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Single-step absorption and phase retrieval with polychromatic x-rays using a spectral detector

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Abstract

In this letter we present a single-step method to simultaneously retrieve x-ray absorption and phase images valid for a broad range of imaging energies and material properties. Our method relies on the availability of spectrally resolved intensity measurements, which is now possible using semiconductor x-ray photon counting detectors. The new retrieval method is derived and presented with results showing good agreement.

X-ray phase imaging has been of interest in the last couple of decades for potential applications in medical imaging and material characterization [1]. A key aspect in phase imaging is the well known “phase problem” which involves detangling the absorption and phase effects from intensity measurements [2]. The most researched methods of x-ray phase imaging are the interferometry-based setups that use elaborate x-ray optics (like multiple gratings or an analyzer crystal) for phase measurements [3,4]. Simplest of the existing phase contrast imaging methods is the in-line phase propagation method which utilizes development of interference patterns at longer sample-to-detector distances when using an x-ray source with a sufficiently large lateral coherence [5, 6]. This method does not require any x-ray optics in the beam path, however typically requires at least two measurements to detangle absorption and phase information from intensity measurements. Such data acquisition schemes involving multiple x-ray exposures are not practical if adaptation to a clinical setting is desired where the speed of acquisition and/or radiation dose is a major concern.

A number of methods were investigated to facilitate phase retrieval from a single x-ray exposure [7–12]. A majority of these methods are valid for only weak phase objects or for small objects with negligible absorption and have very low sensitivity. A notable effort is by Wu et al. [11] where the concept of “phase-attenuation duality” was introduced which is applicable to x-ray energies of 60 – 500 keV that are high enough to neglect the effects related with the photoelectric effect (PE). Although their method can retrieve the phase distribution accurately, it does not provide any absorption contrast which in principle yields the variations in atomic number composition and is considered the current gold standard in radiology. This method is also susceptible to yield poor phase retrieval accuracy when materials of high atomic number (high x-ray absorption) are present in the object. Another promising method for simultaneous retrieval of absorption and phase is by using x-ray energies of 1–20 keV where the PE effects dominate [12,13]. Their approach for phase retrieval is simplified by neglecting the contribution of Compton scattering (CS) in the model for object plane intensity. While this approach is reasonable for imaging energies of few keVs (and hence practical for imaging small samples that require only low penetration),

it fails for medically relevant x-ray imaging energies where CS contributions are significant. In this letter, we bridge the gap between these two methods by proposing a single-step method for simultaneous retrieval of absorption and phase images. This method is valid for a broad range of x-ray imaging energies (1 – 500 keV) and material properties.

Recent advances in x-ray photon counting detectors (XPCD) have provided a new momentum to research in the area of spectral detection and enabled implementations in both biomedical and material imaging [14]. Potential advantages of XPCDs, compared to the energy integrating scintillating detectors (conventionally used in modern radiography) are electronic noise rejection and their energy-resolving capabilities. The latter can be utilized by setting appropriate energy thresholds so that the incoming photons are sorted out into bins based on their energies. In this letter, we first develop the essential mathematical framework and present the solution for the phase problem. Then we demonstrate the applicability of the method by simulating a clinically relevant setup with a microfocus x-ray source and using a currently available XPCD.

Non-interferometric phase retrieval can be achieved by finding solutions of the so-called transport of intensity equation (TIE) which relates the propagation of intensity distribution with the phase distribution of a wave in the paraxial approximation [15]. Assuming slowly-varying intensity distributions on the detector plane, the simplified TIE for a cone-beam (source with sufficient lateral coherence) setup can be written as follows,

$$I_R(E) = \frac{I_{R_1}(E)}{M^2} \left(1 + \frac{R_2}{Mk(E)} \nabla^2 \phi(E) \right) \quad (1)$$

