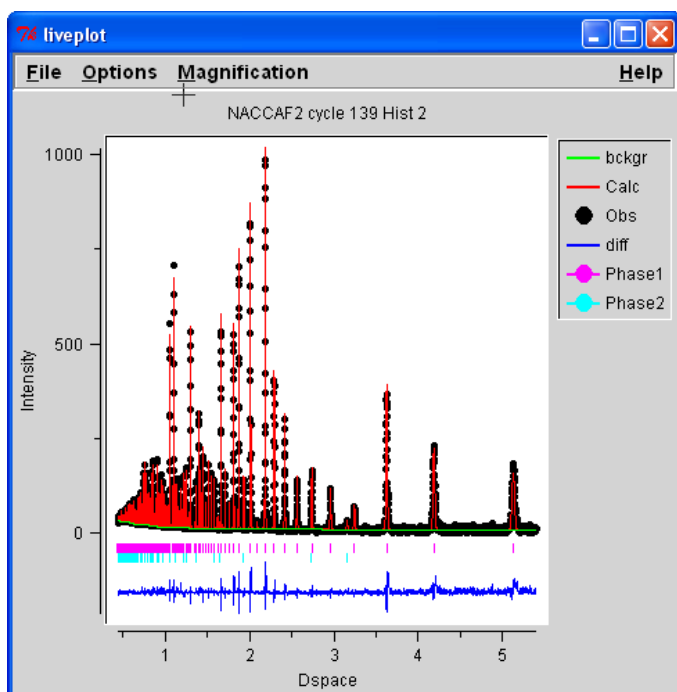


USE OF NAC AS A POTENTIAL LARGE D-SPACE STANDARD FOR POWDER DIFFRACTION PATTERNS

J. Faber, Faber Consulting, Thornton, PA 19373

Instrument standards for powder diffraction focus on the use of NIST standard materials for instrument calibration. The most frequently used standards are Si(SRM-640C), LaB₆ (SRM 660C), corundum (SRM 676 and SRM 1976). However, none of these standard materials contain d-spaces larger than 4.2Å. In the case of neutron TOF experiments on POWGEN at the Spallation Neutron Source (SNS), Na₂La₃Al₂F₁₄ (NAC) has been used to expand the calibrated d-space range to 7.225Å; NAC crystallizes in a bcc lattice, I213. One advantage for neutron powder diffraction is that the absorption cross section is quite modest when compared to X-ray Cu radiation. This has consequences for multiphase analyses. In this paper, we show the results of structural refinement using GSAS.



At least three weak reflections are observed that are not accounted for in the structural model. These are apparent in the difference plot seen in Figure 1.

A substantial improvement in the fit is obtained by adding a second phase, CaF₂. The weight fraction of second phase is ~3 wt.%. The PDF-4+ 2017 was used to help identify this phase.

Qualitative evidence for other phases is also observed. We shall discuss how the signal to noise ratio at large d-space hinders weak phase identification. The instrument upgrades to POWGEN should help to improve this situation.

Figure 1. Rietveld structural refinement of NAC using GSAS.