10$.²¹

Let R be the distance between the object and the image planes (assumed to be the same for all projections). Let us consider the case of a sample with a distribution of refractive index such that at all view angles θ , the sample transmission function $Q_\theta(x', y) = \exp[ik\mathbf{P}_\theta(n-1)(x', y)]$ can be represented in the following form:

$$Q_\theta = \bar{Q}_\theta(1 + \chi_\theta), \quad (4)$$

where $\bar{Q}_\theta(x', y)$ is a slowly varying function on the length scale $h \equiv \sqrt{\lambda R}$ and $\chi_\theta(x', y)$ is small in magnitude, i.e., $|\chi_\theta| \ll 1$.²² Note that the well-known transport of intensity equation²³ (TIE) and the first Born¹⁷ approximations for the image intensity can be obtained using special cases of Eq. (4) with $\chi_\theta \equiv 0$ and $Q_\theta \equiv \text{const}$, respectively.²² When Eqs. (3) and (4) hold, the Fourier transform of intensity distribution $I_\theta^R(x', y)$ in projection images can be approximated by the following expression:¹⁹

$$(\mathbf{F}I_\theta^R)(\xi', \eta) = I_{\text{in}}\{\cos[\pi\lambda R(\xi'^2 + \eta^2)] + \varepsilon^{-1} \sin[\pi\lambda R(\xi'^2 + \eta^2)]\}[\mathbf{F} \exp(-2k\mathbf{P}_\theta\beta)](\xi', \eta). \quad (5)$$

Note that the first term in the curly brackets in Eq. (5) describes the amplitude CTF, while the second term describes the phase CTF.¹⁷ Expressing the projection $(\mathbf{P}_\theta\beta)(x', y)$ via Eq. (5) and substituting the result into Eq. (2) we obtain

$$\Delta(x, y, z) = -\frac{1}{2k\varepsilon} \int_0^\pi \int_{-\infty}^\infty \int_{-\infty}^\infty \exp\{-i2\pi[\xi'(x \sin \theta + z \cos \theta) + \eta y]\} \times \mathbf{F} \ln \mathbf{F}^{-1} \left(\frac{(\mathbf{F}I_\theta^R)(\xi', \eta)}{I_{\text{in}}\{\cos[\pi\lambda R(\xi'^2 + \eta^2)] + \varepsilon^{-1} \sin[\pi\lambda R(\xi'^2 + \eta^2)]\}} \right) |\xi'|d\xi'd\eta d\theta. \quad (6)$$

Equation (6) represents a formula for the reconstruction of the 3D distribution of the complex refractive index, $n=1-\Delta+i\varepsilon\Delta$, from a set of in-line projections $I_\theta^R(x', y)$ measured for all view angles θ from the interval $[0, \pi)$.

Note that at zero object-to-image distance $R=0$ Eq. (6) reduces to the conventional CT reconstruction formula for $\beta=\varepsilon\Delta$. If the absorption contrast is weak, projection images can be collected at a nonzero distance R in order to utilize the phase contrast. In the general case of $R>0$, Eq. (6) contains an extra pair of 2D Fourier transforms compared to the conventional CT. This disadvantage can be eliminated in the case of weak absorption, $2k|(\mathbf{P}_\theta\beta)(x', y)| \ll 1$, by applying the approximation $\exp\{-2k(\mathbf{P}_\theta\beta)(x', y)\} \approx 1-2k\varepsilon(\mathbf{P}_\theta\Delta)(x', y)$ in Eq. (5). As this expression repre-

sents the argument of the logarithm function in Eq. (6), it allows one to use the well-known approximation $\ln(1+x) \approx x$ which is valid for $|x| \ll 1$. As a result, Eq. (6) simplifies to

$$\Delta(x, y, z) = \int_0^\pi \int_{-\infty}^\infty \int_{-\infty}^\infty \exp\{-i2\pi[\xi'(x \sin \theta + z \cos \theta) + \eta y]\}F(\xi', \eta)(\mathbf{F}K_\theta^R)(\xi', \eta)d\xi'd\eta d\theta, \quad (7)$$

with the "transfer" function

$$F(\xi, \eta) = \frac{|\xi|}{2k\{\sin[\pi\lambda R(\xi^2 + \eta^2)] + \varepsilon \cos[\pi\lambda R(\xi^2 + \eta^2)]\}}, \quad (8)$$

and the "in-line image contrast" function $K_\theta^R(x', y) \equiv [1-I_\theta^R(x', y)/I_{\text{in}}]$.

