Embedded-Atom Method Potential for Niobium

Michael R. Fellinger, Hyoungki Park, and John W. Wilkins, Department of Physics, The Ohio State University

Motivation

- Simulation of complex processes in metallic alloys (e.g., Ti-Nb~Gum Metal)
  - plastic deformation
  - phase transformations
- Require large systems (thousands to millions of atoms)
  - first-principles calculations are too expensive ($t_{sim} \sim N^3$)
  - classical interatomic potentials allow large-scale simulations ($t_{sim} \sim N$)

Embedded-Atom Method (EAM) Potentials[1]

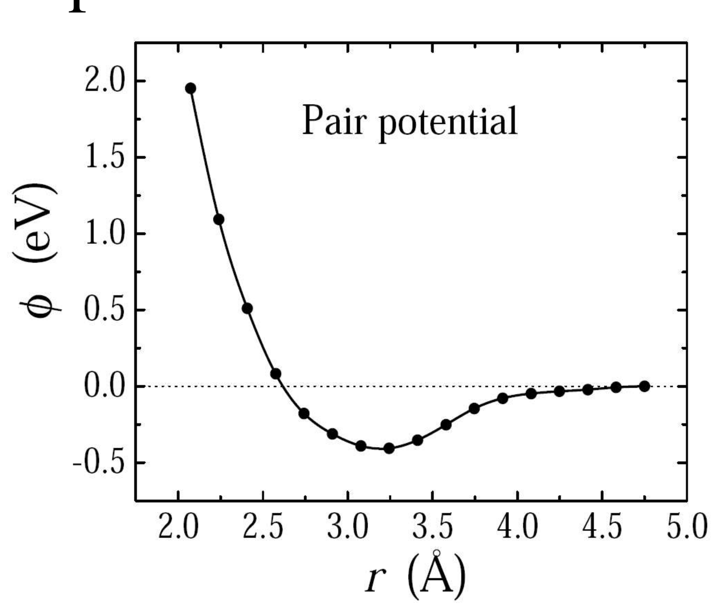
- EAM energy of a collection of atoms:

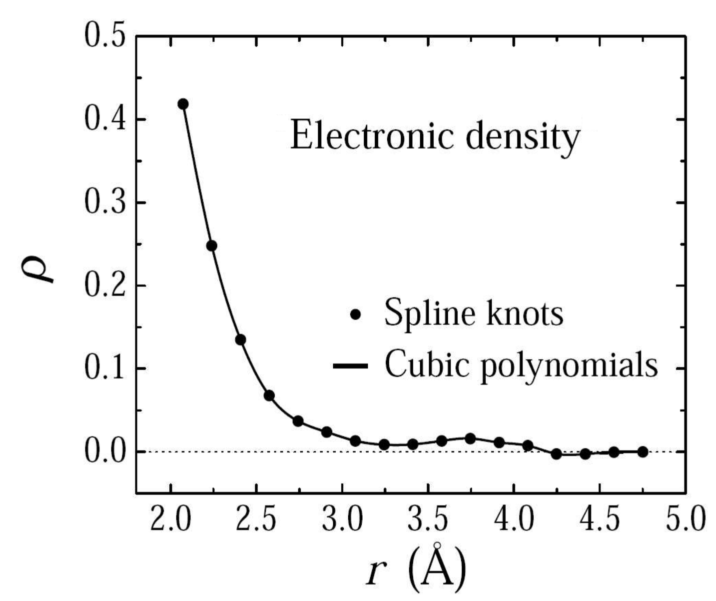
$$E = \sum_{i>j} \phi(r_{ij}) + \sum_i F(n_i) \qquad n_i = \sum_{j \neq i} \rho(r_{ij})$$

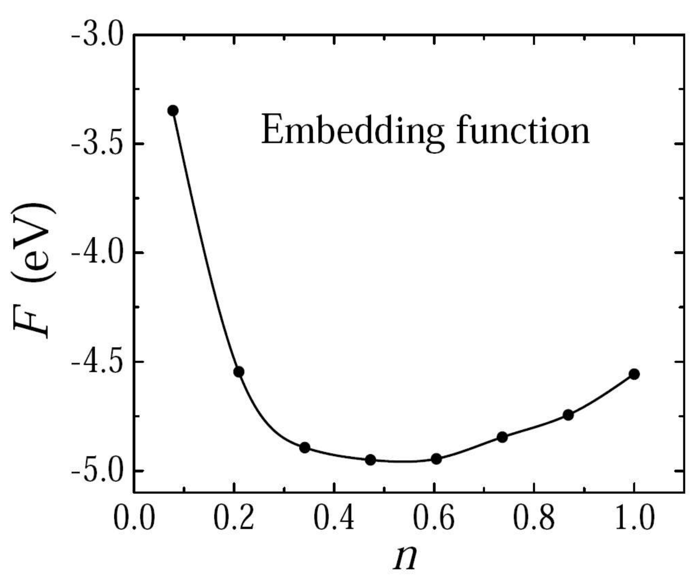
- ϕ is the pair-potential between atoms i and j
- ρ is the electronic density associated with a given atom
- F is the *embedding energy* associated with embedding atom i in the local electronic density n_i
- F is non-linear and implicitly contains many-body effects

