

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Combined X-Ray and Neutron Powder Diffraction Studies of Nanoscale  $\text{Ca}_{5-x}\text{Fe}_x(\text{PO}_4)_3\text{OH}$  Systems** A. KYRIACOU, TH. LEVENTOURI, Florida Atlantic University, B.C. CHAKOUMAKOS, V.O. GARLEA, C.D. CRUZ, Neutron Scattering Science Division, Oak Ridge National Laboratory, A.J. RONDINONE, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, K.D. SORGE, Florida Atlantic University — Multi-substituted hydroxyapatite (HAp) with crystallite size 4-130 nm is the major mineral phase in physiological apatites. Substitutions at all ionic sites affect their physicochemical properties. Fe is one of the minor substitutions at the Ca sites of HAp. It is important because it reduces the solubility of HAp, functioning as a cavities preventive agent, whereas Fe overload leads to a decreased mechanical strength and osteoporosis. Powder x-ray and neutron diffraction methods as well as energy-filtered transmission electron microscopy were used to study the effect of Fe substitution on the crystal structure properties of the  $\text{Ca}_{(5-x)}\text{Fe}_x(\text{PO}_4)_3\text{OH}$  systems. Single phase HAp is identified in systems with  $x \leq 0.1$ . Hematite is formed for higher x. Simultaneous Rietveld refinement of the x-ray and neutron diffraction patterns reveals an unexpected increase of the a-lattice constant. It is attributed to the increase of the Ca1-O3 and Ca2-O1 interatomic distances indicating a local lattice relaxation. Fe substitutes in both Ca1 and Ca2 sites with a preference to the Ca2 site and an occupancy up to 0.05 for x=0.3. Magnetic measurements reveal a transition from the diamagnetic state of the HAp to the paramagnetic of the Fe-doped systems.

A. Kyriacou  
Florida Atlantic University

Date submitted: 11 Nov 2011

Electronic form version 1.4