

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The effects of micro-alloying elements on a BCC iron grain boundaries SUNGHO KIM, SEONG-GON KIM, HONGJOO RHEE, MARK HORSTEMEYER, Mississippi State University — The effects of micro-alloying elements, vanadium and niobium, on a few of BCC Fe grain boundaries are studied using Density Functional Theory calculations to develop an advanced high-strength steel alloy material. The lowest energy configuration of the grain boundaries structures are obtained from the first-principles calculations. The substitutional and interstitial point defect formation energies of micro-alloying elements in the grain boundaries are compared. The segregation energies of micro-alloying elements onto the grain boundaries and its fractured surfaces are computed. The cohesive energy calculations of the grain boundaries with and without micro-alloying elements are performed to investigate the effects of micro-alloying elements on the cohesive strength of the grain boundaries. The tensile and shear tests on the grain boundaries with and without the segregants are carried out to study the effect on the grain boundaries.

Sungho Kim
Mississippi State University

Date submitted: 29 Nov 2011

Electronic form version 1.4