Abstract Submitted
for the 4CF12 Meeting of
The American Physical Society

Engineering direct-indirect band gap transition in wurtzite GaAs nanowires through size and uniaxial strain ANDREW COPPLE, NATHANIEL RALSTON, XIHONG PENG, Arizona State University — One dimensional semiconductor nanowires have been extensively researched in the past years because of their unique characteristics. Group III-V semiconductors show special promise in a wide range of applications, such as field-effect transistors, light-emitting diodes, and optical sensors. The fundamental properties of these materials are essential to their applications, particularly the electronic properties. In this presentation, we report first principles density-functional theory study on the electronic properties of wurtzite GaAs nanowires along the (0001) direction, with the diameter of the wires up to 3.0 nm [1]. It was found that the band gap of GaAs nanowires experience a direct-to-indirect transition when the diameter of the nanowires is smaller than $\sim$2.8 nm. For those thin GaAs nanowires with an indirect band gap, it was found that the gap can be tuned to be direct if a moderate external uniaxial strain is applied. Both tensile and compressive strain can trigger the indirect-to-direct gap transition. The critical strains for the gap-transition are determined by the energy crossover of two states in conduction bands.

[1] A. Copple, N. Ralston, X.-H. Peng, Appl. Phys. Lett.100, 193108 (2012).

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Date submitted: 21 Sep 2012 Electronic form version 1.4