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Optimization and doping of 112 Fe pnictide single crystals[1] AKSHAT PURI, Stony Brook University, JENNIFER MISURACA, Stony Brook University, University of Illinois at Urbana-Champaign, JEDEDIAH K. MORRIS, Stony Brook University, MEIGAN ARONSON, Stony Brook University, Brookhaven National Laboratory — The recent discovery of $Ca_{1-x}La_xFeAs_2$, which when doped with Sb has a T_c of 43K, has led to an increased interest in Fe pnictides in the 112 structure [1]. We have grown plate-like single crystals of $LaFe_{0.6}Sb_2$ 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 ($\sim$ 1 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 Å, c = 10.0341 Å for undoped $LaFe_{0.6}Sb_2$ to a = 4.4343 Å, c = 9.8911 Å for $LaNiSb_2$. 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 $LaFe_{0.6}Sb_2$, 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. [1] Kudo et al. arXiv:1311.1269 (2013).

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