Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Atomistic dislocation simulation of aluminum using a tight-binding method CHEE GAN, Institute of High Performance Computing, Singapore, SIU-SIN QUEK, Institute of High Performance Computing — Atomistic simulation of dislocation in aluminum has been performed using a tight-binding method where the parameters are based on the works of Mehl and Papaconstantapoulous at the Naval Research Laboratory. We study the dissociation of a perfect edge dislocation (the dislocation line is along the $[11\bar{2}]$ direction) of Burgers vector of $\frac{a}{2}[1\bar{1}0]$ into two partials of $\frac{a}{6}[2\overline{11}]$ and $\frac{a}{6}[1\bar{2}1]$ on the (111) slip plane. By performing a large scale atomistic relaxation, we observe a separation of partials of about 14 Å and a stacking fault region. We will comment on the estimate of partials separation predicted by the elasticity theory, which relates to certain quantities such as the stacking fault energy.

Chee Gan
Institute of High Performance Computing, Singapore

Date submitted: 19 Nov 2007 Electronic form version 1.4