A unified statistical framework for material decomposition using multienergy photon counting x-ray detectors

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Purpose: Material decomposition using multienergy photon counting x-ray detectors (PCXD) has been an active research area over the past few years. Even with some success, the problem of optimal energy selection and three material decomposition including malignant tissue is still on going research topic, and more systematic studies are required. This paper aims to address this in a unified statistical framework in a mammographic environment.

Methods: A unified statistical framework for energy level optimization and decomposition of three materials is proposed. In particular, an energy level optimization algorithm is derived using the theory of the minimum variance unbiased estimator, and an iterative algorithm is proposed for material composition as well as system parameter estimation under the unified statistical estimation framework. To verify the performance of the proposed algorithm, the authors performed simulation studies as well as real experiments using physical breast phantom and ex vivo breast specimen. Quantitative comparisons using various performance measures were conducted, and qualitative performance evaluations for ex vivo breast specimen were also performed by comparing the ground-truth malignant tissue areas identified by radiologists.

Results: Both simulation and real experiments confirmed that the optimized energy bins by the proposed method allow better material decomposition quality. Moreover, for the specimen thickness estimation errors up to 2 mm, the proposed method provides good reconstruction results in both simulation and real ex vivo breast phantom experiments compared to existing methods.

Conclusions: The proposed statistical framework of PCXD has been successfully applied for the energy optimization and decomposition of three material in a mammographic environment. Experimental results using the physical breast phantom and ex vivo specimen support the practicality of the proposed algorithm. © 2013 American Association of Physicists in Medicine.

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Key words: material decomposition, energy-level optimization, mammography, statistical analysis

1. INTRODUCTION

Breast cancer is one of the most common cancers in women, and the second leading cause of death among female cancers. However, since it has over a 98% five-year survival rate with early diagnosis,1 its early detection is essential. In particular, the detection of malignant tissues, such as calcifications or carcinomas, is important in the early stage diagnosis of breast cancer.2–4 To distinguish malignant tissues from the physiological structures of normal breasts, a material decomposition approach has been studied. In particular, injected contrast media has been used to detect cancerous tissues.3–5 However, the injection of contrast media can cause a patient inconvenience and motion artifacts due to the multiple measurements required for pre- and postinjection. Moreover, it is well known that contrast media can cause allergic reactions in some patients.6,7

Recently, material decomposition techniques using multienergy x-ray sources or detectors have been demonstrated without contrast media in spectral computed tomography (CT) (Refs. 8–11) and mammography.5,12–16 In most spectral CT applications, a material decomposition method is applied in the reconstructed image domain,8–10 where each image domain pixel can be decomposed into a single material,10 or two or more materials.17–20 In the projection domain, the decomposition methods of two materials have been demonstrated by assuming that the x-ray attenuation coefficient is composed of two bases, namely, photo-electric absorption and Compton scattering.13,21,22 Then, the so-called tissue cancellation method removes the coefficients corresponding one of those two bases as a weighted sum of two different energy measurements.13,22 Other material decomposition of two components has been also successfully demonstrated in mammography in terms of glandular ratio.23–25 Dual energy approach has been also successfully demonstrated for contrast enhanced imaging applications to overcome the motion artifacts, since dual energy material decomposition method can eliminates the necessity of subtraction of a precontrast image.
Decomposition of three materials without contrast agent has been recently attempted in dual energy mammography. Laidevant et al. decomposed a mammography image into water, lipid, and protein based on a previously proposed inverse mapping method assuming that the total object thickness is known. More specifically, inverse mapping methods represent the unknown parameters such as the thickness of material or the ratio between compositions as a polynomial function with respect to dual energy measurements in the sinogram domain. The coefficients of the polynomial are then calculated using the measurements of calibration blocks whose length and material compositions are known. In Laidevant et al., at least 20 calibration blocks are required due to the large number of parameters in quadratic or cubic polynomial fitting. Another inverse mapping method suggested by Kappadath et al. estimated the locations of calcification and the glandular-adipose ratio from dual energy measurements, however, the optimal energy selection or hardware imperfection compensation were not discussed in these approaches. While energy optimization methods have been proposed for dual energy mammography, to our best knowledge we are not aware of any existing works that address the optimal energy selection and three material decomposition in a unified framework.

In this research, we aim to decompose three materials, including carcinoma, using energy resolving photon counting x-ray detectors (PCXD) in mammographic environments. Unlike the conventional approaches, we formulated the material decomposition problem in a statistical estimation framework based on the assumption that the PCXD measurement follows Poisson statistics. The main advantage of this framework is that the problems of the optimal energy selection, system calibration, and material decomposition can be formulated by a unified estimation framework. Furthermore, using calibration phantoms, system imperfection correction can be converted to an attenuation coefficient estimation problem. Under the optimized energy level and attenuation coefficient parameters, the final material decomposition problem can be solved using a convex optimization problem with a positivity constraint.

This paper is organized as follows. Section 2 describes the proposed statistical framework for PCXD measurements and derives an energy optimization method. Then, attenuation coefficient estimation and a material decomposition algorithm are developed in Sec. 3. Methods for experiments are described in Sec. 4, and experimental results are presented in detail in Sec. 5, which is followed by discussion in Sec. 6 and the conclusion in Sec. 7.

2. STATISTICAL FRAMEWORK FOR MATERIAL DECOMPOSITION

2.A. Measurement model

Energy discriminating PCXD simultaneously acquires multienergy measurements by counting the number of photons corresponding to each energy bin in contrast to conventional photon integrating detectors that measure all signals during a time interval. Thanks to the energy discrimination threshold, a great deal of electronic noise can be effectively removed in PCXD. Therefore, a Poisson distribution can be assumed for detector measurements.

Since each PCXD energy bin independently counts the number of photons, the probability density function (pdf) for the measurement $d = [d_1, \ldots, d_M]^T$ is

$$f(d|t) = \prod_{i=1}^{M} \frac{d_i!}{\lambda_i} \exp\left(-\lambda_i\right),$$  \hspace{1cm} (1)$$

where $\lambda_i$ is the expected mean and variance of the $i$th energy bin, and $M$ is the total number of energy bins. For further simplification, the inverse log of normalized intensity is approximated as a linear combination of attenuation coefficients of basis material

$$-\ln \frac{\lambda_i}{I_i} \approx \mathbf{A}^t \mathbf{c} + b_i,$$  \hspace{1cm} (2)$$

where $\mathbf{A}^i$ is the $i$th row of matrix $\mathbf{A}$, representing the effective attenuation coefficients of basis material for the $i$th energy bin, and $b_i$ refers to an offset for the linear approximation of polychromatic measurement, which is originally nonlinear. The meaning of the effective attenuation coefficient will be further discussed later. Here, $I_i$ is the nominal number of photons corresponding to the $i$th energy bin and $t = [t_1, \ldots, t_K]^T$ refers to the thickness of $K$ basis material in projection. Using Eq. (2), the log-likelihood function for Eq. (1) can be approximated as

$$L(t | d) = \ln f(d | t) \approx \sum_{i=1}^{M} \left\{ d_i (-\mathbf{A}^t \mathbf{c} - b_i + \ln I_i) - I_i \exp(-\mathbf{A}^t \mathbf{c} - b_i) - \ln d_i! \right\},$$  \hspace{1cm} (3)$$

