Abstract

This thesis proposes a multi-physics model to couple the electrical, mechanical, thermal and quantum mechanical interactions in semiconductor and their heterostructures. Governing differential equations and constitutive relations among the coupled fields are derived from the principles of irreversible thermodynamics. Variational principle is applied to solve the problem numerically using finite element method. Boundary and interface conditions are derived consistently.

In the first part of the thesis, semiconductor-solid interfaces are considered with the example of III-N thin films. The contributions of individual physical fields in the coupled field interactions on electronic band structures are studied in detail. The effect of various boundary conditions, defused interfaces and doping are analysed using AlN/GaN heterostructures in the present framework.

In the second part, we study three-dimensional Si quantum dots/ nanocrystals embedded in SiO2 matrix. The purpose of this analysis is to introduce atomic continuum framework in the present scheme. The matrix embedded structure is first created using atomistic simulations based on molecular dynamics theory. The scheme is to create simulated annealing so that realistic Si/SiO2 interface is formed. The interface properties namely width, stoichiometry, point defects and their statistics are studied with respect to nanocrystal size. Residual strain due to thermal annealing is computed. The local properties are then applied in the proposed continuum framework via interpolation functions to calculate the electronic band structure of the nanocrystals. The electronic energy bandgap variation with quantum dot diameter is estimated and compared with reported literature. The corrections applied via local strain is observed to improve the accuracy of computation. In the final part of the thesis, we apply the multi-physics model to study semiconductor- fluid interfaces. Semiconductor nanostructures in microfluidic environment are emerging as frontiers in next generation of bioengineering and biomedical fields. The complexity and multi-disciplinary nature of the problem poses a highly challenging task in understanding and designing new designs. In this direction, our model aims at addressing coupled electrical, mechanical and quantum mechanical effects on fluid ow in microfluidic channels consisting of semiconductor nanostructures. To illustrate this, we analyse the effect of nanowire array on electric field and ow in microfluidic channels. A systematic study on the effect of geometry, orientations and inter-nanowire spacing on the physical fields are studied. Nanowire arrays of Si, Si/SiO2 and ZnO in microfluidic channel is considered as examples. Further, their implications on particle trajectories are discussed in the context of trapping and lysing of biological cells. Additionally, we study the effect of electrolytic fluid on the electronic band structure of ZnO nanowires by varying the diameter, tip pointedness and applied electric field.

To summarize, the thesis proposes a fully coupled quantum-continuum multi-physics modelling framework and provide computational examples having potential applications in nanostructure-based devices. The contribution made in this thesis would be useful in advancing the current understanding of nano-scale phenomena involving electro-thermal mechanical interactions, quantum effect, nanostructure heterojunctions, semiconductor- fluid interfaces and several others, and towards developing better tools in designing new nano-electronic devices from concepts to operation.