First Principles Study of Size and Strain Effects on the Electronic Properties of Si and SiC Nanostructures

by

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ABSTRACT

The decrease in size of semiconductor nanostructures can result in a variety of new properties that are absent in the bulk. For example, while bulk silicon (Si) does not emit visible light, photoluminescence (PL) in the visible range is found for Si nanostructures smaller than a critical size. This effect is ascribed to strong quantum confinement. In the case of silicon carbide (SiC), it forms more than 200 different crystalline structures (called polytypes) with varying stacking sequences and each polytype exhibit distinct electronic properties. When SiC nanostructures are fabricated, blue shifts on the optical spectra are observed for different polytypes. These findings have led to the possibility of using Si and SiC nanostructures in technological applications ranging from optoelectronic devices to biological labels.

In industry, band gaps of bulk semiconductors are routinely engineered by employing strains to the materials. At the nanoscale, several experiments have also studied the role of strain on the optical absorptions and emissions of semiconductor nanostructures and found strain has evident effects on modifying the band gap. In this thesis, we show a systematic study on the combined effects of size and strain on the energy gap (E_g) in Si and SiC nanostructures. Secondly, strained Si in the semiconductor industry has been widely used to improve the speed of field-effect-transistors (FETs) resulting from the increased mobility of the electron or hole. Since Si nanowires have been recognized as a potentially critical component in nanoscale devices, we have studied the strain effects on the electronic properties, such as band structures and the effective masses of the electron and hole, in Si nanowires.

In the first part of the thesis, we systematically explore the combined effects of size and strain on the E_g in Si nanoclusters. It has been demonstrated that different types of strain have different effects on the E_g in Si clusters. Hydrostatic strain effects on the E_g display qualitatively novel trends for Si nanoclusters smaller than ~ 2 nm. While the bulk indirect band gap decreases linearly with increasing compressive strain, this trend is reversed for small clusters (≤ 1 nm). In the intermediate 1 ~ 2 nm size range, strain appears to have almost no effect. These results follow from the fact that the bonding/anti-bonding character of the highest-occupied-molecular-orbital (HOMO) and

the lowest-unoccupied-molecular-orbital (LUMO) change non-monotonically with size. Comparing the strain effects between hydrostatic and non-hydrostatic (e.g. biaxial and shear) strains, we found hydrostatic strain has a relatively weak effect on the E_g in the size range 1 ~ 2 nm, while non-hydrostatic strains result in significant variation in the E_g. The evident modifications of the gap by non-hydrostatic strains, which break the tetrahedral bonding symmetry in Si, result from the splitting of degenerate orbitals in the clusters. Further comparing two non-hydrostatic strains, we find shear strain changes the E_g in Si clusters more evidently than that of biaxial strain since shear strain fully destroys the symmetry of Si atoms. Our results suggest that photoluminescence in Si nanoclusters can be engineered by controlling their size and strain. This offers an exciting avenue for designing new classes of optical devices and chemical sensors.

In the second part, we have investigated the size and strain effects on the electronic properties, such as band structures, energy gaps, and effective masses of the electron and hole, in Si nanowires along the <110> direction with diameters up to 5 nm. From the structures of the nanowires, we find that wires expand along the axial <110> direction compared to bulk Si: the expansion is evident for small wires, and there is almost no apparent expansion for wires larger than 4 nm. From the band structures, we find that the <110> wires display a direct band gap at the Γ point. Under uniaxial strain, we find the band gap variation with strain is size dependent. For the 1 ~ 2 nm wire, the band gap is a linear function of strain, while for the 2 ~ 4 nm wire the gap variation with strain shows nearly parabolic behavior. This size dependence of the gap variation with strain may result from the orbital characters of the band edges. In addition, the effective masses of the electron and hole in <110> nanowires are found to be smaller than those of bulk Si suggesting Si wires could be a super material with high electron and hole mobility. We also find strain affects the effective masses of the electron and hole differently – expansion increases the hole effective mass, while compression increases the electron effective mass. The study of size and strain effects on effective masses shows that effective masses of the electron and hole can be reduced by tuning the diameter of the wire and applying proper strain. This result supports the motivation for using Si nanowires as functional components in future nanoelectronics.

In the third part, we have studied the combined effect of polytype and size on the E_g in SiC nanoclusters deriving from three different parent polytypes, namely 3C, 2H and 4H, in the size range of 0.5 nm ~ 2.0 nm. We found that for the clusters smaller than 1 nm, regardless of the parent polytype, identical size - E_g dependency is achieved. For clusters larger than 1 nm, different polytypes exhibit distinct E_g values, systematically approaching their bulk band gaps. The critical size of 1 nm is correlated to the number of bilayers and the stacking sequences within the clusters. These studies suggest how the structure, energetics, and electronic properties are evolved with size in SiC for different polytypes and could have immense impact on future optoelectronics materials and nanodevices.