Investigating the Structure of La$_2$CuGa$_{12}$, Using Neutron Powder Diffraction

JASMINE MILLICAN, National Institute of Standards and Technology, JUNG YOUNG CHO, JULIA CHAN, Louisiana State University, JUDITH STALICK, National Institute of Standards and Technology — Single crystals of a new phase, La$_2$CuGa$_{12}$, have been synthesized using flux growth. Preliminary single crystal X-ray diffraction results suggest La$_2$CuGa$_{12}$ to be isostructural to Ce$_2$PdGa$_{12}$ and crystallize in the $P4/nbm$ space group with lattice parameters of $a \sim 6.179$ Å and $c \sim 15.384$ Å. Residual electron density, which was observed in the Fourier difference map of the single crystal X-ray diffraction data, and the observation of satellite peaks in the data are indicative of the possibility of statistical disorder in La$_2$CuGa$_{12}$. In addition, unusual behavior of thermal parameters for an additional Ga position is observed in the X-ray diffraction data of La$_2$CuGa$_{12}$. Although a preliminary model has been constructed using single crystal X-ray diffraction experiments, due to the two electron difference between $^{29}$Cu and $^{31}$Ga, neutron powder diffraction experiments may be a more suitable probe in accurately determining the structure and site occupancy of the additional Ga atom in La$_2$CuGa$_{12}$. We have employed neutron powder diffraction (BT-1) to investigate the structure in the phase, La$_2$CuGa$_{12}$.