

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Embedded Atom Method Potential for Titanium-Vanadium Alloys**<sup>1</sup> MICHAEL R. FELLINGER, JOHN W. WILKINS, The Ohio State University, Department of Physics — Titanium alloys are important materials for aerospace applications due to their large strength-to-weight ratio and their ability to resist corrosion. Vanadium is an important alloying element for titanium since it stabilizes the high temperature bcc phase of titanium at lower temperatures, and bcc-stabilized titanium alloys generally showed improved hardness and forgeability [1]. Titanium-vanadium is also a reasonable starting point in the study of more complex titanium alloys of commercial importance. The calculation of many alloy properties requires the use of large numbers of atoms simulated over long periods of time. These calculations are currently only feasible through the use of classical interatomic potentials. An embedded atom method (EAM) potential for titanium-vanadium is presented, and thermodynamic and mechanical properties of this alloy are calculated using the potential. The results are compared to density functional theory results and experimental results when available.

[1] M. J. Donachie, Jr., *Titanium: A Technical Guide*, 2nd ed. ASM International: Metals Park, OH (2000).

<sup>1</sup>Supported in part by the DOE. Computing resources provided by OSC and NERSC.

Michael Fellerger  
The Ohio State University

Date submitted: 29 Nov 2007

Electronic form version 1.4