Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**Atomistic Modeling of the Grain Boundary in Silicon** HIROSHI MIZUSEKI, RYOJI SAHARA, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku Univerisity — By combining empirical potential approach with first-principles calculations, we investigate the atomic and electronic structures of grain boundary in silicon to estimate the deleterious effect on photovoltaic properties. Optimized geometries of several boundary structures are obtained by using a Tersoff potential. Moreover, the electronic structures of boundary have been examined using the density-functional theory with the plane-wave pseudopotential method. Calculations show that the electronic properties depend strongly on the atomistic structures, their properties are corresponding to efficiency of photovoltaic cell. This work was supported by the New Energy and Industrial Technology Development Organization (NEDO)

Hiroshi Mizuseki
Institute for Materials Research, Tohoku Univerisity

Date submitted: 20 Nov 2008 Electronic form version 1.4