

Novel Energy Conversion Devices Based on Nanowire Heterostructures

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Overall Vision: When semiconductors are confined to 2, 1 or 0 dimensional structures in the size range of 5-50 nm, their properties can be manipulated in novel ways. Much of the past effort has focused on synthesizing 0-D (quantum dots) and 2-D (quantum wells and heterostructures) nanostructures and studying mostly their optical and electronic properties. Except for carbon nanotubes, 1-D structures have received relatively little attention. The goal of this project is to develop the scientific and engineering foundations of a broad range of energy conversion devices based on 1-D semiconducting nanowire heterostructures. These heterostructures consist of nanowires made of two or more semiconducting materials that are spatially arranged in such a manner that confinement effects are exploited in new and unique ways. We are focusing on energy conversion between thermal, electrical, optical and mechanical forms (see Fig. 1), which requires fundamental understanding of not only the electronic and optical properties, but also their thermal, piezoelectric and thermoelectric ones. Our project is divided into the following technical tasks: (i) synthesis; (ii) characterization; (iii) device design, fabrication, and performance.

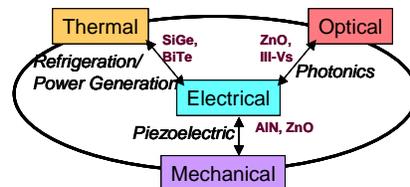


Fig. 1 Various forms of energy conversions that will be achieved using nanowire heterostructures.

Synthesis: Our approach relies on a promising chemical synthesis technique called vapor-liquid-solid (VLS) process that can be used to grow monocrystalline nanowires Si, Ge, SiGe, ZnO and various III-V and II-VI semiconductors. We are using the VLS process to synthesize two types of heterostructures — co-axial heterostructure nanowires¹ (COHNs) and longitudinal heterostructure nanowires² (LOHNs) (see Fig. 2). COHNs allow modulation doping such that nanowires with extremely high charge carrier mobility can be obtained, while LOHNs allow bandgap engineering in 1-D, which could lead to multiple quantum dots or pn junctions integrated within a single nanowire. Engineering the band structure near the Fermi level also allow tailoring of their thermoelectric properties.

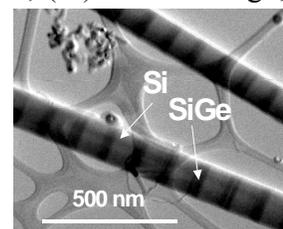


Fig. 2 Longitudinal heterostructure nanowire (LOHN) made of Si and SiGe.

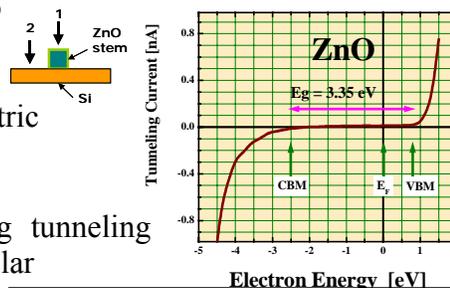


Fig. 3 Scanning tunneling spectroscopy of ZnO nanowires shows Fermi level pinning.

Nanowire Science: Our recent studies using scanning tunneling spectroscopy has shown that ZnO nanowires share similar Fermi level pinning as in bulk material (see Fig. 3). Current work is focused on ballistic electron emission microscopy to study the electronic band structure of

COHNs and LOHNs. While this will eventually lead to manipulation of electronic bandstructure for optoelectronic applications, we have already demonstrated that such nanowire heterostructures can be used as optically pumped nanolasers. Such nanostructures can also be used for non-linear mixing³.

1-D confinement has strong influence on phonon spectra and lifetimes, which could dramatically change their thermal properties. We have developed a new approach to measuring thermal conductivity of individual nanowires⁴ (see Fig. 4). Our studies on single-crystal silicon nanowires suggest that boundary scattering makes thermal conductivity strongly size-dependent, which can be theoretically predicted⁵. What is most interesting, however, is that for nanowires with diameters less than 22 nm, phonon confinement produces additional reduction of thermal conductivity due to changes in the phonon dispersion relation that result in reduction of group velocities as well as possibly changes in scattering rates (see Fig. 4).

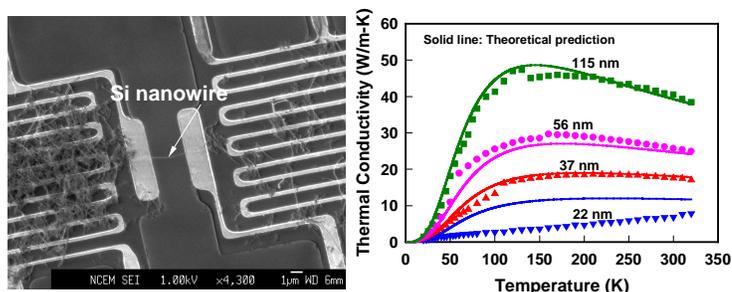


Fig. 4 (Left) Two suspended microheaters are bridged by a single silicon nanowire. By electrically heating one microheater and monitoring the temperature difference between the heaters, one determines the thermal conductivity of the nanowire. (Right) Thermal conductivity as a function of temperature for silicon nanowires 115, 56, 37, and 22 nm in diameter. Solid lines show theoretical predictions using a modified Callaway model accounting for boundary, impurity, and Umklapp phonon scattering.

