Optimization and doping of 112 Fe pnictide single crystals\textsuperscript{1} AK-SHAT PURI, Stony Brook University, JENNIFER MISURACA, Stony Brook University, University of Illinois at Urbana-Champaign, JEDEISHIAH K. MORRIS, Stony Brook University, MEIGAN ARONSON, Stony Brook University, Brookhaven National Laboratory — The recent discovery of Ca\textsubscript{1-x}La\textsubscript{x}FeAs\textsubscript{2}, which when doped with Sb has a \(T_c\) of 43K, has led to an increased interest in Fe pnictides in the 112 structure \cite{1}. We have grown plate-like single crystals of LaFe\textsubscript{0.6}Sb\textsubscript{2} from a self flux. These form in a tetragonal 112 structure with many Fe vacancies, as measured by single crystal x-ray diffraction. The crystal growths were optimized in two ways. Arc melting elemental Fe granules before use resulted in larger (\(~1\text{ cm}^2\)) crystals, and including a rapid cool-down during the growth avoided the formation of a parasitic phase, thus increasing the yield. Doping Ni into the structure resulted in a change in the lattice constants from \(a = 4.4026\text{ Å}, c = 10.0341\text{ Å}\) for undoped LaFe\textsubscript{0.6}Sb\textsubscript{2} to \(a = 4.4343\text{ Å}, c = 9.8911\text{ Å}\) for LaNiSb\textsubscript{2}. Energy dispersive x-ray spectroscopy showed that Ni replaces Fe and also occupies the vacancies, and at 89\% Ni doping, there are no vacancies in the structure. Due to the many vacancies in undoped LaFe\textsubscript{0.6}Sb\textsubscript{2}, the Sb residing near the vacant sites is strongly anharmonic in character; the electronic structure changes with doping and this is seen in the parameter becoming harmonic. \cite{1} Kudo et al. arXiv:1311.1269 (2013).

\textsuperscript{1}We acknowledge the Office of Assistant Secretary of Defense for Research and Engineering for providing the NSSEFF funds that supported this research

Akshat Puri  
Stony Brook University

Date submitted: 15 Nov 2013  
Electronic form version 1.4