ABSTRACT

The need of finding an alternative to the most commonly used HgCdTe alloys as mid-infrared detectors prompted researchers to investigate narrow band gap $InSb_xAs_{1-x}$ ternary alloy systems. The efficiency of InAs- or InSb-based semiconductors to long wavelength radiation helps in fabrication of various devices. For these applications, a detailed understanding of the physics of such semiconductor materials, particularly in the context of electronic band engineering and light-matter coupling, is essential.

Lattice mismatch in semiconductor heterostructures (HSs) is one of the main hindrances in any application. Raman spectroscopy is sensitive to the local strain in the crystal structure. We report weak residual strain along the axis of individual InAs/InSb HS nanowires (NWs), as could be revealed using confocal Raman measurements. The measured value of the strain is within the resolution limit of other commonly used techniques, *e.g.*, high-resolution transmission electron microscopy and selected area diffraction measurements. This intrinsic residual strain can be exploited to modulate the band gap along the axis of these HS NWs. Next we exploit the variation of composition in alloy based HS NWs, to tune the physical properties of these systems. We employ resonance Raman mapping and demonstrate the graded band gap along the axis of individual InAs/InSbAs NWs. We show that the resonance Raman imaging along with the calculated band profile from density functional theory (DFT) can be used as an easy characterization tool to probe the smooth grading of the band gap in these HS NWs. We further carried out the DFT calculations on two HSs: $(InSb)_n$/$InSb_{0.5}As_{0.5}$ and $(InAS)_m$/$InSb_{0.5}As_{0.5}$. Here, n and m are number of unit cell of zinc-blende (ZB) InSb and wurtzite (WZ) InAs. We explain the importance of the modified Becke-Johnson and local density approximation (mBJLDA) and spin-orbit coupling to determine the band structure. We predict the existence of direct and indirect band gaps in some of these systems. We present the layer modulated band gap variation and carrier pockets generation in these HSs. Finally, we focus on light-matter interaction in another type of HS, radial HS NWs, *i.e.* core-shell NWs. We show that the polarization anisotropy has a non-linear variation with the excitation wavelength in InAs/GaSb core-shell NW in comparison to the linear variation for bare InAs NW.

We believe that this thesis presents various fascinating characteristics of As/Sb based HSs.

Keywords: III-V semiconductor, heterostructure, nanowire, zinc-blende, wurtzite, Raman scattering, strain, polarization anisotropy, density functional theory, electronic band structure.