

## Atomistic Simulation of kinks for $1/2a\langle 111 \rangle$ Screw Dislocation in Ta

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### Abstract

Structure, formation energy and mobility of kinks in  $1/2a\langle 111 \rangle$  screw dislocation in metallic Ta have been investigated via low temperature (0.001K) molecular dynamics with a new, first principle based, Embedded-Atom-Model (EAM) potential. We studied  $a/3\langle 112 \rangle$  kinks using a simulation cell containing four dislocations in a quadrupolar arrangement. We impose periodic boundary conditions in the directions perpendicular to  $\langle 111 \rangle$  and fixed boundaries in the  $\langle 111 \rangle$  direction. We find that two, energetically equivalent, core configurations for the  $1/2a\langle 111 \rangle$  dislocation lead to 16 distinguishable kinks. The different mismatches of core configurations along  $\langle 111 \rangle$  direction lead to variations in kink formation energy. The lowest formation energy of a kink pair is determined to be 0.73 eV. We propose an explanation for such variation based on a detailed structure and energy analysis. We also calculate the activation energy for dislocation motion via the double kink mechanism from a dipole annihilation simulation. We help the nucleation of a double kink by introducing a vacancy in the path of one of the dislocations. We find that the migration energy for dislocation motion via double kink formation is 0.016 eV/b, which is more than four times lower than 0.073 eV/b associated with a straight, perfect dislocation moving collectively.

### Acknowledgement

This research work was funded by a grant from DOE-ASCI-ASAP.