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# Influence of surface stoichiometry and quantum confinement on the electronic structure of small diameter $In_xGa_{1-x}As$ nanowires

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## HIGHLIGHTS

- Determination of electronic structures for small diameter $In_xGa_{1-x}As$ nanowires.
- Band gaps, effective masses, and density of states are extracted.
- Comparison of III-V nanowires with silicon nanowires of similar geometries.
- Impact of alloy stoichiometry on the electronic structure.
- Impact of atomic composition of nanowire surfaces on the electronic structure.

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## ABSTRACT

Electronic structures for $In_xGa_{1-x}As$ nanowires with [100], [110], and [111] orientations and critical dimensions of approximately 2 nm are treated within the framework of density functional theory. Explicit band structures are calculated and properties relevant to nanoelectronic design are extracted including band gaps, effective masses, and density of states. The properties of these III-V nanowires are compared to silicon nanowires of comparable dimensions as a reference system. In nonpolar semiconductors, quantum confinement and surface chemistry are known to play a key role in the determination of nanowire electronic structure. $In_xGa_{1-x}As$ nanowires have in addition effects due to alloy stoichiometry on the cation sublattice and due to the polar nature of the cleaved nanowire surfaces. The impact of these additional factors on the electronic structure for these polar semiconductor nanowires is shown to be significant and necessary for accurate treatment of electronic structure properties.

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## 1. Introduction

Transistor scaling results in a set of deleterious performance issues in general referred to as short-channel effects (SCEs). The onset of SCEs led to the requirement for various technology boosters to maintain continued transistor scaling while achieving enhanced performance [1]. Scaling has led to fin-like three dimensional field effect transistors, or FinFETs and most advanced device roadmaps are now including nanowire transistors for 4 nm technologies (although some care is required for defining critical dimensions for new technology "nodes"). Nanowires with gate-all-around architectures and with very small cross-sections provide excellent electrical characteristics with low standby power, and increase the potential for high-density integration. For nanowire diameters less than the Fermi wavelength of free charge carriers, quantum mechanical effects become pronounced. At these critical dimensions, quantum confinement leads to dramatically different electronic band structures with quite different band gaps and effective masses as compared to the same material in bulk form. As channel lengths decrease, carrier scattering is reduced and bulk properties such as charge carrier mobility must be abandoned or redefined for the quasi-ballistic regime.

Due to significantly higher bulk electron and hole mobilities, III-V materials such as $In_{0.53}Ga_{0.47}As$ and the group IV material germanium, respectively, have been suggested as a replacement for silicon as the channel material in advanced complimentary metal-oxide-semiconductor (CMOS) fabrication processes. Other III-V materials such as InAs NWs have also attracted considerable interests for their potential in high-performance applications in optoelectronics [2], as well as low-power logic applications [3]. Notwithstanding the technological challenges of replacing silicon

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in conventional semiconductor manufacturing, there is comparatively little known about the electronic structure of these replacement materials when patterned or grown in nanowires structures with diameters of the order of a few nanometer. Due to advances in bottom up as well as top down fabrication techniques, nanowires with diameters as small as 1 nm have been fabricated. To highlight recent work, we note the preparation of SiNWs with approximately 1 nm diameters for which the oxide sheath was removed and replaced with hydrogen termination; using scanning tunneling microscopy (STM) the band gap widening due to quantum confinement was reported [4]. Recently using a metalorganic chemical vapor deposition (MOCVD) via vapor-liquid-solid (VLS) growth method with gold nanoparticle catalysis, InAs NWs with approximately 2 nm diameter have been observed [5]. This study focuses on $In_xGa_{1-x}As$ nanowires with different crystallographic orientations and cross sections on the order of 5 square nanometer. Alloying on the cation sublattice is considered to be random as observed in the bulk. However, compound semiconductor growth is normally not under equilibrium conditions and the growth or fabrication conditions can lead to cation-rich surfaces or anion-rich surfaces. This leads to a new factor that impacts on the electronic structure of III-V compound semiconductor nanowires at small cross sections. The influence of either cation or anion atoms at the surface of the nanowires is explicitly considered in the calculations, and as will be shown, has a significant influence on the resulting electronic structure. There are previous reports of the electrical properties for InGaAs quantum wells and thin-body transistors [6–8]. However, studies of the electrical properties of $In_xGa_{1-x}As$ nanowires at dimensions of relevance for gate-all-around CMOS technologies with critical dimensions of 4 nm and less are not available. The critical dimensions (cross sectional area) considered are chosen to extract the interaction between quantum confinement and surface effects. The interplay between these effects is relevant for modern nanowire designs, particularly for nanoelectronics and sensing applications. We note that leading nanoelectronics manufacturers are currently developing devices for the 7 nm and 5 nm nodes [9–11]. The challenge for the research community is to explore the surface chemistry and confinement physics for nanowires with critical dimensions approaching atomic scale limits.

