Can machines take over our jobs? – Fact or fiction, mission towards Rietveld refinement

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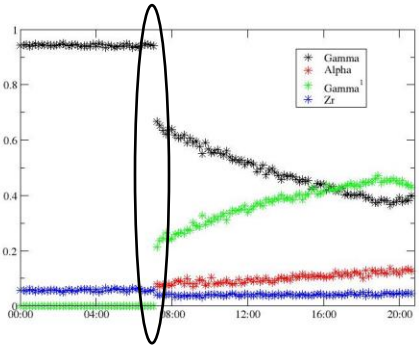
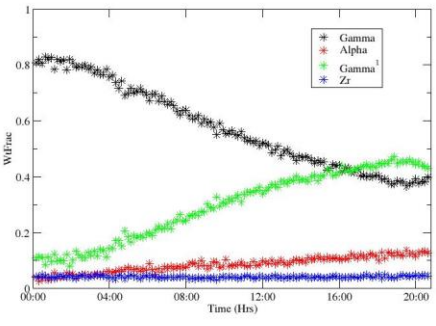
Neutron diffraction is an important characterization technique offering advantages when probing materials systems such as U-Mo, U-Nb and many more. The High Pressure Preferred Orientation (HIPPO) diffractometer at LANSCE (Los Alamos Neutron Science Center) is one of the sophisticated neutron diffractometers in the world capable of doing time resolved studies. Here we present a solution to one of the major problems while analyzing the data collected from HIPPO. When In Situ runs are performed on HIPPO for over 24 hours, it gives out over 10000 data sets for each sample. Each data set is then analyzed using GSAS (a Rietveld refinement software). But with the volume of the data collected it becomes impossible to analyze them individually. So, the final data set is analyzed using GSAS and the rest of the datasets are analyzed by automation using GSAS based bash scripts. But if the starting values for the Rietveld refinement (the lattice parameters in particular) are a bit off from the actual values the computer does not understand that and the Rietveld refinement doesn't converge resulting in some crazy values. So, most days for a scientist working on this is spent on finding good starting values for the Rietveld refinement which takes up most of his/her time. Here we provide an EMULATOR which could potentially take care of this problem by giving us pretty good starting values for the Rietveld refinement, which in turn would make the life of the scientists much easier. GSAS has the potential to simulate diffraction patterns for any material under study. So, we simulated patterns with varying lattice parameters, volume fractions and trained the emulator (emu needs over 1000 simulations to train) using these simulations. The Emu uses these simulations to constrain the uncertainty regarding the calibration parameters. The Emu is then fed with the experimental diffraction patterns. Emu uses this experimental data to predict the lattice parameters. The Emu uses Bayesian analysis via Markov chain Monte Carlo (MCMC). With Emu giving us the starting values for the lattice parameters, it reduces the time spent on Rietveld refinement (guessing the starting values) using GSAS. This would ultimately result in refining over large volumes of data sets using GSAS based bash scripts with as less human intervention as possible.



A plot showing Wt.Frac as a function of time analyzed using automated bash scripts, resulting in an artifact with the jump. It was caused due to poor starting values for the lattice parameter of the Alpha phase.

With human intervention, it takes weeks to analyze the data

With the EMULATOR it takes days/hours to analyze the data



The same plot showing Wt.Frac as a function of time analyzed after discovering the artifact. Data sets near the artifact were then analyzed individually using traditional GSAS with good starting values for the lattice parameter of the Alpha phase.