Because of the nature of elastic boundary conditions in nanowires heterostructures, COHNs and LOHNs would enable dislocation-free interfaces that are not stable in 2-D or thin film form, while also providing access to new stable phases that are metastable in bulk or thin film forms. Figure 5 shows the calculated stability regime for nanowire heterostructures for various diameters and lattice mismatches.

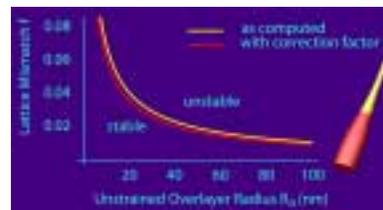
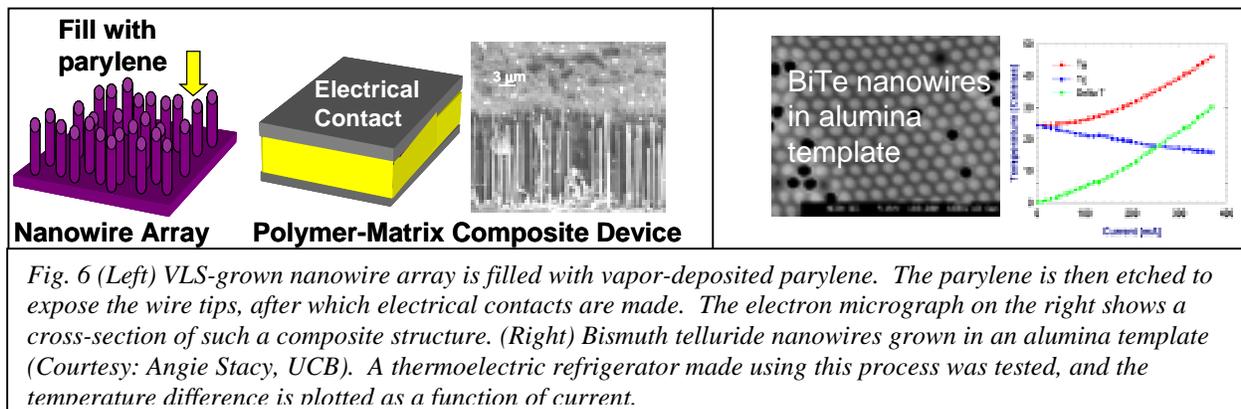


Fig. 6 Stability map of nanowire heterostructure for dislocation-free interfaces.

Nanowire-Based Devices: Based on fundamental understanding of the physics of COHNs and LOHNs, we are developing three types of energy conversion devices. The devices include: (a) thermoelectric refrigerators or power generators; (b) light emitting devices; (c) nanoelectromechanical transducers. The active material in these devices will consist of composites made of unidirectional nanowire arrays embedded in a matrix, such that they can be patterned and integrated into microsystems. We have developed two approaches (see Fig. 6): (i) polymer desposition in VLS-grown nanowire arrays; (ii) nanowire growth in alumina templates.



Semiconducting nanowires with diameters in the 5-10 nm range provide the unique opportunity to develop thermoelectric refrigerators and power generators with performances comparable to or better than gas or vapor based ones. Such solid-state devices could have enormous impact on energy utilization technology as well as on the environment. Figure 6 shows some preliminary results of cooling from a nanowire-based thermoelectric refrigerator. Such device-level testing requires adequate measurement techniques. Figure 7 shows a thermal imaging technique with sub-micron resolution based on visible optics that was developed for this purpose.



Fig. 7 Optical micrograph of temperature distribution with sub-micron resolution

Use of nanowires containing integrated quantum dots can allow efficient and size-tunable optoelectronic conversion. Furthermore, embedding such nanowires in a polymer matrix will produce a light emitting medium with much lower effective index than semiconductors, which will enable efficient coupling with optical fibers and thereby dramatically improve external quantum efficiencies. When combined with single electronics, such quantum dot nanowires offer the possibility of single photonic devices that can significantly impact information storage and processing. Finally, nanowire-based piezoelectric and pyroelectric transducers will lead to high quality factor and high resonant frequency devices that can be used for a variety of applications ranging from molecular sensing and nano-actuators to high-frequency signal processors. We plan to design, fabricate and test such devices in the near future.

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