Abstract for an Invited Paper
for the MAR07 Meeting of
The American Physical Society

Quantum Design of Complex Nanostructured Electronic Materials

ANDREW WILLIAMSON, Lawrence Livermore National Laboratory

Over the last decade, our ability to predict the fundamental properties of nanoscale building blocks such as quantum dots, wires, and slabs has improved dramatically. In particular, first principles modeling techniques can now routinely predict how the structural, electronic, optical, and transport properties of these building blocks depends on their size, shape, composition, and surface structure. In this talk we present the results of three projects designed to build upon these fundamental studies to engineer novel, nanostructured materials with tailored electronic properties. These complex, nanoscale heterostructure materials utilize both the unique properties of their nanoscale building blocks and the interactions between the constituent building blocks to engineer the ideal material properties. (i) We will describe the design of a silicon/germanium nanowire based thermoelectric material whose performance is enhanced by suppressing thermal transport and enhancing electronic transport. This is achieved by engineering the nanoscale confinement and scattering of phonons and electrons. (ii) We will describe the design of a silicon based laser, constructed from silicon nanocrystals embedded in an amorphous silicon nitride matrix. Models of the electronic states in the nanocrystal, the surrounding matrix, and the interface between the two, enable us to optimize the optical efficiency of the emission and electrically pump the laser. (iii) We will describe the use of first principles models to predict the optical response of silicon nanowires. These predictions are used to interpret the results of optical scatterometry metrology which can measure the size and surface roughness of nanoscale electronic devices produced by a combination of lithography and etching. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.