Semiconductor Quantum Nanostructures for Optoelectronic Applications

Sumanta Bose

June 13, 2017

Semiconductor quantum nanostructures, such as 0D quantum dots (QDs), 1D nanorods and 2D nanoplatelets (NPLs), quantum rings (QRs) and quantum wells (QWs) exhibit unique quantum mechanical and optoelectronic properties due to spatial confinement of excitons in one or more dimensions ($\sim 10^{-9}$ m). They have received increasing research interest in recent years owing to their intriguing fundamental properties that can be leveraged for potential applications in optoelectronic and display devices as cost-effective and quantum-efficient luminophores. They have been successfully used to implement and design light-emitting diodes (LEDs), lasers, photodetectors, solar cells, biomedical imagers, etc. This is owing to their morphological bandgap tunability, fast fluorescence lifetime and unique optical characteristics supporting tunable pure-color or wide spectral emission.

Among the wide range of available and newly studied semiconductor quantum nanostructures, firstly (*i*) NPLs and QRs of II-VI materials and alloys thereof, and secondly (*ii*) QDs and QWs of III-V dilute nitride/bismide alloy materials are two families of nanostructures that have emerged as very promising candidates for novel semiconductor device design applications.

In this thesis, we report studies on the aforementioned two families of semiconductor quantum nanostructures. The first part of the thesis focuses on the study of II-VI (CdSe and CdS) NPLs and optoelectronic properties thereof under varying environmental conditions such as geometrical dimensions, temperature, material composition, topology and optical polarization. NPLs are a unique class of atomically flat quasi-2D quantum confined nanocrystals, often synthesized using wide bandgap II-VI materials, having well-defined thicknesses of several monolayers (MLs). Their sizes enable them to be colloidally suspended in solution. Recent advancements in colloidal chemistry has led to the efficient synthesis of high quality single crystal NPL samples having reduced nonradiative recombination paths and enhanced optical properties. They exhibit strong 1D confinement as their thickness is very small compared to the Bohr radius. NPLs possess the wide bandgap tunability of QDs and the short exciton decay time of QWs bringing together advantageous features from two domains. Compared to QDs, they typically have narrower emission spectra, reduced inhomogeneous broadening and suppressed Auger recombination.

Furthermore, the second part of the thesis focuses on the study of quaternary dilute nitride/bismide III-V (InNBiAs, InNBiSb and GaNBiAs) QDs and QWs for their optoelectronic properties and application. Dilute nitride/bismide doped III-V alloys promises increased engineering flexibility in the design of advanced compound semiconductor heterostructure devices. Increased control over key device parameters such as lattice constant, bandgap and band offsets opens the door to improved performance for a wide range of electronic and optoelectronic devices. In dilute nitride alloys, the resonant states couples with the conduction band (CB) states and produces the band anticrossing (BAC) effects. This causes the CB band edge to get lowered compared to the unalloyed case. Similarly, for dilute bismide alloys, the valence band (VB) edge is lifted due to the valence band anticrossing (VBAC) resulting from coupling between its resonant states and VB states. In addition, the spin-orbital-splitting energy can exceed the bandgap in dilute bismuth alloy which can inhibit the Auger recombination, making it an excellent candidate for optoelectronic device applications, particularly suited for optical fiber telecommunication applications.

The core machinery of our modeling and simulation study of semiconductor quantum nanostructures uses an effective-mass envelope function theory based on the 8-band and 16-band $\boldsymbol{k}\cdot\boldsymbol{p}$ models with valence force field considerations. The optical properties calculations are based on the density-matrix equation and takes into consideration the excitonic effects with intraband scattering and temperature effects. For each of the nanostructure studied, we have performed a comprehensive study on a range of optoelectronic characteristics such as the strain tensor profiles, excitonic transition energies, optical transition matrix elements, Fermi factors, spatial change densities, electron-hole wavefunctions, electronic bandstructure/ band lineups, band-mixing probabilities, photoluminescence emission spectra, optical gain/ absorption spectra, maximum and differential gains and transparency properties. Our findings have important implications for the application of II-VI NPLs and QRs; and dilute nitride/bismide III-V QDs and QWs in optoelectronic devices, such as LEDs, lasers, solar cells etc. They serve as an enabler for designing experiments and predicting optoelectronic characteristics in tandem with measurements and fabrication and can be used to tune reiterations parameters to reduce time and cost of device production.