Supplementary

Appendix 1

To facilitate the understanding, the purpose of this section is to further clarify the methodology used to estimate the spectrum. Inspired by Zhao's work (23), model spectra are introduced, which are shown in *Figure S1*. The model spectra were simulated with different thicknesses of aluminum. Assuming that the material maps are known, Eq. [5] can be expressed as:

$$\boldsymbol{P}_{k,L} = \sum_{m=1}^{M_k} c_{k,m} \sum_{E=1}^{N_k} \boldsymbol{s}_{k,m,E} \boldsymbol{\delta} \exp(-\boldsymbol{\mu}_{b,E} \boldsymbol{A}_L \boldsymbol{F}_b - \boldsymbol{\mu}_{w,E} \boldsymbol{A}_L \boldsymbol{F}_w)$$
[34]

where all the parameters except $c_{k,m}$ is known. Thus, Eq. [34] can be expressed as:

$$P_{k,L} = \sum_{m=1}^{M_k} c_{k,m} Q_{k,L,m}$$
[35]

where

N

$$\boldsymbol{Q}_{k,L,m} = \sum_{E=1}^{r_{b}} \boldsymbol{s}_{k,m,E} \delta \exp(-\boldsymbol{\mu}_{b,E} \boldsymbol{A}_{L} \boldsymbol{F}_{b} - \boldsymbol{\mu}_{w,E} \boldsymbol{A}_{L} \boldsymbol{F}_{w})$$
[36]

Considering that $Q_{k,L,m}$ is known, the spectrum estimation problem can be formulated as:

$$\arg\min_{c_k} \frac{1}{2} \left\| \mathcal{F}_L(c_k) - \tilde{P}_{k,L} \right\|_2^2$$
[37]

Considering the physical meaning, $c_{k,m}$ is non-negative and the sum of different coefficients is 1, Eq. [37] can be written as:

$$\underset{c_{k}}{\operatorname{arg\,min}} \frac{1}{2} \left\| \mathcal{F}_{L}(c_{k}) - \tilde{\mathcal{P}}_{k,L} \right\|_{2}^{2} + \lambda_{c} \sum_{k} \left(\left\| c_{k} \right\|_{1} - 1 \right)^{2},$$
s.t. $c_{k} = (c_{k,1}, \dots, c_{k,m}), c_{k,m} \ge 0$

$$[38]$$

There are several methods to solve equation such as multi-variable downhill simplex method (67), an augmented Lagrangian method (68) and BFGS-B (51). Although these methods can provide similar results, for the sake of fast convergence rate, BFGS-B is adopted. Thus, when the material maps are known, c_k can be updated as follows:

Algorithm for spectrum estimation
Input $oldsymbol{c}_k^0$,
1. Repeat
$\boldsymbol{c}_{k}^{t+1} = \operatorname*{argmin}_{\boldsymbol{c}_{k}^{t+1}} \frac{1}{2} \left\ \boldsymbol{\mathcal{F}}_{L}(\boldsymbol{c}_{k}^{t}) - \tilde{\boldsymbol{P}}_{k,L} \right\ _{2}^{2},$
$\boldsymbol{c}_{k}^{t+1} = \boldsymbol{c}_{k}^{t+1} / \operatorname{sum}(\boldsymbol{c}_{k}^{t+1}),$
$\boldsymbol{c}_k^{t+1} = (\boldsymbol{c}_k^{t+1})_{+}$
$t+1 \leftarrow t$,
2. Stop until convergence.

Although Eq. [19] is not the same as equation , the solution for it is similar and step 3 can be replaced as

$$\boldsymbol{c}^{t+1} = \operatorname*{argmin}_{\boldsymbol{c}_{k}^{t+1}} \sum_{k} \frac{1}{2} \left\| \boldsymbol{\mathcal{F}}_{L}(\boldsymbol{c}_{k}^{t+1}, \boldsymbol{F}_{b}^{t}, \boldsymbol{F}_{w}^{t}) - \tilde{\boldsymbol{\mathcal{P}}}_{k,L} \right\|_{2}^{2} + \frac{1}{2\eta_{\boldsymbol{c},k}^{t}} \left\| \boldsymbol{c}_{k}^{t+1} - \boldsymbol{c}_{k}^{t} \right\|_{2}^{2} \ .$$

References

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Figure S1 80 and 140 kVp Model Spectral used in this paper. These spectra are generated with 3-, 4-, 6-, 8-, 12-, 18-mm Al filter.