Abstract Submitted for the MAR10 Meeting of The American Physical Society

Ab initio investigation of grain boundary cohesion in Al alloys¹ SHENGJUN ZHANG, OLEG Y. KONTSEVOI, A.J. FREEMAN, G.B. OLSON, Northwestern University — Strength and hardness of aluminum alloys can be substantially increased by alloying with Mg, Zn, Cu, Si, and other elements. The main drawback of Al alloys is their susceptibility to stress corrosion cracking, which is caused by alloying impurities segregated at grain boundaries. We investigated the embrittling and cohesion-enhancing effects of impurities on a $\Sigma 5(012)[100]$ grain boundary in Al by means of the full-potential linearized augmented plane-wave (FLAPW) method within the framework of the Rice-Wang thermodynamic model and within the ab initio tensile test approach. We calculated segregation energies, analyzed local atomic configurations, electronic structures and spatial charge density distributions around segregated impurities, and identified the roles of atomic size and the bonding behavior of the impurity with the surrounding Al atoms. The results show that He, H and Na are strong embrittlers, Zn is a weak embrittler, while Sc, B, Cu and Mg are cohesion enhancers. We further evaluated the effect of co-alloying with two or more elements on grain boundary strength. This work provides a fundamental basis for the design of high strength Al alloys.

¹Supported by the AFOSR (Grant No. FA9550-07-1-0174) and the Ford-Boeing Nanotechnology Alliance

Oleg Y. Kontsevoi Northwestern University

Date submitted: 20 Nov 2009 Electronic form version 1.4