Optimization Procedure

- The force-matching method[2] is used to construct the potential:
  - Accurate **forces** yield realistic **dynamics**
  - ϕ, ρ, and F are represented as cubic splines
  - The code *potfit*[3] optimizes the spline knots to reproduce a large database of density-functional theory **forces**, **energies**, and **stresses** (**no** experimental data)
  - The fitting database contains snapshots from first-principles MD simulations of structures under various temperature and strain conditions
  - Optimized EAM functions:

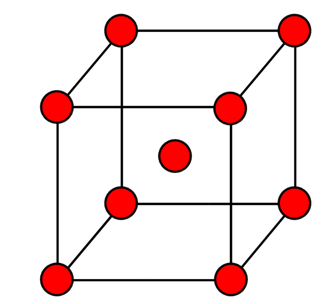




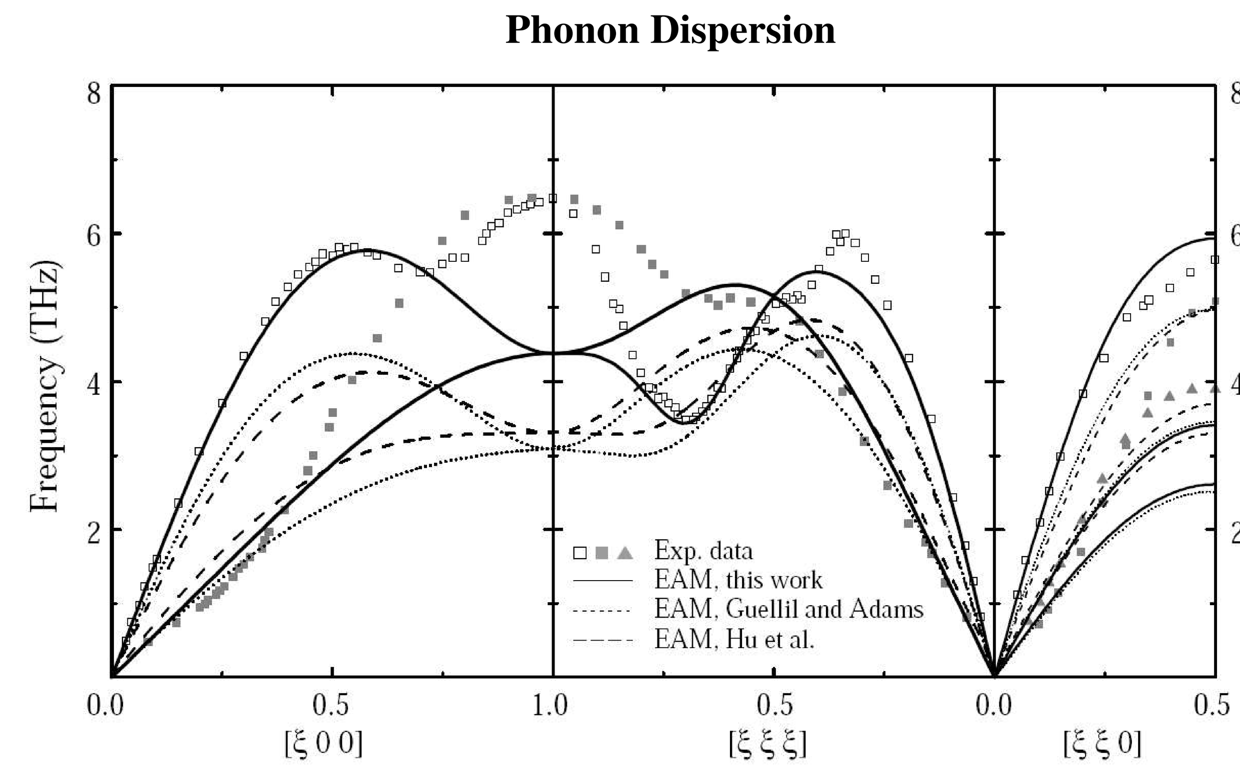


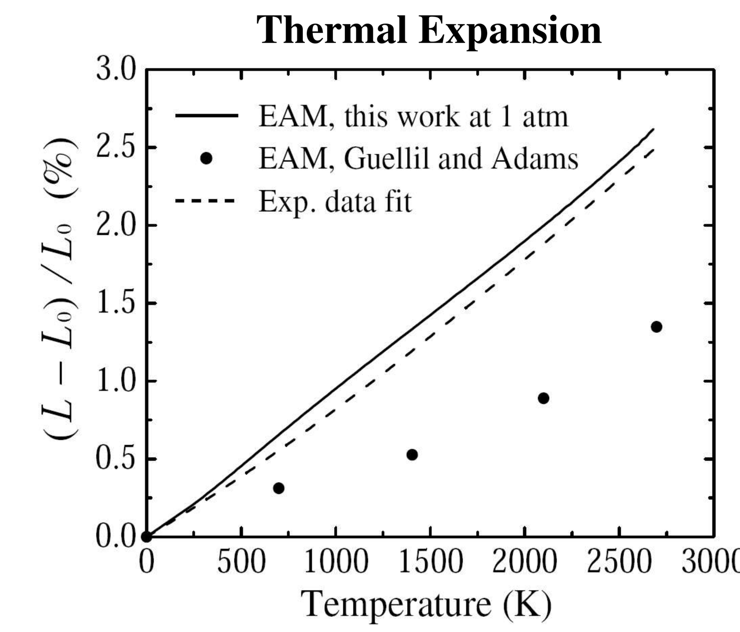
Results for BCC Niobium

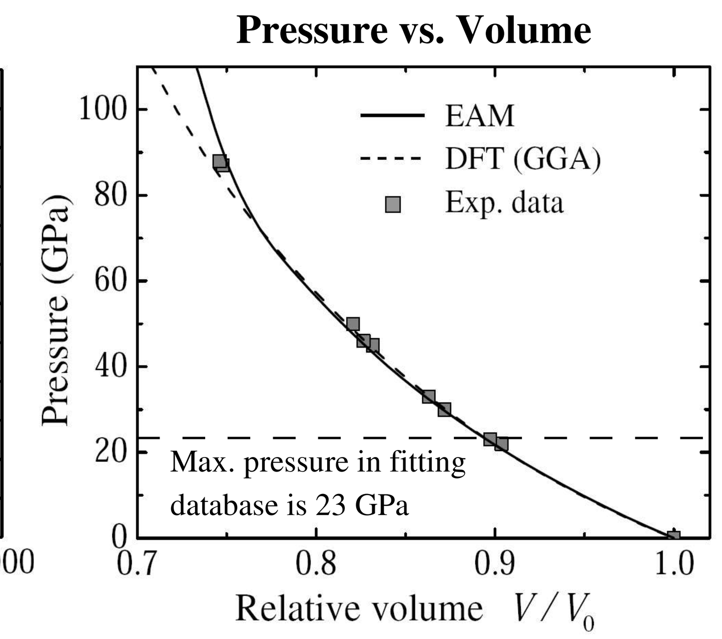
	EAM	DFT (GGA)	Experiment
a (Å)	3.308	3.309	3.303
E_{coh} (eV)	7.09	7.10	7.57
B (GPa)	172	170	173
C_{11} (GPa)	244	246	253
C_{12} (GPa)	136	132	133
C_{44} (GPa)	32	19	31
Q_{vac} (eV)	3.87	...	3.88(0.3)
E^{100}_{surf} (eV/Å^2)	0.147	0.146	Polycrystalline value:
E^{110}_{surf} (eV/Å^2)	0.127	0.131	0.14 - 0.17
E^{111}_{surf} (eV/Å^2)	0.154	0.149	
T_{melt} (K)	2685	...	2742