If it is assumed that the measurement $d_i$ is close enough to $\lambda_i$ such that $d_i \approx \lambda_i$, then a second order Taylor series with respect to $p_i = \mathbf{A}^t \mathbf{c} = -\ln \lambda_i - b_i + \ln I_i$ can be applied around $\hat{p}_i = -\ln d_i - b_i + \ln I_i$. Then, the log-likelihood can be given by

$$L(t | d) \approx \sum_{i=1}^{M} \left\{ d_i \ln d_i - d_i - \ln d_i! - \frac{1}{2} d_i^2 (\mathbf{A}^t \mathbf{c} + \ln I_i - b_i)^2 \right\} = -\frac{1}{2} (y - \mathbf{At} - \mathbf{b})^T \mathbf{A} (y - \mathbf{At} - \mathbf{b}) + c(d),$$  \hspace{1cm} (4)$$

where $y_i = -\ln(d_i/I_i)$, $\mathbf{A} = \text{diag}(d)$, and $c(d)$ is a function of $d$.

2.B. Energy level optimization

In previous research, x-ray dose or material contrast is used to evaluate the energy level optimality in dual source x-ray. For the case of PCXD measurement in material decomposition, Wang and Pelc proposed an optimal energy
weight using sufficient statistics. However, arbitrary control of energy weighting is generally difficult in practice. Hence, we propose a method to determine the optimal energy bin thresholds for PCXD based on the statistical framework derived in Sec. 2.A. Specifically, an energy optimization is derived based on the minimum variance unbiased (MVU) estimator of the unknown materials’ thicknesses. More specifically, with the log-likelihood approximation in Eq. (4), the approximated pdf is in the form of a multivariate Gaussian distribution:

\[ f(d|t) \propto \exp \left( -\frac{1}{2} (y - At - b)^T \Lambda (y - At - b) \right), \tag{5} \]

where the mean of \( y \) is \( At + b \) and its covariance matrix is \( \Lambda^{-1} \). In particular, this pdf can be divided into terms that are dependent and independent to the material thickness variable \( t \) as \( f(d|t) \propto h(d)g(T(d)|t) \), where

\[ h(d) = \exp \left( -\frac{1}{2} (y - b)^T \Lambda (y - b) \right), \]
\[ g(T(d)|t) = \exp \left( -\frac{1}{2} (At)^T \Lambda (At) \exp ((At)^T \Lambda (y - b)). \]

According to the factorization theorem, \( T(d) \) about \( t \) is

\[ T(d) = \Lambda^T \Lambda (y - b). \tag{6} \]

Assuming that approximation (5) is accurate, \( T(d) \) is a complete sufficient statistic since the pdf \( f(d|t) \) is a family of Gaussian distribution, which is well known as a complete distribution family.34

By maximizing the log-likelihood function \( L(t|d) \) given in Eq. (4), the maximum likelihood (ML) estimator \( \hat{t} \) is given by

\[ \hat{t} = (\Lambda^T \Lambda)^{-1} \Lambda^T \Lambda (y - b), \tag{7} \]

if and only if \( (\Lambda^T \Lambda) \) is invertible. Since this ML estimator is unbiased and is a function of a complete sufficient statistic \( T(d) \) of Eq. (6), the estimator \( \hat{t} \) in Eq. (7) is the MVU estimator of \( t \) by the Rao-Blackwell-Lehmann-Scheffe theorem.35 More specifically, the Rao-Blackwell-Lehmann-Scheffe theorem informs us that if an estimator \( \hat{t} \) is unbiased and can be represented by a function of a sufficient statistic, then the estimator is the MVU estimator. Since \( \hat{t} \) in Eq. (7) is given by \( (\Lambda^T \Lambda)^{-1} T(d) \) and is unbiased, it satisfies the conditions for the Rao-Blackwell-Lehmann-Scheffe theorem, so it is a MVU estimator. The implication of Eq. (7) being a MVU estimator is that the estimation error for material decomposition by any unbiased estimation algorithm is always lower-bounded by the variance of the MVU estimator, implying that the proposed decomposition method achieves the ultimate performance limit.

Although \( \hat{t} \) of Eq. (7) is the MVU estimator, its variance varies according to \( A \) and \( \Lambda \), which are determined by energy threshold selection; therefore, the optimal energy bin thresholds can be acquired by minimizing the lower bound of the variance of \( \hat{t} \). If the goal is the simultaneous error minimization for all materials, we need to optimize the average mean squared error (MSE) of \( \hat{t} \), which is given by

\[ \text{MSE} = E[(\hat{t} - t)^2] = E[\text{tr}(\hat{t} - t)(\hat{t} - t)^T] = \text{tr}[E((\hat{t} - t)(\hat{t} - t)^T)] = \text{tr}[\text{Cov}(\hat{t})] = \text{tr}(\Lambda^T \Lambda)^{-1}. \tag{8} \]

Therefore, the trace of a covariance matrix can be used as a metric to minimize in calculating the optimal energy levels. Note that the values of matrix \( \Lambda \) depend on the object compositions and total thickness. Accordingly, the object-specific optimal energy threshold may be acquired by comparing Eq. (8) for different parameters. (On the other hand, if we are interested in reducing the error variance from a particular material at the cost of sacrificing the average MSE across all materials, then we could use the specific diagonal component of the covariance matrix as a cost function.)

Here, it is important to discuss the physical meaning of minimizing Eq. (8). Assuming that the noise variance for selected energy bins is equal, the energy minimization is equivalent to minimizing \( \text{tr}(\Lambda^T \Lambda)^{-1} \). This implies that our optimal energy level selection criterion makes each column of \( \Lambda \) as independent as possible. Since each column of \( \Lambda \) represents the absorption coefficients’ variations according to the energy level for each material (say, malignant, glandular, or adipose tissue), the proposed optimal energy selection criterion selects the energy levels that exhibits more distinct energy dependent attenuation coefficient contrast between the materials. If the energy dependent noise variances are not equal, the proposed optimal energy selection takes the energy dependent noise variance into consideration during the optimization step.

