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Theoretical Study of Electronic and Electrical Properties of Silicon Nanowires

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THEORETICAL STUDY OF ELECTRONIC AND ELECTRICAL PROPERTIES OF SILICON NANOWIRES

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Abstract

Silicon nanowires (SiNWs) are attracting great interest as the most promising building blocks for future nanoscale electronic devices. Remarkable development has been achieved toward the goal of application of SiNWs in industry in the past decades.

The small sizes of SiNWs make their electronic and electrical properties strongly dependent on growth direction, size, morphology and surface reconstruction. A well-known example is the size dependence of the electronic band gap width of SiNWs irrespective of wire direction. As the wire diameter decreases, the band gap of the nanowire widens and deviates from that of bulk silicon gradually. Moreover, the orientation of the wire axis and the surface have a great effect on the electronic properties of SiNWs. Further detailed deeper studies on the structural properties are required to guide the research and application of these nanomaterials.

In this work, systematic studies on the electronic and electrical properties of SiNWs along different orientations were conducted based on density functional theoretical (DFT) calculations. Interesting findings include:

(1) Orientation dependences of electronic band structures of hydrogen-terminated silicon atomic chains: A <110> oriented Si chain showed direct band gap while a <112> chain showed indirect band gap. In addition, the validity of DFT method was confirmed by performing additional GW calculations on these chains.
(2) Unique, tunable electronic band structures of hydrogen-terminated <112> SiNWs: It was shown that the hydrogen-terminated <112> SiNWs kept an indirect gap feature even at extremely small size. Interestingly, the indirect gap of <112> SiNWs could be tuned to direct gap, through changing the cross section shape.

(3) Effects of adsorption and doping of a single boron atom in <112> SiNWs: Although the single boron atom doping in <112> SiNWs showed slight influence on the band structure modification, the atomic adsorption could change the band structure remarkably. Moreover, different adsorbents modified the electronic properties of SiNWs differently, with the electronegative value acting as an index to show the extent of the influence.

(4) Band gap of hydrogen-terminated <112> SiNWs tuned through axial stress: Through structural deformation, the electronic band structure of SiNWs could be tuned. It was found that compression facilitated the indirect-direct gap mutation of <112> wires while extension induced the direct gaps of <110> and <111> wires.

(5) Orientation dependence of transport properties of <112> SiNWs: While <111> SiNWs are semiconductor-like, <112> SiNWs show characteristics of conductors. Furthermore, there is a size requirement of both the electrodes and the conductors placed between the electrodes.

It is expected that this thesis work would be helpful for understanding of both the electronic and electrical properties of SiNWs and provide experimental guidance in materials applications.
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TABLE 3-2-1. Cross sectional area and number of Si and H atoms for the SiNWs.

TABLE 4-1. Models of silicon nanochains/nanowires.
List of Symbols and Abbreviations

Ψ wave function
\( \hat{H} \) Hamiltonian
\( E_F \) Fermi energy level
\( E_g \) band gap
DOS density of states
PDOS projected density of states
LDOS local density of states
VB valence band
CB conduction band
DB dangling bond
LUMO unoccupied molecular orbital
\( \Gamma \) central point in the Brillouin zone
Å angstrom
nm nanometer
eV electron volt
DFT density function theory
MD molecular dynamics
TB tight-binding
GW many-body perturbation
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>LDA</td>
<td>local density approximation</td>
</tr>
<tr>
<td>GGA</td>
<td>generalized gradient approximation</td>
</tr>
<tr>
<td>LCAO</td>
<td>linear combination of atomic orbital</td>
</tr>
<tr>
<td>NEGF</td>
<td>non-equilibrium Green’s function</td>
</tr>
<tr>
<td>SC</td>
<td>self-consistent</td>
</tr>
<tr>
<td>Tr</td>
<td>trace</td>
</tr>
<tr>
<td>ρ</td>
<td>electron density</td>
</tr>
<tr>
<td>I</td>
<td>current</td>
</tr>
<tr>
<td>V</td>
<td>bias</td>
</tr>
<tr>
<td>Δ</td>
<td>energy difference between the CB minima at different positions</td>
</tr>
<tr>
<td>FET</td>
<td>field effect transistor</td>
</tr>
<tr>
<td>PL</td>
<td>photoluminescence</td>
</tr>
<tr>
<td>CVD</td>
<td>chemical vapor deposition</td>
</tr>
<tr>
<td>VLS</td>
<td>vapor-liquid-solid</td>
</tr>
<tr>
<td>OAG</td>
<td>oxide assisted growth</td>
</tr>
<tr>
<td>MBE</td>
<td>molecular-beam epitaxy</td>
</tr>
<tr>
<td>STM</td>
<td>scanning tunneling microscope</td>
</tr>
<tr>
<td>STS</td>
<td>scanning tunneling spectroscopy</td>
</tr>
<tr>
<td>ITO</td>
<td>Indium tin oxide</td>
</tr>
<tr>
<td>SiNW</td>
<td>silicon nanowire</td>
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