Graded Material Inspection by X-ray Computed Tomography

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Abstract
Additive Manufacturing (AM) in particular opens up the possibility of producing functionally graded components, allowing the material composition, and hence for example stiffness, to be specified at a voxel level, in a macroscopically continuously varying manner. Such possibilities not only present a challenge for the design stage, but also for the post-build quality control, where a method of volumetric compositional quality control is required. X-ray Computed Tomography (XCT) has the potential to fulfill this need, especially given that the technique is applicable to the highly complex geometries that can be made by AM, and due to the volumetric output of the inspection. However, further technique development is required to allow XCT to be effectively exploited as a tool of compositional quality control, noting for instance that XCT image greyscales are rarely used quantitatively in an industrial setting, unlike in clinical imaging. This paper describes initial efforts and results towards this objective.

Keywords: graded materials, compositional quality control, material decomposition

1 Introduction
The capability of some advanced Additive Manufacturing (AM) techniques to create functionally graded components, with macroscopically continuously varying composition, specified at a voxel level [1], means a method of post-build volumetric compositional quality control is required. Further development of X-ray Computed Tomography (XCT) is needed for it to be industrially effectively usable in this context. In particular, efforts to date on material decomposition for XCT have been driven by the needs of medical imaging, focusing on elements that are of little industrial relevance, often using photon counting / energy-discriminating detectors that are hardly known industrially [2-4]. This work seeks to expand material decomposition into an industrial context, driven by a need to be able to confirm the macroscopic make up of a component.

In a clinical context, the greyscales of the reconstructed volume are widely used to make deductions about local composition. For this the greyscale values, representing linear attenuation coefficients, are scaled linearly to the Hounsfield scale by first subtracting and then dividing by the attenuation coefficient of water, finally multiplying by 1000. Such quantitative use of image greyscales is essentially unheard of industrially, with most analyses focused on edges. Therefore, there is scope for trying to tackle the challenge of compositional quality control through a more quantitative treatment of industrial XCT greyscales.

Compositional quality control is closely linked to density measurement, as the two are equivalent for the simplest form of compositional grading, where the structure consists only of one material plus air / vacuum. In principle, a linear scaling to the image greyscales of a scan can be applied, dividing by the linear attenuation coefficient observed for a fully dense sample of the same material (in practice, after having subtracted the non-zero greyscale value of the background), to obtain values of fractional density. This could be considered a sample-material specific calibration process. The use of XCT for density measurements has been considered previously [5-7]. However, the two methods found in literature for industrial applications both do not consider the greyscale values, but rather rely on a segmentation of material from the background (either including or excluding identifiable pores, in the former case obtaining an absolute measurement of density from the sample volume measured and a mass balance reading, in the latter obtaining a relative density from the fraction of material in the test volume), so the methods are inevitably sensitive to the surface determination operation. Explicitly segmenting pores in the material has been reported to give poor correspondence to density measurements obtained by the Archimedes (immersion-based) reference technique [5].

For a rigorous compositional assessment of a dual-material graded sample, a second scan, acquired at a different energy, is required. This is because, in principle, a greyscale contrast attributable to a difference in density cannot be distinguished from one caused by a difference in composition. In practice (at the energies considered here) there are two mechanisms of X-ray attenuation (photoelectric absorption and Compton scattering interactions), and the data collection with two effective X-ray energies then allows the abundances of two constituent materials to be uniquely determined. Dual-energy scanning is also widely used for medical contrast agent imaging [2-4], where the two energies are selected to give a clear signal from the absorption edge of the contrast agent in what is otherwise a very challenging multi-material scenario. Sadly, the ability to exploit absorption edges in an industrial context is severely limited by the low energies at which K-edges occur for elements of industrial relevance (e.g. 8.3 keV for Ni), and the correspondingly severely limited penetration, though occasional efforts have been made [8-9].

