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 Papaconstantopoulos at the Naval Research Laboratory. We study the dissociation of a perfect edge dislocation (the dislocation line is along the [112] direction) of Burgers vector of \( \frac{2}{3}[1\bar{1}0] \) into two partials of \( \frac{1}{6}[2\bar{1}1] \) and \( \frac{2}{3}[1\bar{2}1] \) 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.

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Date submitted: 19 Nov 2007

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