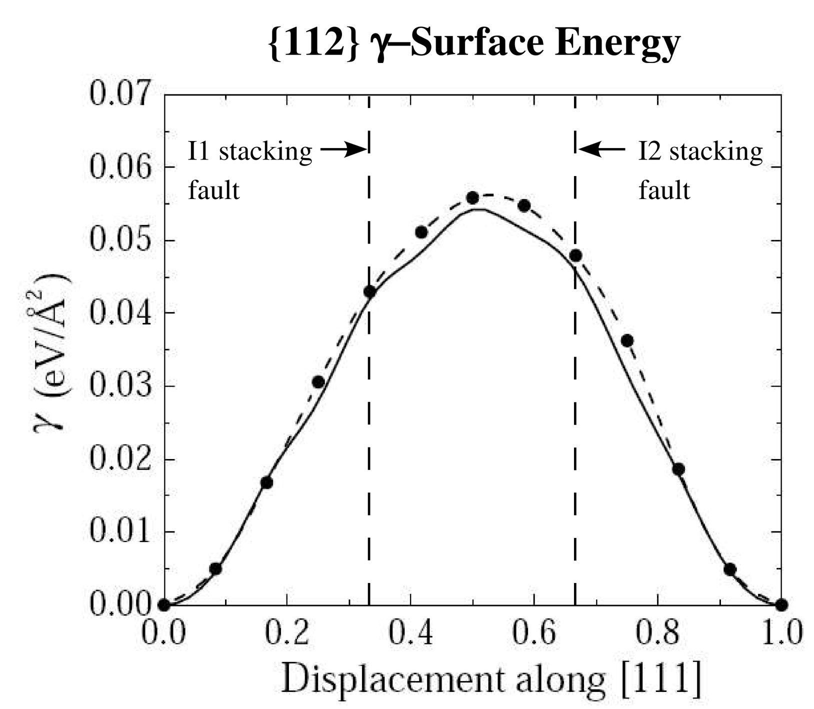


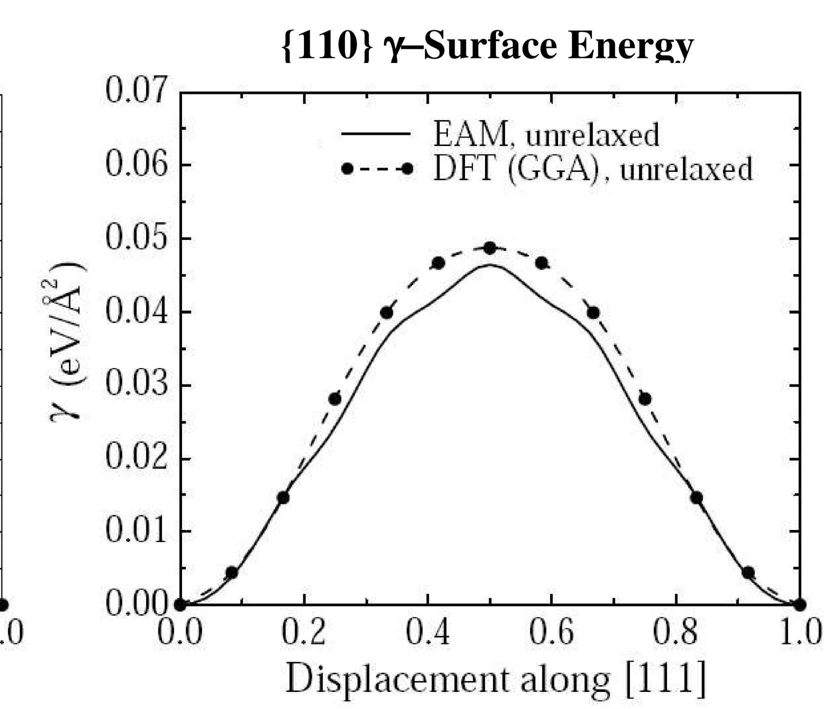
BCC

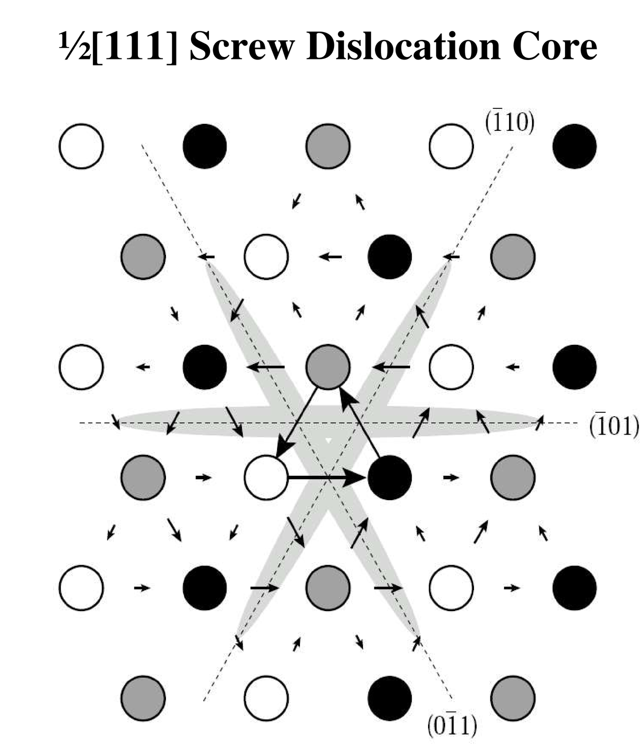












- The EAM potential accurately describes the properties of niobium, even though no surfaces, stacking faults, dislocations, or highly compressed structures are included in the fitting database!

[1] M. S. Daw and M. I. Baskes, *Phys. Rev. Lett.* **50**, 1285 (1984). [2] F. Ercolessi and J. B. Adams, *Europhys. Lett.* **23**, 583 (1994). [3] P. Brommer and F. Gähler, *Modelling Simul. Mater. Sci. Eng.* **15**, 295 (2007).

Funding provided by the D.O.E. Computational resources provided by the Ohio Supercomputer Center.