The present work is an initial examination of XCT as a tool of compositional quality control driven by the needs of functionally graded AM components. The next section describes the methods explored. This is followed by a results section and a detailed discussion prior to final conclusions.
2 Method

2.1 Simulations

As a starting point for developing an understanding of XCT as a tool of compositional quality control for graded materials, simulation studies were conducted on virtual phantoms.

2.1.1 Mono-material

The simulations started with a mono-material phantom design. Here the graduation of material properties is achieved at a macroscopic level by varying the amount of air present in the structure at a microscopic level. The 2D phantom design was generated based on repetitions and permutations of basic 1D binary building blocks (e.g. [1, 1, 0] and [1, 1, 1, 0]) and is illustrated in Figure 1. Each pixel is considered to have a 200 µm edge, and the overall extent of the phantom in the plane is 40 × 64 mm. The design was extended in height (perpendicular to the plane shown) by prismatic extrusion, to make a 3D phantom to be used in the simulations. For the mono-material simulations, the virtual phantom was specified to have been printed in titanium (density 0.005 g/mm$^3$), a material frequently used in its Ti-6Al-4V alloy form in AM for engineering applications.

![Figure 1: Illustration of part of the graded (macroscopic) composition phantom used. In the mono-material configuration, white pixels represent printed material, black air – in the later bi-material configuration the air is replaced by a second solid. The macroscopic density varies monotonically from left to right (direction dependent on two components), with strips (4 mm wide, separated for visual clarity by superimposed red lines) of the same binary building blocks, giving areas of nominally constant macroscopic density.](image)

The phantom was forward projected and then reconstructed in a 2D fan beam geometry to allow the reconstruction output to be compared against the true phantom composition. The exact Siddon projector was used to avoid inaccuracies in the projections given the detailed nature of the phantom [10]. The reconstruction was completed by the standard FDK algorithm (filtered back-projection in the plane imaged) [11]. The geometry of the scan simulated featured an energy-integrating (i.e. conventional) linear detector of 1000 pixels with 400 µm pixel size at a distance of 100 cm from the source. Two geometric magnifications, 5 (“high”) and 1.05 (“low”) were used, giving native voxel sizes in the reconstruction of 80 µm and 389 µm edge length, respectively. In all simulations, 720 projections, evenly spaced around a circular rotation with axis perpendicular to the fan beam, were sampled. Partial volume effects were accounted for by simulating eight rays per pixel, averaging their intensities for the pixel value. Where used, the polychromatic X-ray spectra were generated using the Tucker model [12]. The polychromatic spectrum used was based on an acceleration voltage of 160 kV, a tungsten reflection target and a prefilter of 0.5 mm of copper. The energy of the monochromatic spectrum used for comparison was 150 keV. Where applied, the beam-hardening correction was based on an empirical mapping of polychromatic projection values to monochromatic ones, derived from the simulation of a contiguous block of the phantom material and under the same conditions. Where applied, Poisson noise was added to the projections for a fixed number of incoming photons. Geometric unsharpness from a finite-sized focal spot was neglected, after simulations confirmed the insignificance of this effect for the range of configurations examined. Scatter was neglected for the sake of simplicity and computation speed, though it is recognized that the presence of scatter in a physical set-up could undermine the analysis. Figure 2 provides a representative illustration of the phantom reconstructions obtained, in high and low magnification configurations. Note how for the low magnification set-up some phantom strips, dependent on the coarseness of the microstructure, appear as a uniform greyscale, unlike in the high magnification case.
Having completed simulations in several configurations, the obtained reconstructions were processed to recover the density of the sample along its length. This was done in several ways. The first involved scaling the reconstruction greyscale values through division by the greyscale value of the material peak of the global histogram obtained from the equivalent simulation of a fully dense block sample under the same conditions. The volume fraction figures for plotting were obtained by averaging the greyscale laterally, along central 80% of the phantom strip.