3. MATERIAL DECOMPOSITION ALGORITHM

With an optimal energy level, our goal is to estimate the thickness of material compositions. From the likelihood function in Eq. (5), the cost function is given by

\[ C(A, b, t) = (y - At - b)^T \Lambda (y - At - b), \tag{9} \]

and \( C(A, b, t) \) needs to be minimized with respect to \( A, b, \) and \( t \). Since this optimization problem is highly nonconvex with respect to \( A, b, \) and \( t \), we employ calibration blocks with known thickness \( \{t_b\}_{b=1}^B \) to convexify the problem. More specifically, we first minimize the cost function for the calibration blocks via

\[ \tilde{C}(A, b) = \sum_{b=1}^B (y_b - At_b - b)^T \Lambda_b (y_b - At_b - b), \tag{10} \]

where \( y_b \) denotes the \( b \)th calibration phantom sinogram measurement and \( \Lambda_b \) is a diagonal matrix composed by measurement \( d_b \) in the intensity domain, i.e., \( \Lambda_b = \text{diag}(d_b) \). Such calibration blocks are useful in practice since the attenuation coefficient can differ from numerically calculated values. This may be due to the detector response function, pulse pileup, etc., that can change the detector readings.36,37 Hence, the attenuation coefficient estimation using a calibration block with known lengths can compensate for those imperfections. Note that Eq. (10) is a convex optimization problem with respect to
First, the attenuation coefficient matrix is estimated by minimizing the cost function (10) with respect to Λ and b. Since the optimization problem is quadratic with respect to the columns of Λ = [a₁, ..., aₖ] and b, a standard optimization technique can be applied. Specifically, by computing the derivatives of Eq. (10) for aₖ, the ₖth column of Λ, and b, (K+1) linear equations of the optimal attenuation coefficient columns aₖ and b can be obtained such that

\[
\frac{\partial}{\partial a_k} \tilde{C}(\Lambda, b) = -2 \sum_{b=1}^{B} (\Lambda_{b}\hat{y}_{b,k} - \Lambda_{b}At_{b,k}) = 0, \quad k = 1, 2, \ldots, K, \\
\frac{\partial}{\partial b} \tilde{C}(\Lambda, b) = -2 \sum_{b=1}^{B} (\Lambda_{b}(y_{b} - At_{b}) - \Lambda_{b}b) = 0. \quad (11)
\]

Equations (11) are rearranged in the summation form of aₖ and b as

\[
\sum_{l=1}^{K} \left( \sum_{b=1}^{B} \Lambda_{b}t_{b,l,k} \right) a_t + \sum_{b=1}^{B} \Lambda_{b}b_t = \sum_{b=1}^{B} a_t y_{b_t} \quad (12)
\]

Note that Eqs. (12) can be represented in the form of Mx = Z, where x is vectorized optimal attenuation coefficients, x = [a₁ᵗ, ..., aₖᵗ, bᵗ]ᵗ, and M and Z are matrices composed of A, t, and y. Therefore, the optimal A and b are estimated by rearrangement of M⁻¹Z.

An exemplary estimation of an attenuation coefficient matrix using calibration block measurements is shown in Fig. 1 with comparison to numerical (theoretical) calculation before calibration and real measurements. Recall that a practical PCXD has physical limitations such as detector response, pulse pileup. The pileup occurs where independent events injected with short time intervals are considered as a single event due to the limited count rate of PCXD. This changes the energy level of injected photons as well as the measured number of photons at the detector, as shown in...

**FIG. 1.** Comparison of actual sinogram domain measurements, theoretic prediction (numerical calculation) before calibration, and estimation results using calibration blocks at (a) 10–25 keV and (b) 34–49 keV. Here, (M) and (A) represent muscle and adipose, respectively. (c) Physical mechanism of peak and tail pile-up in PCXD explaining the mismatch between the measurement and theoretical prediction before calibration. Due to the pile-ups, more photons are detected at lower energy bins, which makes the sinogram values lower than the theoretical prediction in 10–25 keV energy bins.
Fig. 1(c). More specifically, due to the peak- and tail-pileup, PCXD counts relatively more photons on lower energy levels, while less photons are counted on higher energy levels. As real sinogram values are calculated by the inverse log of normalized intensity, their values can be lower than the theoretical calculation at low energy levels before calibration, and vice versa in high energy levels, as shown in Fig. 1. However, Fig. 1 shows that, after the calibration, the real measurement values can be accurately reproduced.

### 3.B. Material decomposition algorithm

Here, the proposed material decomposition method is now explained. Based on the statistical model Eq. (4), the optimization problem for \( t \) is given as

\[
\min_{t \geq 0} (y - At - b)^T A (y - At - b),
\]

(13)

where attenuation coefficients \( A \) and offset \( b \) are estimated by Eq. (10), and the positivity of \( t \) was imposed, as thickness cannot be negative. Then, the physical meaning of our material decomposition algorithm is to find the material compositions that fit the noisy measurement as closely as possible by considering noise statistics.

Note that the optimization problem (13) is convex and any optimization algorithm may converge to a global minimizer. However, \((A^T A)\) may have a very large condition number, especially when similar attenuation curves exist between tissue bases due to the lack of sufficient contrast. In such cases, the convergence rate is dependent on the choice of initialization as well as the optimization algorithm. In particular, for some iterative type algorithms, a good initial guess can accelerate the convergence speed significantly, while with a bad initial guess, the value will hardly be updated and it is difficult to converge to the global minimum in this type of ill-posed inverse problem. This is particularly true for iterative coordinate descent (ICD),\(^{39}\) which was employed here thanks to its versatility of exploiting a positivity constraint. Therefore, as will be discussed later, a specific initialization method is provided to accelerate the convergence.

If the total thickness of target object \( T \) is known, the thickness of the \( K \)th material can be expressed using the thicknesses of other materials as \( t_K = T - \sum_{k=1}^{K-1} t_k \). Therefore, in Eq. (5), the mean of \( y \) can be modified as

\[
At + b = \sum_{k=1}^{K-1} a_k t_k + a_K \left( T - \sum_{k=1}^{K-1} t_k \right) + b.
\]

(14)

Based on this, the MVU estimator of \( t \) derived in Eq. (7) can be redefined for the remaining \((K-1)\) basis material \( \hat{t} = [t_1, \ldots, t_{K-1}]^T \) as

\[
\hat{t} = (\hat{A}^T \hat{A})^{-1} \hat{A}^T \hat{A} (\hat{y} - b),
\]

(15)

where \( \hat{y} = y - a_K T \), and the matrix \( \hat{A} \) is composed of attenuation coefficient differences \( \hat{a}_k = a_k - a_K \).

In the following, detailed description of each step of the proposed material decomposition algorithm will be provided.

#### Step 1: Initial material decomposition using matching pursuit (MP)

To accelerate the convergence, the following initialization is used. To improve the decomposition accuracy of basis material, decomposed components are assumed to be sparse in each material basis at each position. Then, an image corresponding to each material is extracted one by one using MP that recursively finds the dominant bases of signals by correlating them with the residuals from the previous iteration in a greedy manner.\(^{30,\,41}\)

Suppose that the actual measurements are in the form of a matrix whose columns correspond to multienergy measurement at each detector pixel: i.e., \( Y = [y_1, \ldots, y_N] \), where \( y_i \) refers to the measurement of the \( i \)th pixel and \( N \) is the number of total detector pixels. Then, for the selection of dominant bases, the most correlated base with the residual at all the detector pixel measurements is found at each iteration. More specifically, let the initial residual \( R_0 = Y \). Then, the dominant basis \( a_{kp} \) at the \( p \)th iteration is determined by finding the most closely aligned basis with the residual at the \((p-1)\)-th iteration, denoted as \( R_{p-1} \) among \( k_p \not\in J_{p-1} \), where \( J_{p-1} \) denotes the set of indices selected up to the \((p-1)\)-th iteration.

