Bismuth-containing GaAs Core−Shell Nanowires

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***Abstract*—This work theoretically investigates the electronic and optical properties of $GaBi_xAs_{1-x}$/GaAs core−shell and GaAs/$GaBi_xAs_{1-x}$/GaAs multi-core−shell nanowires. Our results show a large tuning of absorption wavelength (0.9 μ to 1.6 μ) by varying Bi composition and/or nanowire diameters. The computed polarisation dependent optical spectra indicate the possibility to incorporate such nanowires in photonic devices desiring isotropic polarisation response . Overall our work provides a systematic and detailed understanding of bismuth-containing GaAs nanowire optoelectronic properties which could offer new possibilities for future green photonic technologies.**

***Index Terms*—Nanowires, Bismides, Polarisation, Wavelength**

I. Introduction

Semiconductor nanowires offer highly tunable optoelectronic properties which can be engineered by varying their material profile and/or by changing their geometry parameters. Among many different material candidates including III-Vs, Si/Ge and ZnO, GaAs-based alloy systems have been extensively investigated for the design of core-shell nanowires due to the associated direct band-gap and absorption wavelengths in near to mid-infrared range. More recently, highly mismatched bismide alloys have been incorporated in core−shell nanowires in which a small fraction of Bi is added to form $GaBi_xAs_{1-x}$ alloys [1]. These nanowires have shown highly promising optoelectronic properties which can be exploited for low-energy consumption photonic technologies, as the $GaBi_xAs_{1-x}$ alloys offer the possibility of designing band structures in which the band-gap energy is less than the spin-orbit split-off energy [2]. This novel band structure property associated with $GaBi_xAs_{1-x}$ materials has been predicted to suppress energy hungry loss mechanisms such as CHSH Auger losses and Inter Valence Band Absorption (IVBA) processes in semiconductor devices [3]. In this paper, we discuss our theoretical results based on multi-million-atom tight-binding simulations which provide a detailed understanding of the optoelectronic properties of bismuth containing GaAs core−shell nanowires [4], [5].

II. Results and Discussions

The epitaxial growth of semiconductor nanowires on GaAs substrates has shown large-area dislocation free and uniform formation of vertical nanowire structures such as schematically illustrated in Fig. 1 (a). In order to provide theoretical understanding of their optoelectronic properties, we have atomistically constructed nanowire geometries by randomly placing Bi atoms on As locations in the $GaBi_xAs_{1-x}$ shell region. Fig. 1 (b) shows a zoomed-in portion of one such $GaBi_xAs_{1-x}$/GaAs nanowire with a random distribution of Bi atoms.

A. Methods and Nanowire Geometry

In this work, we have investigated two types of core−shell nanowires as schematically shown in Fig. 1 (c) [top row]. The core region is made up of GaAs material. One nanowire is constructed by single $GaBi_xAs_{1-x}$ shell region whereas the second nanowire shows axial quantum well geometry with two shell regions ($GaBi_xAs_{1-x}$ and GaAs). The nanowire core diameter is 20 nm and the shell diameter is varied between 25 nm and 45 nm. The Bi fraction in the $GaBi_xAs_{1-x}$ shell region is increased from 2% to 15%. The largest nanowire structure in our simulations consists of about 6.3 million atoms, including 0.47 million Bi atoms in the shell region.

The $GaBi_xAs_{1-x}$ and GaAs materials have very different lattice constants which give rise to strain at their interface. The strain relaxation in our simulation is performed based on atomistic valence force field method [6] and the electronic structure is computed by solving sp^3s^* ten-band tight-binding Hamiltonian including spin-orbit coupling [2]. The polarisation dependent optical response is calculated by Fermi's golden rule. To properly investigate the Bi alloying effect, we average the results over five randomly selected Bi configurations in the $GaBi_xAs_{1-x}$ shell region.

B. Wavelength Tuning and Polarisation Response

Fig. 1 (c) [bottom row] shows the dependence of ground-state optical wavelength on the nanowire diameter and Bi fraction in the shell region for both types of studied nanowires.

For $GaBi_xAs_{1-x}$/GaAs nanowires, the wavelength is red shifted when the Bi fraction is increased at 40 nm diameter, as well as when the diameter is increased at fixed 15% Bi fraction. A number of other Bi fractions and diameters are investigated in Ref. [5]. These plots highlight a two-way knob to tune the output wavelength of such nanowires. We predict that 1550 nm wavelength which is relevant for telecomm devices can be realised by adding about 15% Bismuth at 40 nm shell diameter. We also plot the polarisation response of this nanowire at 1550 nm wavelength as inset, showing a highly isotropic dependence which would be promising for optical devices such as semiconductor optical amplifiers.

