Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First Principles Simulations of Beta to Omega Transformation in the Titanium-Molybdenum System ARUN DEVARAJ, NIRAJ GUPTA, SOUMYU NAG, University of North Texas, HAMESH FRASER, Ohio State University, RAJ BANERJEE, SRINIVASAN SRIVILLIPUTHUR, University of North Texas — The omega phase precipitation in beta titanium (Ti) alloys influence the beta to alpha phase transformation, and ultimately the mechanical properties of these alloys. Molybdenum (Mo) and other alloying additions affect both the relative phase stability and the energy barrier of the transformation. In this work we perform first principle calculations using Nudeged Elastic Band Method(NEB) implemented in Vienna Ab initio Simulation Package (VASP) to determine the minimum energy path, and thereby the energy barrier in beta Ti-Mo alloys with up to 20wt.% Mo. We report the energetics of beta to omega transformation path, proposed by De. Fontaine et al (Acta Metallurgica, vol. 19, p 1153 (1971)). The atomic configurations along the minimum energy transformational path will be compared with our 3D atom probe tomography and probe corrected high-resolution scanning transmission electron microscopy results.

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Date submitted: 19 Nov 2010 Electronic form version 1.4