The dominant basis \( a_{kp} \) minimizes

\[
\| P_{a_{kp}} R_{p-1} \|_F^2 = \text{tr} \left\{ R_{p-1}^T P_{a_{kp}} R_{p-1} \right\}
\]

\[
= \| R_{p-1} \|_F^2 - \text{tr} \left\{ R_{p-1}^T P_{a_{kp}} R_{p-1} \right\},
\]

(16)

where \( P_{a_{kp}} \) refers the orthogonal complement of projection defined as

\[
P_{a_{kp}} = I - P_{a_{kp}} = I - a_{kp} (a_{kp}^T a_{kp})^{-1} a_{kp}^T.
\]

Therefore, the index of dominant basis \( a_{kp} \) is acquired by

\[
k_p = \arg \max_{k \not\in J_{p-1}} \frac{1}{\alpha} \| a_{kp}^T R_{p-1} \|_2^2,
\]

(18)

where \( \alpha = a_{kp}^T a_{kp} \). Then, the residual of the \( p \)th iteration and index set are updated as \( R_p = P_{a_{kp}} R_{p-1} \), and \( J_p = J_{p-1} \cup \{k_p\} \).

For the selected dominant basis, the estimator of material thickness is acquired using Eq. (15) as

\[
t_{kp} = (a_{kp}^T a_{kp})^{-1} a_{kp}^T A (\hat{y} - b),
\]

(19)

for each pixel. In the initialization stage, we just need an approximate estimate; so if Eq. (19) provides a negative thickness, it is replaced by zero. More rigorous convex optimization with positivity constraint is performed later in the refinement stage.

If the total thickness \( T \) is known, the aforementioned initialization procedure can be simplified by searching for \( \hat{a}_K = a_K - a_K \), where \( a_K \) denotes the attenuation coefficients of the \( K \)th material. Figure 2 illustrates this initialization procedure.

#### Step 2: Refinement with ICD method

As described above, the optimal \( t \) is acquired by solving

\[
\min_{t \geq 0} (y - At - b)^T A (y - At - b),
\]

(20)
Fig. 2. Initialization of material decomposition algorithm using matching pursuit. Here, $K = 3$ and the total material thickness $T$ is known.

4. METHOD

To verify the proposed algorithm, numerical simulations were first conducted using virtual breast phantoms. Then, real experiments were performed using a physical breast phantom as well as ex vivo specimens.

4.A. Simulation environment

In the simulation, 600 $\times$ 600 detector pixels with 0.1 $\times$ 0.1 mm$^2$ resolution were used. The distance between the source to the detector was set to 660 mm, and the object was assumed to be located on top of the detector. In the simulated data, a virtual 3D breast phantom was used that was composed of 500 $\times$ 400 voxels in the spatial domain with 3 or 5 cm thickness with 0.1 $\times$ 0.1 $\times$ 0.1 mm$^3$ voxel resolution. The phantom was composed of 50% glandular and 50% adipose tissue. Although real breasts are reported to have more adipose tissue than glandular tissue, it is often difficult to find the universally correct composition across all subjects; so, in this paper, we simply assume that a breast tissue is composed by 50% of glandular and 50% of adipose tissue, and we performed experiments under this assumption.

To evaluate the material decomposition quality under inhomogeneous backgrounds, different patterns of glandular and adipose tissue mixture were used as shown in Figs. 3(a) and 3(b). In our virtual phantom, 1-cm thickness muscle blocks were inserted to represent malignant tissues in a breast. More specifically, as shown in Fig. 3(a), six 1-cm thickness muscle blocks were inserted with various diameters as 8, 6, 4, 3, 2, and 1 mm. The resulting slab was put at the bottom, and background slabs were overlaid as shown in Fig. 3(b). To be consistent with real physical phantom experiments, we use the attenuation curves provided by a physical phantom manufactured company, CIRS, Inc. (Norfolk, VA). The attenuation coefficients used for simulation are shown in Table I for several representative keV levels. Note that the reason for using muscle basis instead of carcinoma basis is because their...
The linear attenuation coefficients are very similar as shown in Table I and accordingly we intend to recovery both of them in a same basis.

Monochromatic x-ray measurements were calculated at every 0.5 keV, and polychromatic measurements were synthesized by a weighted sum of monochromatic measurements using the simulated x-ray tube spectrum. X-ray spectrum is generated using Spektr, which was developed based on Boone’s work. To generate a synthetic x-ray spectrum that is consistent with the real system environments, a tungsten anode was assumed, 49 kVp voltage was applied, and Be 0.7 and Ag 0.03 mm filters were used.

For an accurate interpolation of attenuation coefficients at every 0.5 keV interval, an exponential relationship between energy and attenuation coefficient was exploited. An exponential fitting curve is given as in form of

\[
\left( \frac{\mu}{\rho} \right) = \kappa E^\beta,
\]

which is especially useful for mammography using a low energy x-ray, as the attenuation curve significantly changes in these regions. In Eq. (23), the parameters of \(\kappa\) and \(\beta\) were easily solved using the attenuation coefficients at two different energy levels of \(E_1\) and \(E_2\) as

\[
\beta = \frac{\ln \left( \frac{\mu}{\rho} \right)_2 - \ln \left( \frac{\mu}{\rho} \right)_1}{\ln E_2 - \ln E_1},
\]

\[
\kappa = \frac{\ln \left( \frac{\mu}{\rho} \right)_1 \ln E_2 - \ln \left( \frac{\mu}{\rho} \right)_2 \ln E_1}{\ln E_2 - \ln E_1},
\]

where \(\left( \frac{\mu}{\rho} \right)_1\) and \(\left( \frac{\mu}{\rho} \right)_2\) are corresponding attenuation coefficients of \(E_1\) and \(E_2\), respectively. For a realistic simulation, Poisson noises were added into the synthesized measurement images. The signal-to-noise ratio (SNR) was set to 40 dB in the intensity domain. The SNR was computed as

\[
\text{SNR}(\text{dB}) = 10 \log_{10} \frac{\|d_0\|^2}{\|d - d_0\|^2},
\]

where \(d_0\) and \(d\) refer a noiseless image and a noisy image in the intensity domain, respectively. The 40 dB SNR value in simulation was determined considering the specification of our real system that has 45 dB of SNR for a 10–25 keV energy bin under 49 kVp with an 8 mAs dose.

