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Supporting information for article:

Precision lattice parameter determination from transmission diffraction of thick specimens with irregular cross sections

S. R. Stock, M. Laugesen, H. Birkedal, A. Jakus, R. Shah, J.-S. Park and J. D. Almer

Supplemental material

Effect of variable sample to detector distance

In transmission diffraction, Fig. 1 shows the center of mass of the distal metaphysis of a second human metacarpal bone (Mc2) can vary substantially between different x-ray beam paths through the specimen. Consider the parameters of the experiment described in this paper: X-ray energy 71.676 keV (wavelength 0.17300 Å), d_{002} = 3.4325 Å for synthetic hydroxyapatite (hAp, Powder Diffraction File 86-1201) and a nominal sample-detector separation of 2.800 m. The nominal 00.2 diffraction angle is $2\theta = 2.8881°$. If the actual sample-detector separation was 2.805 m, trigonometry shows that a sample with d_{002} = 3.4386 Å would produce a 00.2 diffraction ring at the same 2θ as above. If the actual sample-detector separation was 2.810 m, d_{002} = 3.4447 Å would be responsible for the rings. Displacement-related errors of 0.0061 Å and 0.0122 Å (for 5 mm and 10 mm displacement, respectively) are significant for studies of bone lattice parameters and might very well be encountered in transmission diffraction studies of intact Mc2.

Parameters for laboratory microCT imaging of the specimens

Laboratory microCT was performed with a Scanco MicroCT-40 system. Each specimen was imaged separately with 70 kV tube voltage, 114 μA tube current and 500 projections each with 300 ms integration time. The 20.5 mm diameter field of view was reconstructed on a 1024 x 1024 grid using the Scanco software with 20 μm isotropic volume elements (voxels).