Equations (7) and (8) are the main result of this letter. They represent a phase-and-amplitude computer tomography (PACT) reconstruction formula that allows one to obtain the 3D distribution of the refractive index in a weakly absorbing sample satisfying conditions Eqs. (3) and (4) from a set of in-line projections $I_{\theta}^R(x', y)$.

The proposed reconstruction formula for weak absorption case, Eqs. (7) and (8), is more numerically efficient than the two-stage reconstruction process (consisting of phase retrieval followed by conventional CT reconstruction), as it saves two 2D Fourier transforms [cf. Eqs. (6) and (7)]. The formula has a number of other interesting properties mainly determined by the PACT transfer function $F(\xi, \eta)$.

- (1) In the TIE regime, i.e., when the transmission $Q_{\theta}(x', y)$ is a slowly varying function on the length scale $\sqrt{\lambda R}$ at all θ , the in-line contrast function $K_{\theta}^R(x', y)$ is band limited to the spectral region $\xi^2 + \eta^2 \ll (\lambda R)^{-1}$. In this case the cosine function in the denominator of Eq. (8) can be replaced by 1, and the sine function can be replaced by its argument resulting in a simpler transfer function

$$F_{\text{TIE}}(\xi, \eta) = \frac{|\xi|}{4\pi^2 R(\xi^2 + \eta^2) + \alpha}, \quad (9)$$

where $\alpha = 2k\varepsilon$ is a positive constant.

- (2) In pure PCT one assumes absorption in the object to be negligible, which corresponds to $\varepsilon \rightarrow 0$ in Eq. (8), and, hence, $F_{\text{pha}}(\xi, \eta) = |\xi| / \{2k \sin[\pi \lambda R(\xi^2 + \eta^2)]\}$. In the TIE regime this transfer function becomes $F_{\text{pha, TIE}}(\xi, \eta) = |\xi| / [4\pi^2 R(\xi^2 + \eta^2)]$ which also coincides with Eq. (9) when $\alpha = 0$. The last result was obtained earlier in Ref. 15 using a different approach. In Ref. 16 this result was extended to mixed phase and amplitude objects with almost homogeneous weak absorption [in this case, an additional image $I_{\theta}^0(x', y)$ needs to be acquired at each view angle].
- (3) In conventional (absorption) tomography the transfer function is equal to $F_{\text{abs}}(\xi, \eta) = |\xi| / \alpha$, which corresponds to the limit case with $R \rightarrow 0$ in Eqs. (8) and (9). Obviously, the resultant formula holds even when the absorption is not weak. Although Eq. (7) with transfer functions Eq. (8) [or Eq. (9) in the TIE case] reduces to the known PCT and conventional CT formulas in the absence of absorption and phase contrast, respectively, the assumption of weak absorption is essential for the validity of Eqs. (7) and (8) or Eqs. (7) and (9) in the general case. Indeed, this assumption enables one to discard the ‘‘prism’’ term $\nabla \varphi_{\theta} \cdot \nabla I_{\theta}$, which otherwise affects the intensity distribution in projection images.²² Note that when condition Eq. (3) holds, the latter term is quadratic (and hence, nonlinear) with respect to $(\mathbf{P}_{\theta} \Delta)(x', y)$ and $(\mathbf{P}_{\theta} \beta)(x', y)$.
- (4) It is very important to note that in the pure phase case and in the weak absorption TIE case described by Eq. (9), in contrast to the case of conventional absorption tomography, the transfer function tends to zero for large values of ξ and η . This important feature implies that, as it was previously noted in Ref. 16, unlike the case of conventional CT, the reconstruction formulas in PACT and PCT are numerically stable, i.e., they do not amplify

the high-frequency noise present in experimental projection data.

- (5) Equation (7) with transfer function [Eq. (9)] is also more numerically stable than the previously considered PCT reconstruction,¹⁵ as the presence of factor $\alpha > 0$ in the denominator makes the reconstruction formula described by Eqs. (7) and (9) insensitive to low-frequency noise by preventing the transfer function from diverging at small values of ξ and η . Note that the corresponding significantly more stable behavior of the ‘‘single-material’’ phase retrieval formula¹⁸ compared to the pure-phase one has been already demonstrated in a number of publications.^{18,22,24–26}
- (6) The accuracy of the reconstruction in accordance with Eqs. (7) and (8) or (7) and (9) depends on the accuracy of estimation of the value of ε for the sample. However, the results of the reconstruction are usually not very sensitive to the exact value of ε .²⁶ The dependence is also limited to the low-frequency components of the spatial Fourier spectrum of the sample.