### 4.B. Real system environment

For real experiments, a customized energy resolving PCXD was developed. The detector is composed of four-line detector blocks with 256 Si pixel detectors per block. The detector pixel has 95 × 100 \(\mu\)m resolution and 5.75 mm thickness with edge-on geometry. Since we used line detectors that had gaps between the lines, real experimental data often exhibit some straight line discontinuity in the measurement, which is one of the limitations of the current hardware system. For x-ray generation, a tungsten anode was used with 49 kVp and 20 mA. The x-ray tube inherently includes a Be 0.7 mm filter, and an Ag 0.03 mm filter was added as well. A schematic image of our PCXD system is shown in Fig. 3(c). In this system, the shelf with an object is moving in the direction of the arrow, while the source and line detector are fixed.

### Table I. Linear attenuation coefficients and mass densities of tissues used in the virtual and physical phantoms.

The values are from a document supplied by the manufacturer of the physical phantom, CIRS Inc.

<table>
<thead>
<tr>
<th>Linear attenuation coefficients (cm(^{-1}))</th>
<th>10 keV</th>
<th>20 keV</th>
<th>30 keV</th>
<th>40 keV</th>
<th>60 keV</th>
<th>Density (g/cm(^3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carcinoma tissue</td>
<td>4.9815</td>
<td>0.8136</td>
<td>…</td>
<td>0.2794</td>
<td>0.2152</td>
<td>1.068</td>
</tr>
<tr>
<td>Muscle</td>
<td>5.0532</td>
<td>0.8281</td>
<td>…</td>
<td>0.2804</td>
<td>0.2146</td>
<td>1.062</td>
</tr>
<tr>
<td>Glandular tissue</td>
<td>…</td>
<td>0.6845</td>
<td>0.3439</td>
<td>0.2571</td>
<td>0.2043</td>
<td>1.033</td>
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<tr>
<td>Adipose tissue</td>
<td>2.9269</td>
<td>0.5232</td>
<td>…</td>
<td>0.2261</td>
<td>0.1871</td>
<td>0.967</td>
</tr>
</tbody>
</table>

*Courtesy of CIRS, Inc. (Norfolk, VA).*
the physical phantom and ex vivo specimen, a 400-ms exposure time was used, while the thickness available calibration blocks were exposed for 50 ms. This is because the detector readings for calibration blocks can be averaged across the block to increase the SNR, so a long acquisition time was not necessary for the calibration blocks. A total of 15 homogeneous blocks with three material composition were used as calibration blocks, which includes five thicknesses for each material (from 10 to 50 mm in 10 mm increments).

Breast equivalent materials manufactured by CIRS, Inc. (Norfolk, VA) were used for a physical breast phantom as well as calibration blocks. As mentioned before, the attenuation curves are obtained from CIRS, Inc., who has collected the attenuation coefficients of these breast equivalent materials from previous works such as the ICRU report for glandular tissue, the ICRP report for adipose tissue and muscle, and Theodorakou’s work for breast carcinoma. The physical breast phantom was constructed by stacking 1-cm slabs to achieve the desired total thickness, as shown in Fig. 3(d). Each 1-cm slab is composed of 50% glandular tissue and 50% adipose tissues, and one of the slabs includes 1-cm thickness carcinoma blocks. Six circular-shaped muscle blocks and four carcinoma blocks with 1-cm diameters were inserted into the physical breast phantom with known locations, as shown in Fig. 3(e).

Ex vivo breast specimens were acquired after a total mastectomy with no chemical processing. The specimens were compressed to have a flat thickness, from 3 to 5 cm, during scanning. Since the breast specimens were removed from patients’ bodies and were evenly compressed with a plate in our PCXD system, we can safely assume that the specimens had even thickness in most regions. However, the peripheral regions of the specimen were not fully compressed, so in this region, we decomposed materials without assuming total thickness information and added the results to obtain the estimate of the total thickness. Then, the estimated images were smoothed out such that the thickness changes from the center region to the peripherals did not vary abruptly. Since the peripheral regions are small and do not contain regions of diagnostic importance, such an approximation procedure did not incur performance degradation of the algorithm.

Mean glandular dose (MGD) of ex vivo specimen are estimated as 0.7773 mGy for 5 cm thickness specimen, while 1.0012 mGy for 3 cm thickness specimen. These MGD values are comparable to commercial FFDM mammography whose average MGD value is around 1.5 mGy. In our experimental environment of ex vivo specimen, the specimen is assumed as 50% glandular ratio, and skin entrance exposure is measured with a dosimeter and conversion factors are calculated based on Boone’s method.

4.C. Performance evaluation

In simulated data, the decomposed images were quantitatively evaluated using the root mean squared error (RMSE), percentage error (PE), and the contrast to noise ratio (CNR).

More specifically, the RMSE of material \( j \) is calculated by

\[
RMSE_j = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (t_{j,i} - g_{j,i})^2},
\]

(25)

where \( N \) is the number of pixels; \( t_{j,i} \) and \( g_{j,i} \) refer to the decomposed thickness and the ideal thickness of the \( i \)th pixel of the \( j \)th material, respectively. After calculating the RMSE is for each material, we calculate the average RMSE including all \( K \) materials, as follows:

\[
RMSE_{\text{total}} = \sqrt{\frac{1}{K} \sum_{j=1}^{K} RMSE_j^2}.
\]

(26)

We also calculated the percentage error using the following formula:

\[
\text{PE}_j = \frac{\text{RMSE}_{\text{obj}}}{\bar{g}} \times 100(\%),
\]

(27)

where \( \text{RMSE}_{\text{obj}} \) refers to the RMSE of material \( j \) of the selected region whose ground truth is not zero; \( \bar{g} \) is the average ground truth thickness of the selected region. Note that this percentage error can only be calculated for the object regions where the ground-truth value is nonzero. The CNR was calculated by

\[
\text{CNR} = \frac{|S - N|}{\sigma},
\]

(28)

where \( S \) and \( N \) refer to the intensities of the signal and the noise, respectively, and \( \sigma \) is the noise standard deviation.

In real experiments, detection of malignant tissue was qualitatively evaluated based on its known location. In ex vivo data, a radiologist finds the tumors and then marks their locations, which were used as the ground truth for the malignant tissue locations. More specifically, after the multi-energy system measurement, the specimens were imaged using a conventional digital mammography with a dual-track anode tube (GE Senographe DS), and a radiologist marked the malignant region on the enhanced images. These marked images are used as ground-truth for qualitative performance evaluation.

The proposed material decomposition results are then compared to those obtained with conventional inverse mapping methods in Kappadath et al. and Laidevant et al. Both algorithms represent the material thickness in polynomials using dual energy measurements, and the polynomial coefficients were estimated based on calibration phantom measurement. In previous works, dual source measurements were applied, so if multienergy measurements of a PCXD system are applied, more polynomial coefficients are required. Therefore, to compare our results to previous methods, we selected two energy bins out of our PCXD measurements for previous methods. To minimize the attenuation coefficient correlation between measurements in order to allow for a fair comparison, bins corresponding to the lowest and the highest energy ranges were selected, which provides the best decomposition results among possible choices.
TABLE II. Calculated optimal energy bin thresholds for the decomposition of muscle, glandular, and adipose tissues.

