Translation of CT data into voxel-specific micromechanics-based elasticity tensors

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Aims
The use of computer tomography (CT) imaging is steadily increasing in the ever growing bone implant/surgery and tissue engineering market, although commercial exploitation of CT data for structural design purposes is still based on trial-and-error approaches. This is because X-ray attenuation information is reduced to geometric grey level evaluation, and mechanical properties such as stiffness are often derived from empirical regression functions between grey values, mass density, and elastic constants. As a remedy, we here introduce a technique for (i) conversion of voxel-specific attenuation coefficients into chemical composition, and (ii) translation of these volume fractions, via micromechanics laws, into voxel-specific, inhomogeneous and anisotropic material properties. The application of this method is demonstrated for two classes of materials, namely commercial ceramic (carbonated hydroxyapatite) bone biomaterials, and extracellular bone matrix. Currently, this technique is being made compatible with the commercial software of SKYSCAN.

Method
Commercial porous biomaterial granules made of synthetic carbonate-substituted hydroxyapatite¹ for bone replacement or tissue engineering, with two different diameter size distributions of 0.7 and 2 mm, were scanned with a micro-CT scanner (Skyscan 1172, Skyscan, Belgium) at a resolution of 3.49 μm. A mouse femur was scanned with a micro-CT scanner (Skyscan 1172) at a resolution of 6.78 μm.

The grey scale values (GS) of a computer tomographic image are linearly related to voxel-specific X-ray attenuation coefficients $\mu$, the attenuation coefficient of one voxel is the sum of the attenuation coefficients of the single constituents within this voxel, weighted by their volume fractions. These two basic relationships are used for computing the voxel-specific (nano)porosity of ceramic bone biomaterials, and the composition of extracellular bone matrix, in terms of the volume fractions of the bone mineral (hydroxyapatite), of the organic matter (90% of which is collagen), and of the water in the nanopores spaces between the collagen molecules or the mineral crystals.

For computing voxel-specific elasticity tensors from the aforementioned voxel-specific chemical information, we use homogenization procedures in the framework of continuum micromechanics³. As concerns the carbonated hydroxyapatite biomaterial, a single-step homogenization scheme is employed⁴.⁵. Within a material volume (representative volume element – RVE) with a characteristic length of several microns (coninciding with the considered voxel), we discern, as material phases, spherical pores and solid crystals. The latter are represented as spheres, needles, or discs. Besides shape, the material phases are
characterized by their volume fractions (nanoporosity for the pores, and the rest of the RVE filled by the crystals), by “universal” (sample-independent) stiffnesses (zero for the pores, and that of hydroxyapatite for the crystals), as well as by their interactions, here by direct mechanical interaction as in a polycrystal (mathematically realized by means of a self-consistent scheme). As concerns the extracellular bone matrix of the mouse femur, the volume fractions of hydroxyapatite, of collagen, and of water plus non-collageneous organics serve as input for a multistep homogenization scheme for the elasticity of bone materials\(^6\), which is based on ‘universal’ (tissue-independent) elastic properties of hydroxyapatite, of water, and of collagen. The first homogenization step refers to an observation scale of several nanometers, where crosslinked collagen molecules form a contiguous matrix, which is ‘perforated’ by intermolecular, water-filled spaces. We call the homogenized material ‘wet collagen’. At the fibrillar observation scale (100-500 nanometers), wet collagen and mineral crystal agglomerations penetrate each other, building up the mineralized fibril. The last homogenization step refers to a material volume with 5 to 10 microns characteristic length (coinciding with the considered voxel), where mineralized fibrils are embedded as inclusions into the extracellular mineral foam (a porous polycrystal), forming together the extracellular bone matrix. For each scale, the morphology of the phases is defined in terms of spheres or cylinders, and a suitable homogenization scheme is considered: the Mori–Tanaka scheme is used for composite materials such as the extracellular bone matrix or wet collagen, and the self-consistent scheme is employed for all other material volumes (with polycrystalline morphology).

Results

Colour representations of (nano)porosity of biomaterials and of volume fractions of extracellular bone matrix are depicted in Figures 1 and 3. The corresponding distributions of isotropic elasticity in case of ceramic biomaterials, and of transversely isotropic elasticity in case of the mouse femur, are shown in Figures 2 and 4.

Figure 1: Reconstructed micro-CT image of a ceramic bone biomaterial (voxel size 3.49 microns): (a) typical slice, and (b) colour representation of (nano)porosity for one image
Figure 2: Distribution of voxel-specific isotropic elasticity in the ceramic bone biomaterial depicted in Figure 1, in terms of colour representations of (a) Young's modulus [GPa], (b) Poisson's ratio.

Figure 3: Colour representation of volume fractions of (a) bone mineral, (b) organic matter, and (c) water, for a micro-CT image of a mouse femur, settings: photon energy $E=10$ kEV, mean extracellular matrix mass density $\rho^\text{ec} = 2.0$ g/cm$^3$. 
Figure 4: Distribution of voxel-specific transversely isotropic elasticity in the mouse femur, in terms of colour representation of engineering stiffness constants: (a) transverse Young’s modulus $E_{11}$ [GPa], (b) axial Young’s modulus $E_{33}$ [GPa], (c) axial shear modulus $G_{23}$ [GPa], (d) Poisson’s ratio $\nu_{12}$ in isotropic plane, and (e) axial Poisson’s ratio $\nu_{13}$; settings: photon energy $E=10$ kEV, mean extracellular matrix mass density $\rho^e = 2.0$ g/cm$^3$.

**Conclusion**

We have presented a new concept for translating CT data into nanoporosity of ceramic scaffold materials and into the chemical composition of extracellular bone matrix, and for voxel-specific (multiscale) homogenization of elastic properties, based on the composition and microstructure of the materials. These mathematical relations are currently translated into a Graphical User Interface, as to demonstrate the functionality of the new concept and to allow for user-specific settings and refined data input and output. Finally, the software is currently made compatible with SKYSCAN’s package “CT-Analyser” (CTAn)$^\text{7}$.

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References: