Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Simulations of the Optical Properties of Silicon Nanoparticles Embedded in Silicon Nitride SEBASTIEN HAMEL, Lawrence Livermore National Laboratory, ANDREW WILLIAMSON, GIULIA GALLI, LUCA DAL NEGRO, Massachusetts Institute of Technology, JAE HYUNG YI, VICTOR NGUYEN, YASHA YI, JURGEN MICHEL, LIONEL C. KIMERLING — There is currently a strong interest in the material science community in the optical properties of silicon nanoparticles embedded in silicon nitride. These nanostructures are CMOS-compatible materials which exhibit efficient and fast light emission. The optical properties of these embedded silicon nanoparticles are studied using first-principles Density Functional Theory simulations. We present simulations of the structural, electronic and optical properties of nitrogen-doped silicon nanoparticles both in the gas phase and embedded in a silicon nitride environment. These simulations point to the crucial role played by nitrogen atoms bonded to the surface of small ($\sim$ 1nm) silicon nanoparticles in the light emission mechanism of SiN_x films. We compare the calculated optical gaps and radiative lifetimes of the nanoparticles with recent experimental measurements of light-emitting silicon-rich silicon nitride films obtained by PE-CVD deposition followed by low temperature (500-900 °C) thermal annealing. 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.

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Date submitted: 04 Jan 2006 Electronic form version 1.4