Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Development of an Embedded-Atom Method Potential for Niobium[1] MICHAEL R. FELLINGER, JOHN W. WILKINS, The Ohio State University — An embedded-atom method (EAM) potential [1,2] is developed for pure niobium as the first step in the construction of an EAM potential for titanium-niobium alloys. The potential is constructed using the force-matching method [3]: the functions comprising the potential are represented as cubic splines, and the spline knots are chosen such that the potential optimally reproduces a large database of forces, cohesive energies, and stresses computed via density functional theory. The code potfit [4] optimizes the splines using a combination of simulated annealing and conjugate gradient-like minimization algorithms. EAM results are compared to DFT and experimental results for the lattice constant, cohesive energy, single-vacancy formation energy, fcc-bcc and hcp-bcc structural energy differences, elastic constants, and phonon dispersions.

[1] M. S. Daw and M. I. Baskes, Phys. Rev. Lett. 50, 1285 (1983).
[2] M. S. Daw and M. I. Baskes, Phys. Rev. B 29 6443 (1984).
[3] F. Ercolessi and J. B. Adams, Europhys. Lett. 26, 583 (1994).
[4] P. Brommer and F. Gähler, Modelling Simul. Mater. Sci. Eng. 15, 295 (2007).

[1]Supported in part by the DOE. Computational resources provided by OSC.

Michael Fellinger
The Ohio State University

Date submitted: 18 Nov 2008 Electronic form version 1.4