Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Effects of point defects on the electrical properties of aluminum antimonide: a first principles investigation[1] VINCENZO LORDI, DANIEL ÅBERG, PAUL ERHART, Lawrence Livermore Lab — A first principles study is conducted of the effects of point defects on the electrical properties of bulk AlSb, a material of interest for room temperature gamma radiation detection. Detailed calculations were performed for all native defects, including vacancies, antisites, interstitials, and split interstitials, and also for a variety of impurities (H, C, Si, Ge, Sn, P, O, S, Se, Te). Formation energies of each defect in different charge states were calculated to determine the equilibrium defect density and net carrier density. Carrier scattering rates for each defect were calculated using perturbation theory to determine the effects on electron and hole transport. The most detrimental, as well as innocuous, defects were identified. Relative solubilities of the impurities were examined along with their scattering rates to find efficient dopants that minimize mobility degradation. Finally, carrier trapping cross sections and energy levels were calculated to study the role of each defect in deep level trapping.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.

Vincenzo Lordi
Lawrence Livermore Lab

Date submitted: 27 Nov 2007 Electronic form version 1.4