Alternative approaches for converting the greyscale values of the reconstruction to a density measure were also trialed, driven by a desire to avoid needing to refer to a supplementary scan of a fully dense sample subjected to the same inspection conditions. The second approach attempted to recover the reference value for the greyscale value of a fully dense component from the histogram of the phantom itself, using the position of the maximum of the material peak of the greyscale histogram, either for the full image or a region of interest, containing the densest elements of the phantom.

The third attempt also considered the (global) greyscale histogram of the reconstruction, and attempted to apply a typical ISO50 segmentation [13], splitting the histogram half-way between the air and material peaks to separate the two entities in the image and then using the binary representation of the material presence to derive a fractional density.

### 2.1.2 Bi-material

For the bi-material simulations, the same graded phantom design as before was used, but this time the effective air gaps of the set-up described in the last section were filled with iron (density 0.008 g/mm$^3$), another element of great engineering importance.

Fig. 3 provides a representative illustration of the phantom reconstructions obtained, corresponding to Fig. 2 for the mono-material case.

For the single energy scans, the analysis mirrored that for the mono-material phantom, using a reference scan of a simple, fully dense object, imaged under the same conditions as the phantom. The difference here was that two reference scans, one for each component material, was required, and the volume fraction of one material in the phantom was obtained by linear interpolation.
between the attenuation coefficients observed for the two materials. This approach assumes that there is no third material (such as air) in the structure, that would mean there is no unique material combination to produce an observed effective linear attenuation coefficient.

In addition to the simulations corresponding exactly to those for the mono-material phantom, dual-energy scans were simulated, too. Whilst there are multiple ways of in practice collecting dual-energy information (including fast-kV switching, use of an energy-sensitive detector and two separate, simultaneously operating imaging lines, see [14]), the most accessible option industrially is sequential scanning with different source parameters, so that is the set-up envisaged here. The two polychromatic scans were based on acceleration voltages of 120 and 200 kV, respectively, using a 1 mm copper pre-filter in the latter case (none for the former). The monochromatic simulations performed for comparison used photons at 110 keV and 190 keV, for low- and high-energy scans, respectively.

For the dual-energy scans, a simple, image-based decomposition is reported on here. This is based on analytically solving the linear simultaneous equations formed for the linear attenuation coefficients of the two scans [15]. This sort of approach is more industrially accessible, but also less capable than alternative possibilities such as an Empirical Dual Energy Calibration (EDEC) [16-17], or a full projection-based method [18-19].

2.2 Experimental Plan

To demonstrate the value of the approach initially explored by simulation, functionally graded material samples were designed, manufactured and subjected to XCT scanning, prior to analysis of the scan data. Given the coarse nature of the graded structure, and the relatively compact sample size, a low magnification XCT scan was used to explore the compositional assessment capabilities, whilst a high-resolution XCT scan, analyzed by segmentation of the component materials (see Section 1), was used for validation.

2.2.1 Mono-material

For the mono-material case, a sample geometry, based on varying strut thicknesses in a regular lattice, was designed by MTC and manufactured on a Stratasys J750 printer in Stratasys Vero [20-21]. One instance of the sample is pictured in Fig 4. The geometry is also being printed in titanium on a metal AM system.

![Figure 4: Photograph of the polymer mono-material sample created.](image)

2.2.2 Bi-material

Whilst there are numerous AM systems that offer multi-material printing capabilities, for example enabling pre-operative planning aids to be printed with multiple colors and varying transparency, such capabilities are not widespread yet for AM of mechanically functional components. Based on the capabilities currently available at the MTC, it was decided to make the bi-material samples by resin in-fill of instances of the mono-material samples presented in the preceding section.

3 Results

3.1 Simulations

3.1.1 Mono-material

The initial results obtained, using a reference scan for mapping greyscales to density values, are shown in Fig. 5. Poisson noise was added to the projections prior to reconstruction.
Figure 5: The material volume fraction computed for the mono-material phantom, inspected at low and high magnifications. On the left the results for the monochromatic spectrum are shown, on the right, those for the polychromatic spectrum, with and without beam-hardening correction (bhc). This correction allows results to be obtained that closely match the monochromatic performance, though with more noise. The lower magnification smooths out the values obtained, but otherwise the high and low magnification outputs are equivalent, despite the previously highlighted degradation in image quality associated with the latter.