For double shell (or quantum well) GaAs/$GaBi_xAs_{1-x}$/GaAs nanowires, the overall dependence of wavelength on nanowire diameter and Bi fraction is very similar to $GaBi_xAs_{1-x}$/GaAs nanowires. The wavelength is

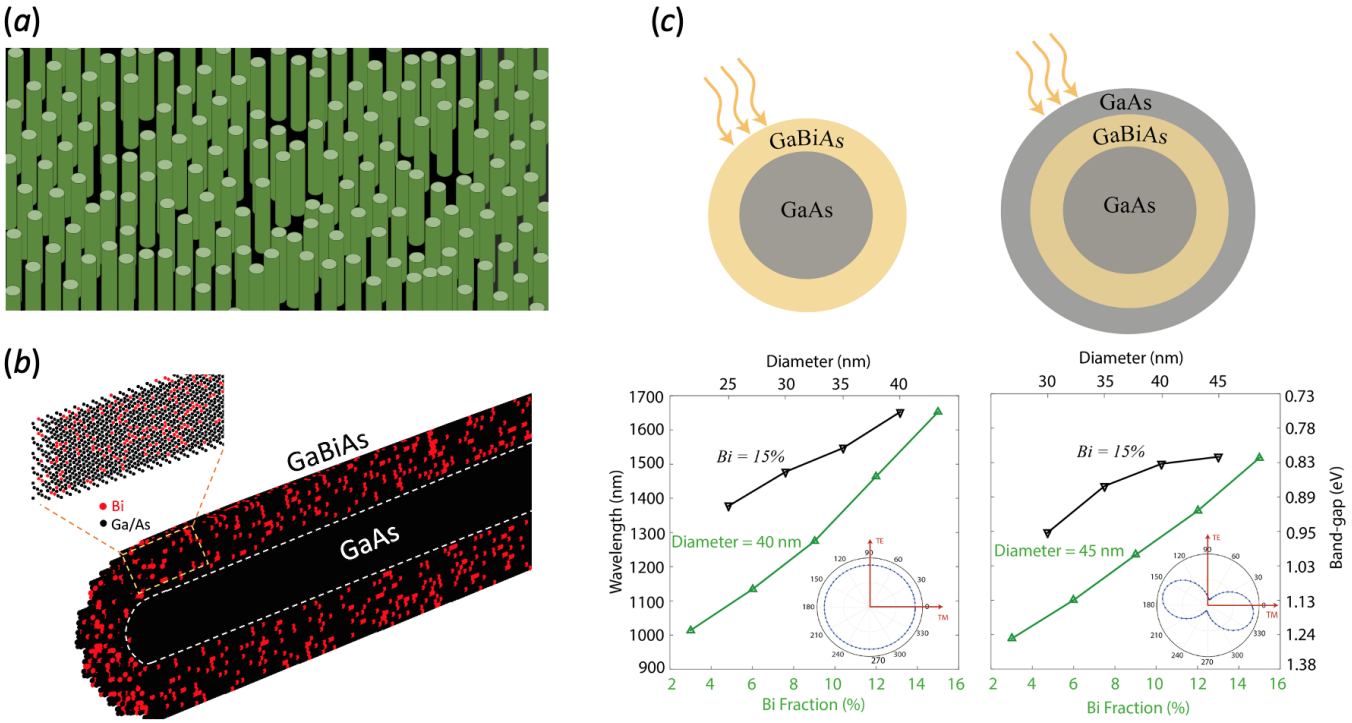

Fig. 1. (a) Schematic diagram of an array of vertical nanowires. (b) One $GaBi_xAs_{1-x}$/GaAs nanowire is zoomed in to indicate atomistic structural construction in which Bi atoms randomly replace As atoms in the GaAs shell region. (c) (Top Row) Schematic diagram of investigated $GaBi_xAs_{1-x}$/GaAs and GaAs/$GaBi_xAs_{1-x}$/GaAs nanowires shown. (Bottom Row) Absorption wavelength is plotted as a function of the nanowire shell diameter (at 15%) and Bi fraction (at 40 nm or 45 nm diameter). (Insets) The insets show polarisation dependent optical transition spectra.

red shifted by increasing nanowire diameter and Bi fraction. However, one interesting difference is that the wavelength shift as a function of nanowire diameter becomes relatively flat at higher Bi fraction. This behaviour of wavelength dependence is a consequence of internal strain modulation by the GaAs outer shell region which is discussed in Ref. [5]. We also show polarisation dependent optical response as inset which is starkly different from the $GaBi_xAs_{1-x}$/GaAs nanowires and exhibit a strong direction dependence.

III. Conclusions and Outlook

In conclusion, we have investigated the electronic and optical properties of $GaBi_xAs_{1-x}$/GaAs core−shell and GaAs/$GaBi_xAs_{1-x}$/GaAs multi-core−shell nanowires by carrying out large-scale atomistic tight-binding calculations. Our work reveals interesting properties of these nanostructures and provide an understanding of wavelength and polarisation dependence on Bi fractions and nanowire diameters. We also investigate internal strain profiles and spatial distributions of the confined electron and hole states which are consistent with the observed optoelectronic behaviour.

The idea of including $GaBi_xAs_{1-x}$ material in nanowires is relatively new and has recently started to gain traction. For such nanowires to be incorporated in future photonic devices, significant progress is needed in the next few years, with challenges to overcome in epitaxial growth and characterisation with Bi fractions ranging from 10-15%. Another promising nanowire material would be to include both Bi and N in the nanowire shell region forming $GaBi_xN_yAs_{1-x-y}$ alloys which can provide additional control over strain and optical wavelength tuning [7].

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