<table>
<thead>
<tr>
<th>Object thickness</th>
<th>Energy thresholds (keV)</th>
<th>Glandular 25%</th>
<th>Glandular 50%</th>
<th>Glandular 75%</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 cm</td>
<td>10 23 35 49</td>
<td>10 23 35 49</td>
<td>10 23 35 49</td>
<td></td>
</tr>
<tr>
<td>4 cm</td>
<td>10 23 35 49</td>
<td>10 24 35 49</td>
<td>10 24 35 49</td>
<td></td>
</tr>
<tr>
<td>5 cm</td>
<td>10 24 35 49</td>
<td>10 24 36 49</td>
<td>10 24 36 49</td>
<td></td>
</tr>
<tr>
<td>6 cm</td>
<td>10 24 36 49</td>
<td>10 25 36 49</td>
<td>10 25 36 49</td>
<td></td>
</tr>
</tbody>
</table>

5. EXPERIMENTAL RESULTS

5.A. Simulation results

The minimum bound of the energy threshold was set to 10 keV to avoid the dark current that exists up to 6 keV in our PCXD system. The optimal energy level, listed in Table II, is calculated by the minimization of numerically computed $\text{tr}(A^T A)^{-1}$ for all possible energy bin combinations. The optimal energy levels are obtained for various compositions such that 25%, 50%, and 75% of glandular ratio, and for various total thicknesses from 3 to 6 cm. We found that the optimal energy bin threshold is more dependent on the x-ray spectrum rather than the material composition ratio for given experiment scenario (it also depends on the choice of material basis as well). For a target composed of 50% glandular and 50% adipose tissue, theoretical optimal energy levels were [10–23, 23–35, 35–49] keV for a 3-cm object, which maximizes the energy-dependent contrast after considering the noise statistics. However, in our prototype system, each detector pixel exhibits different energy sensitivity, so it was necessary to modify the current offsets of each pixel to acquire consistent energy measurement. Accordingly, our hardware was shown to perform consistently with 25 and 34 keV energy levels without artifacts. Hence, we used [10–25, 25–34, 34–49] keV as the optimal energy in the real experiments. As shown in Table III, the trace value of the alternative choice with respect to the theoretical optimum was nearly equivalent, whereas the trace value of an arbitrarily selected energy bin was five times larger. A similar trend was observed in the optimal energy level of a 5-cm-thick object, where an arbitrarily selected energy bin has almost four times larger trace value when compared to that of the optimal energy threshold.

Material decompositions using the optimized energy level and arbitrarily selected energy thresholds are compared in Fig. 4 for the decomposition of a 3-cm virtual breast phantom in simulation. In the simulation, theoretical optimal energy levels [10–23, 23–35, 35–49] keV were applied because we do not need to consider hardware limitations in a computer simulation. Arbitrarily chosen energy levels were set to [10–30, 30–40, 40–49] keV. More background contamination was observed in the muscle image from the arbitrarily selected energy levels than that from the optimal energy bins, as shown in Fig. 4. To make the difference clearer, the areas with more background contamination are shown in zoom and the specific regions are indicated by arrows, as shown in Fig. 4. The corresponding RMSE values confirm the validity of the energy optimization algorithm, as described in Table IV. In addition, CNR values are compared as shown in Table IV for the case of muscle blocks. Here, the noise level is calculated from the whole background region, excluding muscle location from the muscle decomposition image. For the CNR of ROI 1 and ROI 2, values of $S$ were calculated by averaging the values obtained from white boxes 1 and 2, respectively, in Fig. 4. As described before, we minimized the average RMSE values for all materials simultaneously rather than for specific materials; hence, there are cases in which a RMSE value for a specific material basis can be larger than its counterpart obtained from the nonoptimized energy level (for example, the RMSE value for muscle from a 3-cm phantom in Table IV). However, average RMSE values are consistently better than those of the nonoptimized energy level. We could have changed the energy level optimization criterion to minimize the RMSE error for a specific material basis by minimizing the corresponding diagonal component of the error covariance matrix. However, this would have been at the cost of increasing of average RMSE values across multiple material bases, which we tried to avoid.

TABLE III. Traces of the covariance matrices for the theoretically (th) optimal, experimentally (exp) optimal, and nonoptimal energy bin selections in virtual phantom simulation.

<table>
<thead>
<tr>
<th>Object thickness</th>
<th>Energy levels (keV)</th>
<th>$\text{tr}(A^T A)^{-1}$</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 cm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimal (th)</td>
<td>10 23 35 49</td>
<td>1.1627 × 10^6</td>
<td>1</td>
</tr>
<tr>
<td>Optimal (exp)</td>
<td>10 25 34 49</td>
<td>1.2821 × 10^6</td>
<td>1.1027</td>
</tr>
<tr>
<td>Nonoptimal</td>
<td>10 30 40 49</td>
<td>5.3259 × 10^6</td>
<td>4.5807</td>
</tr>
<tr>
<td>5 cm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimal (th)</td>
<td>10 24 36 49</td>
<td>2.6489 × 10^6</td>
<td>1</td>
</tr>
<tr>
<td>Optimal (exp)</td>
<td>10 25 34 49</td>
<td>2.7364 × 10^6</td>
<td>1.0331</td>
</tr>
<tr>
<td>Nonoptimal</td>
<td>10 30 40 49</td>
<td>8.8518 × 10^6</td>
<td>3.3417</td>
</tr>
</tbody>
</table>

TABLE IV. RMSE, average percentage error, and CNR of material decomposition results from different energy level selection criteria in virtual phantom simulation.

<table>
<thead>
<tr>
<th>Object thickness</th>
<th>RMSE of 3 cm phantom (mm)</th>
<th>CNR</th>
<th>ROI 1</th>
<th>ROI 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Muscle</td>
<td>Glandular</td>
<td>Adipose</td>
<td>Total</td>
</tr>
<tr>
<td>Optimal</td>
<td>4.95</td>
<td>4.04</td>
<td>3.18</td>
<td>3.04</td>
</tr>
<tr>
<td>Arbitrary</td>
<td>4.76</td>
<td>4.30</td>
<td>3.56</td>
<td>3.28</td>
</tr>
<tr>
<td>RMSE of 5 cm phantom (mm)</td>
<td>CNR</td>
<td>ROI 1</td>
<td>ROI 2</td>
<td></td>
</tr>
<tr>
<td>Optimal</td>
<td>7.85</td>
<td>5.85</td>
<td>4.16</td>
<td>4.29</td>
</tr>
<tr>
<td>Arbitrary</td>
<td>8.51</td>
<td>6.25</td>
<td>4.38</td>
<td>4.57</td>
</tr>
</tbody>
</table>
To verify the robustness of muscle decomposition with respect to thickness variations, we performed additional simulation using a virtual phantom including 16 muscle blocks of varying thicknesses and sizes (see Fig. 5 and Table V). For this simulation, virtual phantoms with backgrounds of 50% glandular tissue and 50% adipose tissue were used with muscle blocks inserted. We performed the experiments for two levels of total thickness of 3 and 5 cm. The decomposition accuracy was verified using the RMSE value and the percentage error of decomposed muscle (carcinoma) blocks in Table V. Note that the accuracy of the proposed method increases as the muscle thickness increases. We also found that the decomposition results are less dependent on the block size. The decomposition results shown in Fig. 5 for the case of 3 cm total thickness illustrates that the proposed method provides visible muscle (carcinoma) block decomposition with less noise.

