Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Prediction of dislocation junction strength in hexagonal close-packed crystals[1] CHI-CHIN WU, PETER CHUNG, Army Research Laboratory, COMPUTATIONAL MATERIALS SCIENCE RESEARCH TEAM — Determination of dislocation junction strengths in *hcp* crystals is important in order to understand and control the fundamental mechanisms in plastic deformation in new lightweight metals and to reduce the density of deleterious dislocations in wide band-gap wurtzite semiconductors. The many factors that may be involved, such as combinations of available slip systems, native material properties, and local morphology due to growth conditions, make systematic investigations via combinatorial experimental approaches challenging. Utilizing discrete dislocation (DD) simulations, we determine yield surfaces comprised by loci of critical stresses required to unzip junctions. Then, using a comparative study of different binary junctions formed by non-coplanar dislocations using different pairs of Burgers vectors on different intersecting planes in Mg and Be crystals, we find that the shape and orientation of yield surfaces are most sensitive to the planes on which the junction forms but independent of the elastic properties. The latter only appears to affect the size of yield surface which is consistent with known behavior in fcc crystals. This work particularly detects similarities and differences in dislocation junctions in hcp crystals.

[1]with support from ORAU under the contract No. W911QX-04-C-0129

Chi-Chin Wu
Army Research Laboratory at Aberdeen Proving Ground

Date submitted: 08 Nov 2012 Electronic form version 1.4