Abstract Submitted
for the TSF06 Meeting of
The American Physical Society

X-ray Diffraction and Polarized X-ray Absorption Study of Single Crystal LiFePO₄

GAN LIANG, Sam Houston State University, RON BENSON, Rigaku/MSC, JIYING LI, DAVID VAKNIN, Iowa State University, MARK CROFT, Rutgers University — Large size LiFePO₄ single crystals have been grown by standard flux growth technique with the LiCl as the flux. Single crystal x-ray diffraction (XRD) and synchrotron polarized x-ray absorption spectroscopy (XAS) measurements have been performed on the crystals. The XRD measurements were performed at T = 293 K using Mo $K_α$ radiation ($\lambda = 0.7107\text{Å}$) to a resolution corresponding to $\sin\theta/\lambda = 0.6486 \text{ Å}^{-1}$, with $2\theta_{\text{max}} = 54.9^\circ$. A total number of 1330 reflections were processed with 350 unique data. The obtained crystal structure data were the following: lithium iron (II) phosphate, LiFePO₄, orthorhombic, space group $Pnma$, lattice constants: $a = 10.3172 (11) \text{ Å}$, $b = 6.0096(8) \text{ Å}$, $c = 4.6775 (4) \text{ Å}$, Z = 4, formula weight: 157.76, density: 3.613, $\mu = 55.562 \text{ cm}^{-1}$. The bond lengths between Fe and O and between P and O were obtained. The polarized XAS was performed at the Fe $K$-edge with the x-ray $E$-vector along the $a$-, $b$-, and $c$-axis. The XAS results show that the Fe ions in the LiFePO₄ single crystals are divalent. We also observed a big shift in both the energies of the pre-edge $1s \rightarrow 3d$ transition feature and the main edge when the polarization direction of the $E$-vector changes from along $a$-axis to along $c$-axis.

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Date submitted: 18 Sep 2006

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