To quantify the decomposition accuracy of various total thickness and glandular/adipose ratio, we performed another simulation experiment using a virtual phantom including 16 blocks, as similar to above experiment. Each blocks are composed of varying adipose ratio from 20% to 80%; and their thicknesses vary between 3 and 6 cm, while the thickness of muscle is set to 1 cm.

Figure 6 illustrates the material decomposition results along with the ground-truth. In every case, the muscle is decomposed quite well. While the decomposition results of glandular and adipose are not good for higher ratio of adipose, we can still identify their locations qualitatively in the decomposition results.

To test the robustness of the assumed total thickness in our algorithm, the material decomposition results were compared according to the error of the assumed total thickness. The RMSE values, depending on the total thickness variation, are

---

**Fig. 4.** Material decomposition results of the 3-cm virtual phantom using (top) the optimal energy level, (middle) a nonoptimal energy level, and (bottom) the ground truth. Muscle images are shown at 0–15 mm (0–10 mm in the magnified image), and other images are shown at the 0–35 mm scale. To make the difference more clear, area with more background contamination are zoomed and the specific regions are pointed by arrows.
FIG. 5. Material decomposition simulation for various muscle block thickness when the total thickness is 3 cm. The muscle blocks have various thickness from 5 to 20 mm and size from 2 to 8 mm. The images are shown at a 0–35 mm scale except muscle blocks, which are shown at 0–20 mm scale.
FIG. 6. Material decomposition simulation for various total thickness and glandular-adipose ratio. The muscle blocks have constant 1 cm thickness, while total thickness of blocks vary 3–6 cm and adipose ratio 20%–80%. The images are shown at a 0–45 mm scale except muscle blocks, which are shown at 0–15 mm scale.
Table V. RMSE and percentage error values of muscle (carcinoma) blocks of various thicknesses and sizes in 3- and 5-cm block phantom simulations using the proposed method. Columns indicate block size while rows indicate block thickness.

<table>
<thead>
<tr>
<th>thickness (mm)</th>
<th>2 mm</th>
<th>4 mm</th>
<th>6 mm</th>
<th>8 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>4.41 (88.14%)</td>
<td>4.42 (88.31%)</td>
<td>4.41 (88.16%)</td>
<td>4.40 (88.05%)</td>
</tr>
<tr>
<td>10</td>
<td>5.41 (54.06%)</td>
<td>5.45 (54.45%)</td>
<td>5.39 (53.88%)</td>
<td>5.41 (54.06%)</td>
</tr>
<tr>
<td>15</td>
<td>3.99 (26.58%)</td>
<td>3.93 (26.23%)</td>
<td>3.92 (26.14%)</td>
<td>3.94 (26.28%)</td>
</tr>
<tr>
<td>20</td>
<td>2.69 (13.45%)</td>
<td>2.60 (12.98%)</td>
<td>2.59 (12.95%)</td>
<td>2.58 (12.88%)</td>
</tr>
</tbody>
</table>

5.B. Real experiments

Material decompositions using the optimized energy level and arbitrarily selected energy bin thresholds are also compared in Fig. 8 for the tissue decomposition of a 3-cm physical phantom after 20 ICD iterations. To make the difference clearer, the areas with more background contamination are shown in zoom and the specific regions are indicated by arrows, as shown in Fig. 8. Note that both the muscle and the carcinoma blocks are decomposed into a muscle basis since the carcinoma tissue and the muscle have very similar attenuation characteristics, as shown in Table I. Hence, we considered these materials to be the same materials and decomposed them into the same muscle basis. With the arbitrarily chosen energy levels, [10–30, 30–40, 40–49] keV, the malignant tissue image has more background noise than that of the optimal energy measurement decomposition, as indicated by the arrows in the magnified view of the malignant tissue image. These results confirm that the proposed energy optimization method is indeed useful in practice.
### TABLE VI. RMSEs of various methods with respect to the total thickness error in virtual breast phantom simulation. The RMSE values were calculated for muscle blocks with 10 mm thickness and 10 mm width.

<table>
<thead>
<tr>
<th>Total thickness error (mm)</th>
<th>RMSE of 3 cm phantom (mm)</th>
<th>RMSE of 5 cm phantom (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed method</td>
<td>12.21 7.91 3.69 1.46 5.41</td>
<td>6.00 2.25 3.89 7.64 8.92</td>
</tr>
<tr>
<td>Conventional (Laidevant)</td>
<td>6.03 3.15 3.34 6.27 9.32</td>
<td>6.09 7.46 8.89 9.81 10.00</td>
</tr>
</tbody>
</table>

In Fig. 9, the material decomposition results for a 3-cm physical breast phantom are compared according to various methods. The images are decomposed into malignant (in the muscle basis), glandular, and adipose tissues using the measurements acquired at [10–25, 25–34, 34–49] keV. All the inserted carcinoma and muscle blocks were detected in the muscle basis in the proposed algorithm. Although some circular shapes of inserted blocks are not clearly visible, this might be due to the thick glandular tissue overlap. Note that the irregularity of the decomposed carcinoma blocks is due to the variability of the anatomic structural noise in layers surrounding each mass. Still, the proposed algorithm shows

Fig. 8. Material decomposition results of the 3-cm physical phantom using (top) the optimal energy level and (bottom) a nonoptimal energy level. Malignant tissue images, decomposed into a muscle basis, are shown at a 0–5 mm scale, and the other images are shown at a 0–35 mm scale. To make the difference more clear, areas with more background contamination are zoomed and the specific regions are pointed by arrows.
decomposition for all bases better than that of the conventional methods. In the conventional methods, inserted malignant tissue blocks are decomposed with massive background structures in the case of the Kappadath method, or only a few inserted blocks were detected by the Laidevant method.

For all ex vivo specimens, [10–25, 25–34, 34–49] keV energy levels were also used. The measurements are decomposed into muscle (malignant tissue), breast, and adipose tissues, and results were acquired after 20 iterations of ICD. The malignant tissue region is also accurately decomposed into a muscle basis in both of the specimens, as shown in Figs. 10 and 11, which were very similar to the ground truths provided by a radiologist. Furthermore, in the breast tissue image shown in Fig. 11, the glandular structure of the breast is clearly visible when using the proposed method, as indicated by the dotted circle. Although the adipose region is similarly decomposed in the conventional methods, the proposed algorithm can lead to better decomposition of malignant tissue and breast tissues. For example, in Figs. 10 and 11, parts of the normal tissue regions are decomposed as malignant tissues, as indicated by the white arrows for the case of the conventional methods. Specifically, in the results obtained using the Kappadath method, more noise was visible. In particular, in the magnified view of muscle shown in Fig. 10, calcification speckles are not clearly discernible due to high noise.

The total thickness accuracy has been also tested on ex vivo data to confirm the simulation results in a real environment. As shown in Fig. 12, decomposed carcinoma...
images are relatively unaffected up to a total thickness error of 2 mm.

6. DISCUSSION

While our numerical simulation results also confirmed the advantages of the proposed energy level optimization and material decomposition algorithm, the results using the real physical phantom and ex vivo data showed much clear advantages of the proposed methods. Note that the decomposition results from numerical study are dependent on the accuracy of the numerical modeling of forward measurement process, so algorithmic advantages may not be clearly in numerical simulation. On the other hand, such inaccuracy of the forward modeling is not present in real measurement, so we believe that it is more easy to demonstrate the algorithmic advantages of the proposed method using the real experiment results.
FIG. 11. Material decomposition results of an ex vivo specimen using various methods. In the results of the conventional methods, parts of normal tissue regions are decomposed as malignant tissues, as pointed out by white arrows. The total thickness of the specimen is 3.1 cm, and images are shown at a 0–36 mm scale.

There exists many source of performance differences between the method in Laidevant et al. and the proposed method. It turns out that the decomposition of muscle (considered as carcinoma), glandular, and adipose is even more difficult than the decomposition of protein, water, and lipid (P-W-L) because the similarity of the density and attenuation coefficients among materials makes the decomposition problem more ill-posed. Recall that the densities of protein, water, and lipid are 1.35, 1.0, and 0.95 (g/cm³), respectively, while those of muscle (carcinoma), glandular, and adipose (M-G-A) are very similar to each other as shown in Table I. This leads to \( \text{tr}(A^TA^{-1}) = 3.0377 \times 10^5 \) in P-W-L compositions, while it is \( 1.1627 \times 10^6 \) in M-G-A composition as given in Table III. This implies that the M-G-A decomposition is more difficult than that of P-W-L decomposition.

Note that in Table V, the errors that make up the RMSE are mostly negative in terms of muscle decomposition with
exact total thickness, since muscle (carcinoma) blocks are underestimated, and parts of muscle and adipose tissue are decomposed into glandular tissue. This result also appears in Figs. 5 and 6, where some decomposition values of the proposed method especially for glandular overlapped with thin muscle blocks, are much larger than the ground truth. The reason that some values (especially in glandular) in the proposed method are much whiter is that some of the muscle and adipose components are assigned to the glandular value because these components are usually underestimated. However, since this is not a simple matter of off-sets, we may need a more sophisticated technique to correct this problem, which is beyond the scope of this paper.

As shown in numerical simulation results in Fig. 7 and Table VI, under sufficiently accurate estimate of the total thickness, the RMSE values of the proposed method was the smallest. In Table VI, the results of the Kappadath method are most insensitive among the various methods for the discrepancy of total thickness for various ranges of thickness error, and the Laidevant method tends to fail for overestimated total
thickness and there were no muscle decomposition using this method (this is why the RMSE value is 10.0 mm in Table VI).

Since Kappadath’s method uses only calcification thickness and the ratio of glandular and adipose tissue of the calibration blocks, the results are less sensitive to the total thickness error. However, in our experimental results the decomposition results determined using Kappadath’s method were not as accurate as those of other methods when the exact total thickness is available. In the Laidevant method, if the total thickness is overestimated, all of the muscle blocks tend to be decomposed into other materials with less density. Therefore, the RMSE value goes to the maximum thickness, 10.00 mm, as shown in Table VI. However, in our method, the decomposition error is consistently reduced as the total thickness estimation becomes more accurate, and for the true thickness the RMSE value of the proposed method is the smallest. In addition, Fig. 12 showed that the decomposition results using the conventional methods were more sensitive to thickness estimation error for real \textit{ex vivo} specimen as well. For example, in the case of the Laidevant method, the image variation was severe, even with the small thickness variation of 2 mm.

The Kappadath method was relatively consistent, regardless of the total thickness accuracy; however, the decomposed images were less accurate and noisier than those of the proposed method.

However, recall that our main algorithm is derived based on the assumption that the total thickness is known. According to Mawdsley et al., \textsuperscript{50} errors in total thickness of up to 15 mm can occur. Our \textit{ex vivo} experiment showed that over 2 mm error, the results of our reconstruction were not accurate, either. Therefore, to make the algorithm more useful in a real imaging environment, a sophisticated method, such as that used in Tyson et al., \textsuperscript{51} which can improve this accuracy to less than 1 mm using a compression paddle would be necessary. However, even sophisticated methods do not measure breast thickness accurately toward the periphery, where the breast is not in contact with the paddle, so we need a more sophisticated reconstruction technique to address such issues. This problem is beyond scope of this paper, and needs to be investigated in the future.

One limitation of our proposed method relative to Laidevant et al. is that our basis materials are not the basic component such as protein, lipid, and water. In practice, there are many suspicious findings in breast tissue other than invasive cancer that do not fall into the categories of invasive, adipose, and fibroglanular, e.g., fibroadenomas, ductal carcinoma \textit{in situ}, or just a variant of benign breast tissue. In Laidevant et al., the assumption of the breast being composed of protein, water, and lipid always holds, and all findings will be fractional variations of these components. Even though our algorithm has been developed for decomposition muscle, glandular, and adipose, the method can be equally applied for other basic material decomposition similar to those of Laidevant et al. Since the proposed unified statistical framework still holds for such decomposition, we believe that our method may have advantages. Such extension could be potentially useful and need further investigation, which will be reported elsewhere.

7. CONCLUSION

A material decomposition algorithm and an energy optimization algorithm for PCXD were proposed under a unified statistical framework. A PCXD energy optimization scheme was derived by the minimum variance unbiased estimation principle, and the scheme’s accuracy was validated by simulation and real experiments. The proposed algorithm successfully decomposed malignant tissue from PCXD measurements in simulation, physical breast phantom, and \textit{ex vivo} data.

In simulation study, we observed that there still exist significant errors in quantitative values from the proposed material decomposition results. However, considering that this is a single view imaging rather than a tomographic method and that the linear attenuation curves for some materials are quite similar, the estimation problem is severely ill-posed and there may exist a fundamental performance limit for estimating the thickness accurately. Therefore, we are not claiming that the main contribution of this work is the tomographic accuracy of the thickness estimation in an absolute sense; rather, we claim that the proposed method provides better results compared to those of existing methods in many aspects.

Although the decomposed material accuracy depends on the thickness error, for errors of up to 2 mm thickness, the proposed method in many aspects provides good reconstruction results in both simulation and real \textit{ex vivo} breast phantom experiments, especially compared to existing methods. Hence, we believe that the proposed method has great potential to detect carcinoma tissue from breast tissue through three material decomposition. Moreover, as the proposed method requires fewer parameters and provides a unified optimization framework for various system calibrations, we believe that our algorithm is quite useful in practice.

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