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X-ray Diffraction and Polarized X-ray Absorption Study of Single Crystal $LiFePO_4$ GAN LIANG, Sam Houston State University, RON BENSON, Rigaku/MSC, JIYING LI, DAVID VAKNIN, Iowa State University, MARK CROFT, Rutgers University — Large size $LiFePO_4$ 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 (λ = 0.7107Å) to a resolution corresponding to $\sin\theta/\lambda$ = 0.6486 $Å^{-1}$, with $2\theta_{max} = 54.9^\circ$. A total number of 1330 reflections were processed with 350 unique data. The obtained crystal structure data were the following: lithium iron (II) phosphate, $LiFePO_4$, orthorhombic, space group *Pnma*, lattice constants: a = 10.3172 (11) Å, b = 6.0096(8) Å, c = 4.6775 (4) Å, Z = 4, formula weight: 157.76, density: 3.613, μ = 55.562 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 $LiFePO_4$ 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 $\boldsymbol{E}$-vector changes from along a-axis to along c-axis.

Gan Liang
Sam Houston State University

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