8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

ELECTRONIC STRUCTURES OF MECHANICALLY DEFORMED SILICON NANOWIRES

R.Q. Zhang, A.J. Lu and S.T. Lee

Center of Super-Diamond and Advanced Films (COSDAF) & Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China
E-mail: aprqz@cityu.edu.hk and URL: personal.cityu.edu.hk/~aprqz/research.html

Key Words: *Silicon Nanowires, Electronic Band Structures, First-Principles Calculation.*

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 explorations on the structural and electronic properties are needed to guide the research and application of these nanomaterials.

In this presentation, we describe our recent density-functional theoretical study on the electronic band structures of hydrogenated SiNWs altered by applying axial stresses. We found that an axial compression could cause an indirect-to-direct band gap transition in [112] SiNWs while extension induced the direct gaps of <110> and <111>wires. As direct energy band may induce strong light-emission properties of Si, the possibility of indirect-to-direct band transition via axial stress has fundamental implications in exploiting SiNWs for optoelectronic applications.