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Sublattice Melting in $\mathbf{Na}_x\mathbf{V}_2\mathbf{O}_5$[1] RAYMOND OSBORN, MATTHEW KROGSTAD, STEPHAN ROSENKRANZ, PETER ZAPOL, ANH NGO, JOHN VAUGHEY, Argonne Natl Lab, JACOB RUFF, CHESS, Cornell University — We have developed efficient methods of measuring single crystal diffuse scattering, using synchrotron x-rays, that provide new insights into cation disorder in electrode materials. Large volumes in reciprocal space are transformed into 3D pair distribution functions (3D-ΔPDF) that image defect-defect correlations in real space, allowing a model-independent view of short-range order. We demonstrate this with data on β-$Na_xV_2O_5$ with $x = 0.2$ and 0.4 over the temperature range 100K to 500K. The sodium intercalants partially occupy sites on two-rung ladders penetrating the framework of vanadium oxide pyramids and octahedra, with no long-range order at room temperature and above. However, at $x = 0.4$, the length scale of sodium-sodium correlations increases significantly below 200K with the emergence of forbidden Bragg peaks below an order-disorder transition. The 3D-ΔPDF show that the sodium ions occupy alternate sites on each ladder rung, with a zig-zag configuration that is in phase with neighboring ladders. The growth in the length scale of sodium-sodium correlations with decreasing temperature is clearly seen in real space images that allow a quantitative determination of the interionic interactions that impede ionic mobility.

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