

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Atomistic models of Si nanocrystals embedded in Si-rich nitride and oxide matrices¹ TIANSHU LI, DAVIDE DONADIO, Dept. Chemistry, UC Davis, FRANCOIS GYGI, Dept. Applied Science & Dept. Computer Science, UC Davis, GIULIA GALLI, Dept of Chemistry & Dept Physics, UC Davis — Several experimental techniques have been recently developed to precipitate Si nano-crystals in nitride and oxide amorphous matrices, and photo-luminescence of these nanoparticles has been reported by several authors. However the role played by the nanocrystal/host interface in determining the optical properties of the nanocrystals is not yet understood and no atomistic model of the interface is available. Using techniques recently developed to study nucleation in supercooled liquid silicon, we derive realistic models of nanocrystal/matrix interfaces; in particular, we simulate the nucleation of crystalline Si nanoparticles from Si-rich nitride and oxide supercooled liquids, by means of molecular dynamics coupled to advanced sampling techniques. Such an approach allows one to closely mimic experimental conditions, without any assumptions on either the shape of nanocrystals or the defect concentration at the interface. The composite structure obtained in our simulations can then be used as input for *ab initio* calculations to investigate the opto-electronic properties of the nanocrystals.

¹This work is supported by DOE/BES DE-FG02-06ER46262 and DOE/SciDAC DE-FC02-06ER25794.

Tianshu Li
Dept. Chemistry, UC Davis

Date submitted: 14 Dec 2009

Electronic form version 1.4