We believe that due to its favorable properties discussed above the PACT reconstruction formula will find many applications in biomedical imaging and nondestructive testing of samples exhibiting weak absorption contrast.

¹F. Natterer, *The Mathematics of Computerized Tomography* (Wiley, New York, 1986).

²M. Born and E. Wolf, *Principles of Optics*, 7th expanded ed. (Cambridge University Press, Cambridge, 1999).

³U. Bonse and M. Hart, *Appl. Phys. Lett.* **6**, 155 (1965).

⁴A. Snigirev, I. Snigireva, V. Kohn, S. Kuznetsov, and I. Schelokov, *Rev. Sci. Instrum.* **66**, 5486 (1995).

⁵S. W. Wilkins, T. E. Gureyev, D. Gao, A. Pogany, and A. W. Stevenson, *Nature (London)* **384**, 335 (1996).

⁶A. Momose, T. Takeda, and Y. Itai, *Rev. Sci. Instrum.* **66**, 1434 (1995).

⁷U. Bonse and F. Busch, *Prog. Biophys. Mol. Biol.* **65**, 133 (1996).

⁸F. A. Dilmanian, Z. Zhong, B. Ren, X. Y. Wu, L. D. Chapman, I. Orion, and W. C. Thomlinson, *Phys. Med. Biol.* **45**, 933 (2000).

⁹K. M. Pavlov, C. M. Kewish, J. R. Davis, and M. J. Morgan, *J. Phys. D* **34**, A168 (2001).

¹⁰C. Raven, A. Snigirev, I. Snigireva, P. Spanne, A. Souvorov, and V. Kohn, *Appl. Phys. Lett.* **69**, 1826 (1996).

¹¹P. Cloetens, M. Pateyron-Salome, J. Y. Buffiere, G. Peix, J. Baruchel, F. Peyrin, and M. Schlenker, *J. Appl. Phys.* **81**, 5878 (1997).

¹²S. C. Mayo, T. J. Davis, T. E. Gureyev, P. R. Miller, D. Paganin, A. Pogany, A. W. Stevenson, and S. W. Wilkins, *Opt. Express* **11**, 2289 (2003).

¹³G. Gbur and W. Wolf, *Opt. Lett.* **27**, 1890 (2002).

¹⁴M. A. Anastasio and D. Shi, *Proc. SPIE* **5535**, 361 (2004).

¹⁵A. V. Bronnikov, *Opt. Commun.* **171**, 239 (1999).

¹⁶A. V. Bronnikov, *J. Opt. Soc. Am. A* **19**, 472 (2002).

¹⁷A. Pogany, D. Gao, and S. W. Wilkins, *Rev. Sci. Instrum.* **68**, 2774 (1997).

¹⁸D. Paganin, S. C. Mayo, T. E. Gureyev, P. R. Miller, and S. W. Wilkins, *J. Microsc.* **206**, 33 (2002).

¹⁹T. E. Gureyev, Ya. I. Nesterets, D. M. Paganin, A. Pogany, and S. W. Wilkins, *Opt. Commun.* **259**, 569 (2006).

²⁰<http://physics.nist.gov/PhysRefData/FFast/Text/cover.html>

²¹X. Wu and H. Liu, *J. X-Ray Sci. Technol.* **12**, 273 (2004).

²²T. E. Gureyev, A. Pogany, D. Paganin, and S. W. Wilkins, *Opt. Commun.* **231**, 53 (2004).

²³M. R. Teague, *J. Opt. Soc. Am.* **73**, 1434 (1983).

²⁴T. E. Gureyev, A. W. Stevenson, D. M. Paganin, T. Weitkamp, A. Snigirev, I. Snigireva, and S. W. Wilkins, *J. Synchrotron Radiat.* **9**, 148 (2002).

²⁵L. D. Turner, B. B. Dhal, J. P. Hayes, A. P. Mancuso, K. A. Nugent, D. Paterson, R. E. Scholten, C. Q. Tran, and A. G. Peele, *Opt. Express* **12**, 2960 (2004).

²⁶T. E. Gureyev, T. J. Davis, A. Pogany, S. C. Mayo, and S. W. Wilkins, *Appl. Opt.* **43**, 2418 (2004).