Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Thermal transport size effects in self-assembled Germanium quantum dots in single-crystal silicon JEAN-NUMA GILLET, University of Colorado at Boulder — Superlattices with low thermal conductivity have been used to design 1-D thermoelectric materials. With them, it is challenging to obtain a thermoelectric figure of merit $ZT > 1$. Self-assembly is used to fabricate Ge quantum-dot (QD) arrays. High ZT is expected in these self-assembled Ge QDs arrays in Si since they are single crystals. We prove that high-density 3-D Ge QD arrays in diamond-cubic Si exhibit low thermal conductivity. This property can be used to design 3-D thermoelectric devices. To study the thermal behavior of these 3-D 'phononic crystal' nanocomposites, we create an atomistic model of a supercell consisting of Si unit cells. Inside each supercell, we substitute Si atoms with Ge atoms to form a QD. The thermal conductivity has been shown to reduce below 0.2 W/m/K. Such a result is realized by ensuring minimum group velocities. Further reduction is expected from multiple scattering. We are concerned with the size dependence of the thermal conductivity upon the Ge volumic composition f. From preliminary results with constant f, we obtain an exponential-like thermal-conductivity decrease when the supercell size is increased.

Jean-Numa Gillet
University of Colorado at Boulder

Date submitted: 23 Dec 2008 Electronic form version 1.4