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# Enabling three-dimensional densitometric measurements using laboratory source X-ray micro-computed tomography

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ABSTRACT

We present new software allowing significantly improved quantitative mapping of the three-dimensional density distribution of objects using laboratory source polychromatic X-rays via a beam characterisation approach (c.f. filtering or comparison to phantoms). One key advantage is that a precise representation of the specimen material is not required. The method exploits well-established, widely available, non-destructive and increasingly accessible laboratory-source X-ray tomography. Beam characterisation is performed in two stages: (1) projection data are collected through a range of known materials utilising a novel hardware design integrated into the rotation stage; and (2) a Python code optimises a spectral response model of the system. We provide hardware designs for use with a rotation stage able to be tilted, yet the concept is easily adaptable to virtually any laboratory system and sample, and implicitly corrects the image artefact known as beam hardening.



## Code metadata

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| Current code version | *1.0* |
| Permanent link to code/repository used of this code version | https://github.com/ElsevierSoftwareX/SOFTX-D-17-00053 |
| Legal Code License | *Apache 2.0* |
| Code versioning system used | *SVN* |
| Software code languages, tools, and services used | *Python 2.7* |
| Compilation requirements, operating environments & dependencies | *The main Python modules that users may need to install are numpy, matplotlib, scipy, tifffile* |
| If available Link to developer documentation/manual | https://ccpforge.cse.rl.ac.uk/svn/tomo_bhc/trunk/doc/ |
| Support email for questions | ronald.fowler@stfc.ac.uk |

## Software metadata

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| Legal Software License | *Apache 2.0* |
| Computing platforms/Operating Systems | *Linux, Windows, MacOS* |
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| Support email for questions | ronald.fowler@stfc.ac.uk |

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## 1. Introduction

Three-dimensional (3D) densitometry can be conducted using monochromatic X-ray imaging (synchrotron) and tomographic reconstruction [1,2]. The relationship between attenuation and a homogeneous object's thickness is linear for a single X-ray energy (e.g. [3]). Single energy calculated attenuation is also linear since the detector response, in theory, is constant (see [4] for a discussion of detectors and sources).

Measuring density quantitatively and accurately using a typical laboratory X-ray imaging setup, however, is non-trivial. This is because conventional impact X-ray sources produce polychromatic beams (which can change from scan to scan), and attenuation is strongly dependent on X-ray energy (Fig. 1). Furthermore, conventional detectors do not differentiate energy (only flux) and do not have uniform response over the whole energy range. Finally, there may be no practical way of placing precisely known thicknesses of the exact material of interest into the beam, which would allow an internal calibration between attenuation and thickness to be made (for that material only).

The detected signal is an outcome of the combination of three variables: the incoming spectrum, the sample-specific interaction with that beam, and the response of the detector. Our aim here is to make quantitative densitometry practical, and adaptable to any laboratory setting, by demonstrating a method of characterising the beam spectra that can be easily integrated into day-to-day laboratory procedure. Once the beam is characterised using our code, correction factors for any given material can be calculated with respect to that material's attenuation of a monochromatic beam. With the correction applied to the projection data, the reconstructed tomograms are a quantitative and reproducible measure of that objects' density, and with beam-hardening minimised.

## 2. Background

In theory, if the proportions of different energies and the composition of the specimen are known, a good estimate of density can be derived from the reconstructed X-ray image. All that is required in order to calculate the attenuation and thus density of the object the beam passes through is knowledge of the X-ray spectra used, and the response function of the detector. The non-linearity in the response due to polychromatic X-rays can then be corrected to a linear relationship between response and sample thickness.

X-ray spectra can be calculated, which gives a good approximation for the energies emitted from polychromatic X-ray sources. Yet these values are not precisely known for real X-ray tubes and there are a number of other uncertainties, such as the efficiency of the detectors, which influence the signal recorded. Today's industrial X-ray radiography and tomography equipment does not attempt to apply corrections based on calculations from measurements made from the beam itself. Instead, the density phantoms suitable for some purposes are provided and are used as calibration standards to apply to images ([5]; see also method notes in [6]). Qualitative correction routines that improve the visual appearance of the result – but do not provide an estimate of the true absorption properties – are also provided by scanner manufacturers. While the artefacts appearing in such images may be neglected for some purposes, these can at best complicate the analysis and at worst lead to spurious results.

During a tomography acquisition, the average X-ray path lengths common to a single voxel are shorter when that voxel is near the edge of the object (Fig. 2a). This causes 'beam hardening' to manifest as image cupping in tomographic reconstructions based upon linear absorption. The artefact manifests as relative brightening at the edges of reconstructed objects and darkening in the middle (Fig. 2b). Without correction of the original projection data (i.e. the response per pixel) this artefact precludes accurate densitometry. For objects that actually have a radial distribution of density such as a tooth or a bone, or chemically zoned crystals, the beam hardening effect becomes confounded with the very property the experiment is intended to measure (see Fig. 3).

Understanding and overcoming image artefacts inherent to the polychromatic nature of laboratory-source X-ray spectra is thus a vital task (e.g. [7]). This is because the greyscale value assigned to a reconstructed voxel is routinely used to digitally map an object's features, in order to extract textural [8] and chemical information [9]. Applications that rely on high confidence when using the greyscale value as a key image parameter range from geological and environmental [10–13] to biomedical [14], to transport and energy [15] and material engineering applications [16]. Due to this numerical 'smearing', however, beam hardening artefacts have long posed a major limitation to quantitative 3D image analysis.

## 3. Our approach

In this contribution, we report an advance in the development of a method of three-dimensional densitometric measurement by characterising the polychromatic beam and the detector response [17–21]. First, the scan settings are decided upon, and then that beam is characterised. The beam is used to take projection data through different thicknesses of materials of known attenuation (that bracket that of the object). The images provide raw intensity data that can be then compared to a modelled system [17]. Since the model is not exact, it is necessary to adjust some of the parameters to obtain an optimal fit to the measured data.

Measurements are conducted using a nonlinear optimisation process to obtain a function that represents the X-ray energy response of the system [17]. Where the specimen material composition is known, the function can be used to generate a calibration curve for that material using published X-ray attenuation values, for instance see [22]. This approach produces a curve approximating the real, non-linear relationship between total polychromatic beam attenuation and the expected attenuation with monochromatic radiation [20] which may be easily and simply applied in existing tomography equipment.

A current limitation of this algorithm is that the resulting correction curve is specific to a single phase. If, for example, the material of interest is encapsulated or held in place by resin, or surrounded by soft tissue etc., the presence of this second phase will decrease the accuracy of our approach. In cases where one phase contributes little to the attenuation, the method still gives an accurate estimate of the dominant phase. Similarly, for multi-phase specimens where there is a macroscopically uniform distribution of the phases, the method gives good overall beam-hardening correction that can improve the segmentation of the individual phases. An enhanced version of this method for more accurate densitometric measurement in dual phase systems is under development [23].

Our approach is distinct from filtration, which works to remove low energy X-rays from the beam, thereby narrowing the window of beam energy used toward an ideal case (see first paragraph). Since the ideal case is not possible in the laboratory (even if a single energy was achieved the flux would be too low for imaging in any practical scenario), filtration serves to reduce the effects of beam hardening, but does not provide quantitative densitometry.

## 4. Method developments

### 4.1. Hardware

It has long been common practice to use a step wedge of aluminium as an attenuation standard (e.g. [24]). Aluminium is