Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Phase Stability and Deformation Behavior of Mo-Si-B System and effect of alloying[1] OLEG Y. KONTSEVOI, ARTHUR J. FREEMAN, Northwestern University — Molybdenum silicides are promising materials for ultra-high temperature applications above 1300 $^\circ$C. One of the main drawbacks is their brittleness at low temperatures, which may be improved by additions. We employ first principles calculations with the highly precise FLAPW method to investigate the effect of alloying with $3d$, $4d$ and $5d$ transition metals on phase stability, cleavage and shear characteristics of the 3-component system Mo – Mo_3Si – Mo_5SiB_2. We determined site preference, phase partitioning of alloying elements, and their effect on shear behavior and preferred deformation modes. We show that in Mo_3Si alloying with $3d$ transition metals results in a significant reduction of energy barriers to shear deformation (softening effect), while $4d$ and $5d$ additions increase shear barriers (hardening effect). In Mo_5SiB_2, $3d$ transition metals (except for Ti) act as weak softeners, while $4d$ and $5d$ show mixed behavior – hardening for early elements and softening for late ones. The softening potency of additions increases with atomic number, but exhibits non-monotonic behavior as a result of a competition between size and electronic effects. The results are discussed in conjunction with possible pathways to ductility enhancement through alloying.

[1]Supported by the AFOSR (Grant No. FA 9550-07-1-0174)

Oleg Y. Kontsevoi
Northwestern University

Date submitted: 13 Dec 2011 Electronic form version 1.4