where $\phi(E)$ is the phase of the x-ray wave with wavenumber $k(E)$, $I_{R_1}(E)$ is the intensity at object plane (at distance R_1 from the source) and $I_R(E)$ is the intensity at detector plane (at distance R_2 from the object plane) for x-ray energy E and $R = R_1 + R_2$. $M = R/R_1$ is the magnification factor for the image on detector plane. ∇^2 represents the two-dimensional Laplacian defined on the detector plane. The intensity distribution on object plane can be expressed in terms of the line integrals of x-ray attenuation along the x-ray path,

$$I_{R_1}(E) = I_{in}(E) \exp \left(- \int \mu(E) d\ell \right) \quad (2)$$

with $\mu(E)$ as the linear attenuation coefficient distribution of the object and $I_{in}(E)$ as the incident intensity. Integration limits for $d\ell$ are from 0 to the detector coordinate. After combining equation 1 and 2, and using an approximation of Rytov-type [16] which is valid for weakly scattering objects, we get an expression of the form,

$$-\log \left(\frac{M^2 I_R(E)}{I_{in}(E)} \right) = \int \mu(E) d\ell + \frac{R_2}{Mk(E)} \nabla^2 \phi(E) \quad (3)$$

with left hand side as the flat-field corrected data term. Note that the right hand side consists of the two unknown functions $\mu(E)$ and $\phi(E)$. Thus, even using multiple-energy measurements, a unique solution for the projected $\mu(E)$ and $\phi(E)$ is not feasible at this step, because, $\phi(E)$ has a non-linear energy dependence unlike $\mu(E)$ and is unknown prior to measurements. To overcome this problem, we express the unknowns in terms of energy independent material quantities, i.e., the effective atomic number Z and the electron density ρ_e . This can be achieved by decomposing the attenuation coefficients into absorption and scattering components [17],

$$\mu(E) = NK \frac{Z^5}{e^3(E)} + NZ\sigma_{KN}(E) \quad (4)$$

where the first and second terms on the right hand side correspond respectively to the PE and CS contributions to the total attenuation. This technique is well-studied in material/basis decomposition methods when multiple energy data are available. In equation 4, N is the concentration, K is a dimensionless constant, $\alpha(E)$ is the normalized energy of the incident radiation with respect to that of a single electron and $\sigma_{KN}(E)$ is the crosssection of an electron that can be computed based on the Klein-Nishina equation [18]. Phase, on the other hand, is linearly proportional with the projected electron density ρ_e and can be expressed as,

$$\phi(E) = -\frac{2\pi r_e}{k(E)} \int \rho_e d\ell \quad (5)$$

with r_e as the classical electron radius. By substituting equation 4 and 5 into 3, we finally arrive at the following expression of the form,

$$-\log\left(\frac{M^2 I_R(E)}{I_{in}(E)}\right) = \frac{K}{e^3(E)} a_1 + \left(\sigma_{KN}(E) + \frac{2\pi r_e R_2}{Mk^2(E)} \nabla^2\right) a_2 \quad (6)$$

where a_1 and a_2 are the energy independent unknown projections defined as:

$$a_1 = \int \rho_e Z^4 d\ell \quad a_2 = \int \rho_e d\ell \quad (7)$$

Intensity measurements at two energies provide sufficient data to retrieve the two unknown projected quantities, a_1 and a_2 , from the set of two linear equations based on expression 6. From a_1 and a_2 , the absorption and phase images can be obtained according to expression 5 and the first term on the right hand side of expression 6, respectively. While this retrieval method can produce reasonably accurate results with simply two energy bins, in the simulation model described below, we will briefly discuss the benefits of using XPCDs with multiple-energy bins and a noise regularization strategy.