An alternative presentation of the results to focus on the errors of the derived composition is shown in Fig. 6, for which the compositional values across each phantom strip were reduced to a single number, avoiding the interface regions. The error bars are derived from obtaining multiple values using a laterally sliding window along the length of each strip (avoiding the strip ends).

Figure 6: The results seen in Fig. 5 analyzed in terms of the deviation from the ground truth volume fraction. On the left the results for the monochromatic spectrum are shown, on the right, those for the polychromatic spectrum, with and without beam-hardening correction (bhc). The graphs emphasize the improvement obtained by using beam-hardening correction for the polychromatic spectrum, as well as the fact that the monochromatic results remain better.

Both alternative analysis routes proved to be problematic. For the second method, even when the histogram was restricted to a region of interest in the reconstruction, focused on the densest elements of the phantom, the recovered value was lower than the desired value by several percent, giving rise to substantial density overestimates (deviation rising with density). This demonstrated that, without a section of the sample known to be fully dense in the field of view of the scan, any attempt to avoid a separate reference scan should be treated with great caution. The third method, based on an ISO50 binarization, gave rise to substantial overestimates of the fractional density, especially at low magnification, rendering this approach useless in this context.

3.1.2 Bi-material

The results are shown in Fig. 7, now considering only the high magnification setting, having confirmed in the mono-material tests that there are no unwanted complicating factors associated with different magnifications. For the polychromatic data, two forms of beam-hardening correction were applied, one for each of the two component materials. Note Poisson noise was not added to the simulations for the results presented in this section.
Figure 7: The volume fraction of material 1 (titanium) computed from a single scan, under different inspection configurations: a monochromatic spectrum, a polychromatic spectrum, and the polychromatic spectrum, but applying either the beam-hardening correction for titanium (Ti-bhc) or iron (Fe-bhc). It is apparent that the latter provides the best option in this scenario for recovering performance close to that of a monochromatic inspection (mostly obscured by the ground truth line).

The results obtained for the analytical dual-energy scheme are shown in Fig. 8. Note that this approach allows the two material volume fractions to be recovered separately, both are plotted, subtracting the fraction from 1 for the second material (iron).

Figure 8: The volume fraction of material 1 (titanium) computed for a dual-energy inspection using the analytical decomposition. On the left, the results are shown for the monochromatic case, on the right for the case of a polychromatic spectrum, with iron beam-hardening correction applied. The latter is seen to give poor performance near the edges of the sample. In line with the performance seen in Fig. 7, only these simulation variants are considered – the others fail badly.

3.2 Experiments

Given delays in the manufacture of the samples, it was not possible to complete the XCT data collection and analysis of the results in time for the conference manuscript deadline, but the experiments will be reported on in the conference presentation.

4 Discussion

The simulations with the mono-material phantom reveal few surprises, but do provide reassurance that there are no clear confounding effects associated with imaging a microstructure sample at a macro level, a potential problem given e.g. partial volume effects. The results further confirm what might have been suspected, that the beam-hardening associated with a polychromatic spectrum of a lab XCT scanner can undermine the analysis and should be managed by applying an effective beam-hardening correction. The photon scatter likely to contribute to an experimental output is similarly expected to be detrimental to the measurements. The most striking output of the simulations on the mono-material phantom is the confirmation that it is likely to be impossible to avoid a reference scan of a fully dense sample. Additionally, the failure of the ISO50-based approach means that attempting to assess the density by segmentation of the scan volume for a sample containing pores below the resolution of the scan is not to be recommended.
The bi-material phantom simulations confirm that this scenario is much more challenging than a mono-material set-up. However, by making the assumption that no third material (e.g. air) is present in the structure, a promising ability to derive the material volume fraction can be observed. This not only applies for a hard-to-implement monochromatic set-up: applying the beam-hardening correction for the more absorbing of the two constituent materials of the phantom to the polychromatic data worked convincingly, and much better than the other material’s beam-hardening correction. Further work is required to see whether this generalizes to other material systems. The dual-energy scanning avoids the assumption about the lack of a third material, but necessitates more data collection. The analytical material decomposition was seen to work reasonably well for the monochromatic and iron beam-hardening corrected datasets, though the latter is severely compromised at the edges of the sample, most likely due to remnant beam-hardening. Clearly, one could also explore the application of a more advanced decomposition scheme for the dual-energy scanning [16-19], but any such approach would be less accessible industrially than a pure image-based method.

