

Quantitative assessment of bone's ultrastructural orientation by a novel 3D scanning SAXS method

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The arrangement and orientation of the ultrastructure plays an important role in the mechanical properties of inhomogeneous and anisotropic materials, such as polymers, wood, or bone. In this study, a novel method is presented, which allows deriving the three-dimensional (3D) orientation of the material's ultrastructure in a quantitative and spatially resolved manner. The proposed 3D scanning small-angle X-ray scattering (3D scanning SAXS) method was applied to a section of a human vertebral trabecular bone specimen. A micro-focus X-ray beam was used to raster scan the sample for different rotation angles that covered almost the full 360° range, excluding a small angular range, where the bone section was practically parallel to the X-ray beam. A mathematical framework was developed to describe the relation between the two-dimensional (2D) information regarding bone's ultrastructural orientation, which is retrieved from the X-ray diffraction patterns for the different rotation angles, and the local 3D orientation of the bone ultrastructure. This allowed deriving the local 3D orientation of the bone ultrastructure with high certainty, by fitting the theoretical model to the experimental data (mean and median coefficient of determination equal to 0.94 and 0.99, respectively). The bone's ultrastructural orientation has been visualized by a 3D orientation map using vector fields, which revealed links between trabecular bone microarchitecture and local ultrastructure. Moreover, the 3D orientation maps may help to quantify and understand structure-function relationships linking bone ultrastructure and bone mechanics. Finally, the proposed 3D scanning SAXS method can also be used in other research fields such as material science, to derive the 3D orientation of ultrastructural material components on a local level.

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