Let us consider a XPCD which registers detected photons to N different energy bins (B_i : $i=1, \dots, N$) according to their energy. Then, expression 6 can be approximated as,

$$-\log\left(\frac{M^2 [I_R(E)]_{B_i}}{[I_{in}(E)]_{B_i}}\right) = \frac{K}{e^3(\tilde{B}_i)} a_1 + \left(\sigma_{KN}(\tilde{B}_i) + \frac{2\pi r_e R_2}{Mk^2(\tilde{B}_i)} \nabla^2\right) a_2, \quad i=1, \dots, N \quad (8)$$

with $[I(E)]_{B_i}$ representing the measured intensity corresponding to x-ray photons of energy within bin B_i and $\tilde{B}_i$ representing the photon energy corresponding to the median of the photon counts in that bin. Equation 8 can easily be expressed using the matrix notation: $D = GA$ where A is the solution vector, D is the data vector, G is the matrix consisting of the energy dependent coefficients. Increasing the number of energy bins results in a larger number of spectrally resolved data, leading to an improved accuracy in the retrieval solutions. However, more bins with narrower energy windows imply a small number of photons to be detected in each bin and in turn deteriorates the signal-to-noise ratio (SNR). Thus, a regularization strategy to consider the unequal distribution of noise within the bins is necessary for stable solutions. We used weighted least-square method applied in Fourier domain to obtain the solutions:

$$A = (G^T W G)^{-1} G^T W D \quad (9)$$

where W is the weighting matrix constructed according to the SNR of the detected x-ray quanta in each energy bin:

$$W = \text{diag} \left[\frac{S_1}{\sigma_1}, \dots, \frac{S_i}{\sigma_i} \right], \quad i=1, \dots, N \quad (10)$$

with S_i is the total counts at bin i and $\sigma_i^2 = S_i$ is the corresponding noise variance.

We numerically tested the method using a clinically relevant cone-beam setup with a microfocus x-ray source having a 20 μm focal-spot size. R_1 and R_2 were both selected as 1 m. We modeled a 120 kVp tungsten anode spectrum discretized in 1 keV steps. The detector pixel size was 55 μm and the detector quantum efficiency was computed for a 300 μm thick cadmium-zinc-telluride detection layer. The modeled system had eight energy bins, separated by the thresholds at 29, 35, 40, 45, 51, 58 and 66 keV. The phantom consists of six kinds of different standard materials: aluminum (Al), alumina (Al_2O_3), hydroxylapatite (HA), polytetrafluoroethylene (PTFE), polyoxymethylene (POM) and polymethylmethacrylate (PMMA). The respective diameters of the materials were 0.14, 0.12, 0.03–0.06, 0.2, 0.4 and 0.27 mm. The first three represents strongly absorbing materials and the last three represents weakly absorbing materials. The material properties, cross sections, and atomic form factors were calculated according to the values taken from NIST database [19].

The resultant retrieved values of absorption (PE) and phase are given in figure 1 together with the calculated true values. The retrieved phase image contains grainy artifacts, which is typical due to the low-pass filtering property of the inverse Laplacian operator. A detailed analysis was conducted by calculating the relative errors (RE) of the retrieved values with respect to the true values (i. e. $\delta x = 1 - x^{\text{ret}}/x^{\text{true}}$). Figure 2 demonstrates the calculated errors obtained for each material by averaging the REs over the associated circular regions. The retrieved absorption values of weakly absorbing materials are slightly underestimated with relative errors about 0.15–0.2. We found that the retrieval errors can originate from the inaccuracies in modeling of the PE absorption term, particularly arising at low-energies. Therefore, the energy dependence term, i. e., $1/e^3$ factor in expression 4, could be tuned appropriately for objects of very high or very low absorption contrast for improved accuracy.

In summary, we developed a single-step noninterferometric method for simultaneous x-ray phase and absorption retrieval. We showed the applicability of this method using XPCDs for clinically representative dose levels and for various types of materials. Due to simplicity and applicability to a wide range of imaging energies and material compositions, this method has the potential for applications in medical imaging and material sciences. Since this method is single-step and involves no x-ray optics and detector motion, it is ideally suitable for tomographic imaging of other related physical quantities such as the complex refractive index, effective atomic number and/or electron density map in the object.

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Fig. 1. Retrieved values of the (a) absorption and (b) phase images at 35 keV. The true values of (c) absorption [cm^{-1}] and (d) phase [rad] images at 35 keV.

Fig. 2.
The relative errors of retrieved absorption and phase distribution of each material with respect to the true values.