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Effect of Strain and Diameter on Electronic and Charge Transport Properties of Indium Arsenide Nanowires

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Abstract — The impact of uni-axial compressive and tensile strain and diameter on the electronic band structure of indium arsenide (InAs) nanowires (NWs) is investigated using first principles calculations. Effective masses and band gaps are extracted from the electronic structure for zero strain and strained nanowires. Material properties are extracted and applied to determine charge transport described within the effective mass approximation and by applying the non-equilibrium Green's function method. The transport calculations self-consistently solve the Schrödinger equation with open boundary conditions and Poisson's equation for the electrostatics. The device structure corresponds to a metal oxide semiconductor field effect transistor (MOSFET) with an InAs NW channel in a gate-all-around geometry. The channel cross sections are for highly scaled devices within a range of 3×3 nm^2 to 1×1 nm^2. Strain effects on the band structures and electrical performance are evaluated for different NW orientations and diameters by quantifying subthreshold swing and ON/OFF current ratio. Our results reveal for InAs NW transistors with critical dimensions of a few nanometer, the crystallographic orientation and quantum confinement effects dominate device behavior, nonetheless strain effects must be included to provide accurate predictions of transistor performance.

1. Introduction

Field-effect transistors (FETs) are on target to be manufactured with sub-7 nm critical dimensions within the next few years[1]. Electronic properties of materials at these length scales vary significantly with respect to the bulk due to increase in the surface-to-volume ratio and quantization effects arising at small critical dimensions[2,3]. Due to large quantum confinement effects in NWs, there is substantial band gap widening relative to the bulk energy gap. In addition to band gap widening, the direct or indirect nature of a semiconducting material can be