

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Understanding Vibrational Spectra of Silicon Nanocrystals DUNDAR YILMAZ, CEM SEVIK, Texas A&M University, CEYHUN BULUTAY, Bilkent University, TAHIR CAGIN, Texas A&M University — After the discovery of light emission from porous Si, nanostructured Si became a promising material for opto-electronic applications. For two decades lots of both experimental and theoretical works done in order to understand mechanisms behind the interaction of light with low dimensional forms of Si. In this work we employed MD simulation technique. The simulation details are similar to our earlier work except we used Large Scale Atomistic Molecular Modeling Package Software (LAMMPS) with ReaxFF package as an integrator. We used constant pressure constant temperature (NPT) ensemble with a simulation box size around 4.2 nm. We inserted silicon nanocrystals into amorphous silicon dioxide matrix with diameter ranging from 2 nm to 3.2 nm using a scheme defined in our previous work⁷. We also simulated free standing hydrogen passivated nanocrystals with same diameters to compare effects of oxide matrix on the nanocrystals. The effect of strain on vibrational spectra of Silicon Nanocrystals is studied as a function of nanocrystal diameter using reactive molecular dynamics simulations technique for both embedded and hydrogen passivated nanocrystals. With use of refined parameters our calculations reproduce the redshift of the Raman active transverse optical peak of Si-Si vibrations with decreasing the nanocrystal size.

Dundar Yilmaz
Texas A&M University

Date submitted: 18 Nov 2010

Electronic form version 1.4