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Strain manipulated direct-indirect band gap transition in GaAs nanowires XIHONG PENG, ANDREW COPPLE, NATHANIEL RALSTON, Arizona State University — One dimensional nanostructures of group III-V semiconductors have drawn broad research interests in recent years due to their potential applications in nano-electronics. In particular, GaAs has been considered as a promising channel material for the high speed NMOS beyond Si based technology. In this project, electronic structures of GaAs nanowires at both wurtzite and zinc blende phases were studied using first-principles Density Functional Theory (DFT) calculations. 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 a specific value [1]. 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 strain is applied. We found many types of strains, such as tensile and compressive uniaxial strain, radial strain, strain along a specific orientation in the cross-section of the nanowires, 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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