## 2. Methods

Fig. 1 shows the relaxed structures for three crystallographic orientations of GaAs nanowires considered in this study; these structures form the basis for the generation of the nanowires with differing alloy composition. All atomistic visualizations are rendered using VESTA [12].

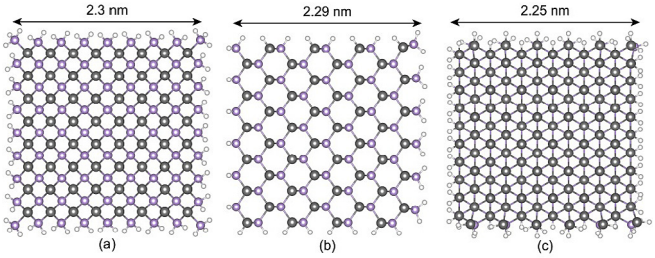


**Fig. 1.** Cross-section of GaAs NWs for (a) [100], (b) [110], and (c) [111] wire orientations composed of As (purple), Ga (grey) and pseudo-H (white) atoms. Note that pseudo-hydrogens of appropriate charge are chosen for each surface atom to provide a defect free surface. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The electronic band structures of small cross section, approximately square, $In_XGa_{1-X}As$ nanowires are investigated for different alloy compositions and for different crystallographic orientations using density functional theory. The impact of different surface character (*i.e.* cation or anion) is also considered. Silicon nanowires of similar cross sections and with the same orientations as for the III-V nanowires are also calculated for comparison. Using the Kohn-Sham eigenvalues to approximate band structures, the effect of band folding due to quantum confinement is determined. Band folding results in significantly different electronic structures in the nanowires compared to their bulk form as is reflected in large changes to the band gap energies and effective masses at the conduction and valence band edges. Knowledge of these physical parameters that can be directly extracted from the electronic band structures is key to accurate calculations of charge transport through nanoscale transistors [7]. Electron effective masses govern charge transport and as a first approximation give an indication of the change in electron mobility as critical dimensions are reduced. The direct and indirect nature of a band gap is crucial for engineering of photonic devices; the magnitude of the band gap controls the thermal operation of a semiconductor in a transistor, and as well controls and/or limits source-to-drain tunneling.

A representative structure is selected at each nanowire alloy composition from a large set of geometries generated by randomly occupying each site of the cation sublattice with either an In or Ga atom with probability proportional to the alloy stoichiometry. The nearest neighbor distributions about each of the arsenic atoms in each nanowire generated in this manner is calculated leading to a distribution of In and Ga nearest neighbors. Specific nanowire configurations with nearest neighbor averages matching the positions of the peaks in the ensemble nearest neighbor distribution are chosen to represent the set of alloy configurations accessible at a given stoichiometry.

All calculations are performed using the Vienna *ab initio* simulation package (VASP) [13–15] using the Pedrew-Burk-Ernzerhof (PBE) exchange-correlation functional [16] and the projected augmented wave method [17,18]. A plane wave cut-off energy of 460 eV is chosen. A *k*-point grid of 11 × 1 x 1 is used to converge the electronic energy. The lattice parameters for all nanowires are relaxed and atomic positions are optimized to a force tolerance of less than 10 meV/Å per atom. A primary goal of the calculations is to understand the impact of the cation sublattice stoichiometry on electronic structure and physical properties as extracted from the band structures. The pseudo-hydrogen approach to surface terminations as described in, for example, ref. [19] is used. Pseudo-hydrogen atoms with fractional charges are widely used to chemically saturate surface dangling bonds in III-V materials to obtain an ideal passivation with no defect states in the nanowire band gap. Electrical properties of $In_XGa_{1-X}As$ nanowires are investigated by determining the band gaps and effective masses from the electronic structure calculations. The electron effective masses are calculated using an approximation of the second derivative $\partial^2E/\partial k^2$ at the conduction band minima using a 5 point stencil method [20].

The band gap energy is an important factor in design of tunneling devices [21] and also has a significant impact on the ON-OFF current ratio in metal-oxide field effect transistors (MOSFETs) [22–24]. The effective masses can be considered in a first approximation as indicating the relative electron mobility for nanowires of different crystallographic orientation with a smaller effective mass suggesting higher electron mobility – assuming a similar order of magnitude in various electron relaxation processes between the various III-V nanowires examined. On the other hand, a small effective mass is concomitant with a lower density of states (DoS) leading to a lower inversion charge density [3] for device applications. Lower inversion charge density and phenomena such as

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