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Diffusion and possible freezing phases of Li-ions in $LiFePO_4$[1]
YUEN YIU, Ames Laboratory, Iowa State University, RASMUS TOFT-PETERSEN, Helmholtz-Zentrum Berlin, GEORG EHLERS, Oak Ridge National Laboratory, DAVID VAKNIN, Ames Laboratory, Iowa State University — Elastic and inelastic neutron scattering studies of $LiFePO_4$ single crystal reveal new Li-ion diffusion properties relevant to its function as Li-battery materials. In the past decade there has been broad interest in $LiFePO_4$ and its related compounds, largely due to the applications of these materials as cathodes in Li- batteries. This is owing to these materials' high charge-discharge ability and conductivity, both of which are by virtue of the Li-ions' high mobility. In this talk, we present our findings on the temperature and directional dependence of Li-ions' diffusion in $LiFePO_4$. $LiFePO_4$ adopts the olivine structure at room temperature (Space group: *Pnma*), which contains channels along principal crystalline directions that allow Li-ion motion. Elastic neutron scattering reveals lowering of symmetry from the Pnma structure below room temperature, which can be interpreted as the freezing of Li-ions, and can be subsequently linked to the reported decrease in Li-ion conductivity. Inelastic neutron scattering, in the 35K to 720K temperature range, shows temperature dependence, as well as anisotropy (i.e. along 0K0 versus 00L) of Li-ion diffusion.

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