In general, the results suggest that XCT can be used as an industrial tool of compositional quality control, subject to constraints and caveats. For example, clearly, beam-hardening is a problem, especially in a true multi-material scenario. Moreover, what algorithms have been devised for multi-material beam-hardening correction [22-23], are not directly applicable to a graded-material inspection, as these algorithms rely on the segmentation of the different materials in the image – impossible for a compositionally graded structure. However, it might be possible to use an initial decomposition (e.g. see Fig. 7) as a fractional segmentation for an improved beam-hardening correction and hence decomposition. Additionally however, scatter is likely also to compromise the accurate derivation of local sample composition.

Whilst the paper here has considered graded samples of one to two materials, the need may arise in due course to assess the local composition of graded structures containing three or more constituent materials (including air). Given that, in the lower X-ray energies examined here, there are only two types of photon-matter interaction for each material (both with quasi-linear energy dependencies), adding further energy channels to the inspection (e.g. “triple-energy XCT”) will still not allow the three (or more) materials to be decomposed uniquely, due to the (in the absence of practically usable absorption edges in the absorption spectra of the materials) lacking linear independence. The options for tackling this scenario are twofold. Firstly, one can complete one scan at such a high energy that a third photon-matter interaction (pair production) plays a role in the X-ray absorption observed. This in principle would then provide a linearly independent measure of the sample absorption, and hence allow a three-way decomposition to be achieved unambiguously. Secondly, one can exploit prior knowledge about the sample / make reasonable assumptions, a possibility we will discuss further.

For instance, in the simplest form, the assumption of volume conservation, allows us to confirm that there is (essentially) no air in the structure for the results of Fig. 8, as we can see that (to a close approximation) the volume fractions for the two constituent materials sum to unity. Of course any assumption implies a degree of risk as the result of the analysis will be wrong if the assumption is not satisfied, which for volume conservation may in practice occur numerically due to noise in the (reference) scans. Under such circumstances it may be better to solve for the properties of the constituent materials rather than to try to measure these directly [24]. For tackling n-fold material decompositions, assumptions quickly become essential, for example to locally reduce the problem to a 3-fold decomposition that can be tackled by a dual-energy inspection [25]. In the context of AM inspection, where the nominal local composition is known, such a reduction of an intractable n-fold decomposition problem to a series of local 3-fold decompositions should be readily achievable for all practical graded material inspection challenges of the foreseeable future, though one must accept the contamination of the results in the interfaces between the identifiable 3-material regions.

5 Conclusions

XCT is being further developed as a tool of compositional quality control, driven by the needs of advanced AM methods, building on methods used in medical imaging. Initial simulations have allowed the most promising analysis approaches to be identified, with experimental demonstration and validation to follow. The results also have immediate implications for the assessment of density in the presence of pores below the resolution limit of the scan. Further work is needed to refine the use of XCT in this context, especially with respect to confounding effects due to beam-hardening and scatter.

Acknowledgements

This work has been funded by the MTC from UK High Value Manufacturing Catapult support, as part of NB’s secondment to MK’s group at DKFZ. Parts of the reconstruction software were provided by RayConStruct® GmbH, Nürnberg, Germany. We thank NB’s MTC colleagues Ollie Hartfield, Chris Burchell and Shaun Smith for the design, manufacture and scanning, respectively, of the samples.

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