Determination Of 3d Strain Behavior Of The Mineral Phase.

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Introduction: Introduction: Bone toughness is rooted at the ultrastructural level. A novel approach was attempted in this study to quantify the deformation of bone mineral crystals at the ultrastructure level using synchrotron X-ray scattering techniques. Mineral crystals in bone are distributed in different orientations. In a previous study, we developed a 2D model of strain distribution in the mineral phase of bone based on the orientation dependent deformations of individual crystal subsets. In this study, we intended to develop a novel methodology for defining the 3D strain tensor of the mineral phase so as to quantify age-related changes in the in situ mechanical behavior of the mineral phase in bone.

Methods: Methods: Cylindrical compressive specimens (Φ3.0×5.0mm) were harvested from the mid-diaphyses of five male human cadaveric femurs: 51.6±1.8 years (N=5). A monochromatic high-energy X-ray beam from a synchrotron source was irradiated to the center of the specimen, which was deformed in a progressive cyclic loading scheme. Concurrently, WAXS patterns were recorded sequentially at each incremental strain level [1]. Bone specimens were kept moisturized throughout the experiment.

From the synchrotron X-ray scattering measurements, six lattice planes in a mineral crystal, namely (002), (310), (213), (113), (221) and (222), were selected to measure the mineral strains of the crystal in the normal direction to the planes. The strains calculated in the normal direction to the plane surface were converted to Euler angles to be used in Equation 2. The strains were measured on a 2D area detector at different azimuth angles (χ) corresponding to the angle between each lattice-plane-normal and the longitudinal direction.

The strain tensor in a 3D orthogonal co-ordinate system is given as shown by the 3×3 matrix (Equation 1). Six different equations are obtained using the equation shown below (Equation 2) forming a system of linear equations with six variables. The right hand side of Equation 2 is the strain value obtained on the lattice plane normal to the surface. The coefficients fij are calculated as described below. The strains measured in the detector plane were used for out of plane deformations, with the assumption that the mineral crystals along the loading direction are transversely isotropic in deformation. Where the coefficients fij for εij were calculated using the following relation: f11 = d2; f12= 2de; f22=e2; f23=2ce; f33=c2; where a = sinθcosω + sinχcosθsinω; b=cosχcosθ; c=sinθsinω -sinχcosθcosω; d= a cosΦ -bsinΦ; e=asinΦ + bcosΦ [2]

Fig. 1a Euler Angles depicting rotation of plane with respect to laboratory coordinates. 1b Determination of strain tensor of individual subsets of mineral crystals(η) using different lattice planes. 1c Euler angles calculated by fixing a coordinate system on the sample surface with S3 axis as the surface normal.

Results: Results: The resulting strain values are as shown in the table below (Table 1).

Strain values in shear can be noticed as consistently high compared to the normal strains along the loading axis.

Discussion:
Discussions: The 3D stress tensor (σij) can be obtained from the 3D strain tensor assuming a linear elastic model.

Significance: The strain tensors obtained can be used to characterize the Elastic stress-strain behavior of the mineral phase for a subset of crystals. In this study we have established a strain tensor for mineral crystallites oriented along the loading axis, further work to obtain strain tensors for mineral crystal subsets oriented along different axes would provide stress-strain behavior as a function of the orientation distribution of the mineral phase.

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Table 1. 3D Strain Values (%)

<table>
<thead>
<tr>
<th>Strain (%)</th>
<th>Cycle 1</th>
<th>Cycle 2</th>
<th>Cycle 3</th>
<th>Cycle 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{11}$</td>
<td>-0.236</td>
<td>-0.378</td>
<td>-0.379</td>
<td>-0.455</td>
</tr>
<tr>
<td>$\varepsilon_{12}$</td>
<td>-0.979</td>
<td>-1.623</td>
<td>-0.659</td>
<td>-0.0138</td>
</tr>
<tr>
<td>$\varepsilon_{22}$</td>
<td>0.003</td>
<td>0.060</td>
<td>0.442</td>
<td>0.759</td>
</tr>
<tr>
<td>$\varepsilon_{13}$</td>
<td>-1.020</td>
<td>-1.631</td>
<td>-0.716</td>
<td>-0.094</td>
</tr>
<tr>
<td>$\varepsilon_{23}$</td>
<td>-0.271</td>
<td>-0.613</td>
<td>-0.059</td>
<td>0.336</td>
</tr>
<tr>
<td>$\varepsilon_{33}$</td>
<td>-0.621</td>
<td>-0.974</td>
<td>-0.348</td>
<td>0.118</td>
</tr>
</tbody>
</table>

$$f_{\text{11}}\varepsilon_{11} + f_{\text{12}}\varepsilon_{12} + f_{\text{22}}\varepsilon_{22} + f_{\text{13}}\varepsilon_{13} + f_{\text{23}}\varepsilon_{23} + f_{\text{33}}\varepsilon_{33} = \frac{\lambda}{2d_0 \sin \theta} - 1$$