Phase diagram of Na$_{1-x}$Ca$_x$V$_2$O$_4$ compounds synthesized at high pressure

TAMAS VARGA, JOHN MITCHELL, Argonne Natl Lab, KAZUNARI YAMAURA, DAVID MANDRUS, Oak Ridge Natl Lab, JUN WANG, Argonne Natl Lab — Ambient pressure CaV$_2$O$_4$ and high-pressure NaV$_2$O$_4$ crystallize in the CaFe$_2$O$_4$ structure type containing double chains of edge-sharing VO$_6$ octahedra. Recent measurements on NaV$_2$O$_4$ reveal low-dimensional metallicity and evidence of half-metallic ferromagnetism. In contrast, CaV$_2$O$_4$ is an antiferromagnetic insulator. To explore the evolution of these ground-state behaviors, we have prepared a series of Ca-doped NaV$_2$O$_4$ compounds with the formula Na$_{1-x}$Ca$_x$V$_2$O$_4$ (x=0-1) using high-pressure synthesis. The lattice parameters of Na$_{1-x}$Ca$_x$V$_2$O$_4$ samples change with nominal x according to Vegard’s law. The metallic state in NaV$_2$O$_4$ is dramatically altered by Ca doping. Samples with higher Ca concentrations (x=0.6-0.8) exhibit a metal-insulator transition around 150 K. Samples at the Na end (x=0-0.2) show a broad antiferromagnetic transition in the 120-160 K range in accordance with earlier reports. With increased Ca doping, the antiferromagnetic transition is suppressed to $\sim$70 K at the Ca-endmember. Transport measurements show an insulator-metal transition at x$\sim$0.4. Comparison to existing studies at the Ca- and Na-rich ends will be discussed along with a schematic (T-x) phase diagram for the Na$_{1-x}$Ca$_x$V$_2$O$_4$.