Lecture 2: Physical Origins of Empirical Potentials

January 13, 2010

Stillinger-Weber Potential for Silicon

- F. H. Stillinger and T. A. Weber, "Computer simulation of local order in condensed phases of silicon," *Physical Review B* **31** (1985) 5262-5271.
- Cited more than 1300 times.
  - diamond as stable allotrope at low pressure, lattice constant, atomization energy
  - melting point and liquid structure in reasonable agreement with experiment

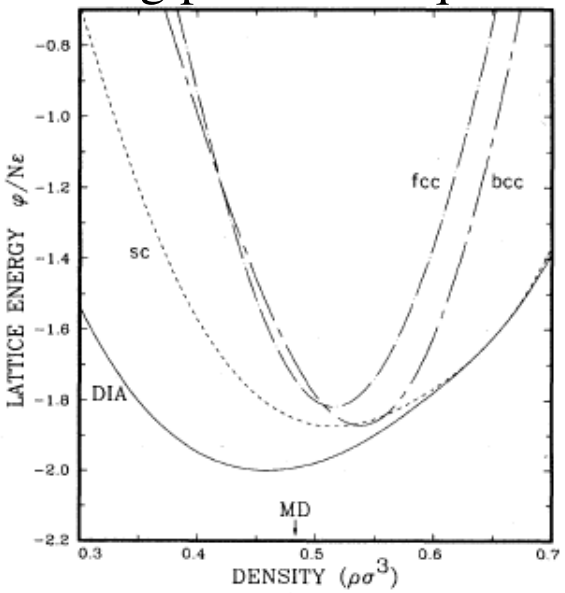


FIG. 1. Lattice energy (per atom) vs density for the nonadditive Si potential. Equation (2.7) provides the parameter set used for the interactions. The arrow locates the density at which our molecular-dynamics calculations were performed. (See text for label legend.)

TABLE I. Comparison of structure-factor positions in k space. (Units for k are Å^{-1}.)

Feature[a]	Molecular dynamics[b]	Experiment[c]
First peak	2.53	2.80
Shoulder	3.25	3.25
Second peak	5.35	5.75
Third peak	8.16	8.50
Fourth peak	10.60	11.20

[a]Refer to Fig. 6.
[b]For $T^*=0.0817$.
[c]From Waseda and Suzuki, Ref. 2, Fig. 1, for liquid Si at 1460 °C.

Performance of SW Silicon

	Experiment	SW Silicon
C11, GPa	151.6	166
C12, GPa	76.5	64
Thermal conductivity, W/m-K @ 500 K	76	230±47

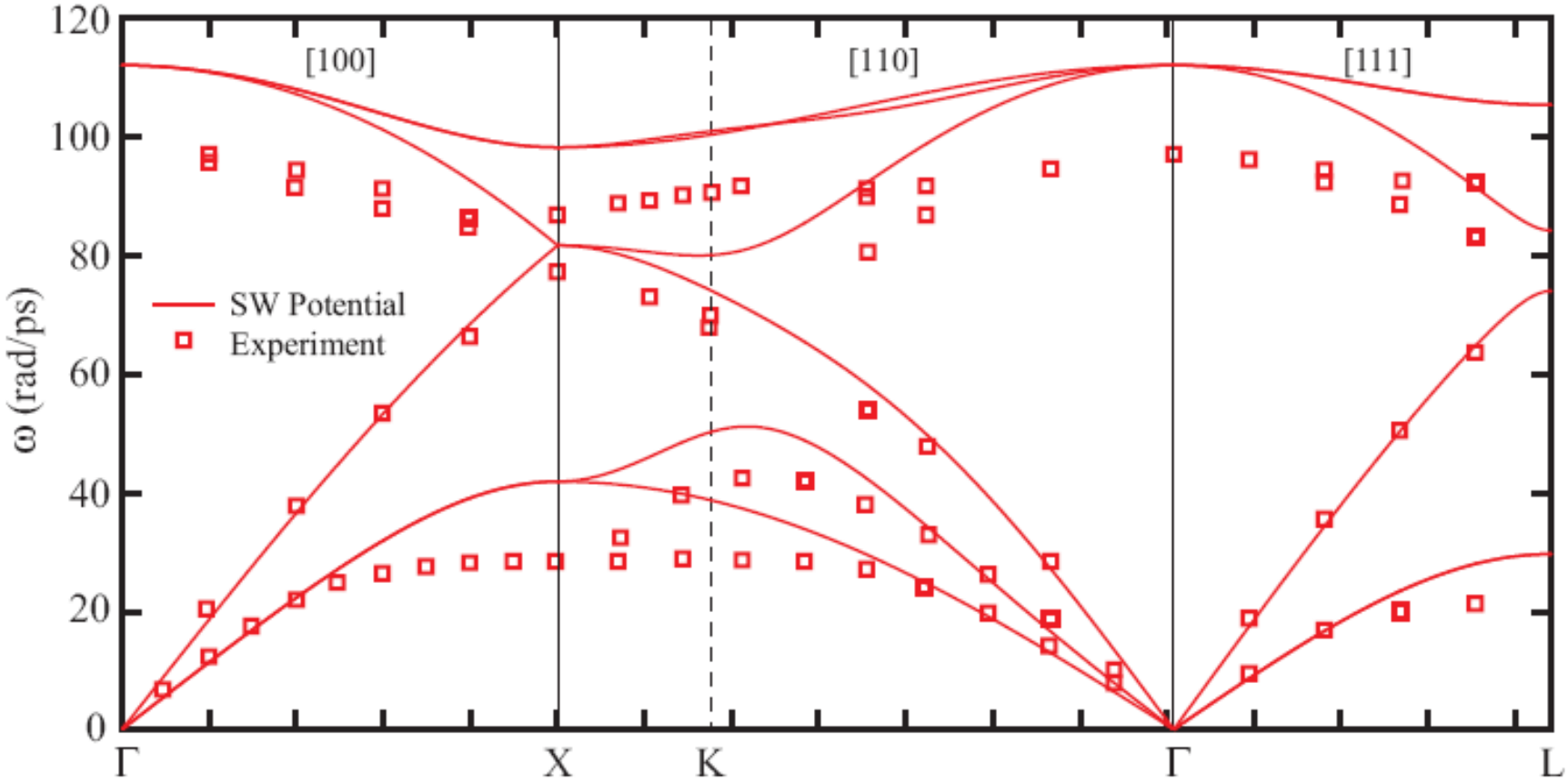
From Eric Landry's PhD thesis (CMU, 2009).

TABLE I. Grüneisen parameters.

	Experiment	*ab inttio*	Tight binding	Tersoff	Stillinger–Weber
$\gamma_{LTO}(\Gamma)$	0.98	1.00	0.98	1.32	0.80
$\gamma_{TA}(X)$	−1.40	−2.18	−1.12	−0.20	−0.04
$\gamma_{TO}(X)$	1.50	1.50	1.37	1.60	0.89
$\gamma_{LOA}(X)$	0.90	0.97	1.02	1.27	0.83

The Gruneisen parameters are related to thermal expansion. From Porter et al., *JAP* **81** (1997) 96-106.

More SW Silicon Performance



Phonon dispersion curves are related to the atomic vibrations.
From Eric Landry's PhD thesis (CMU, 2009).

Thermal Conductivity from Si Potentials

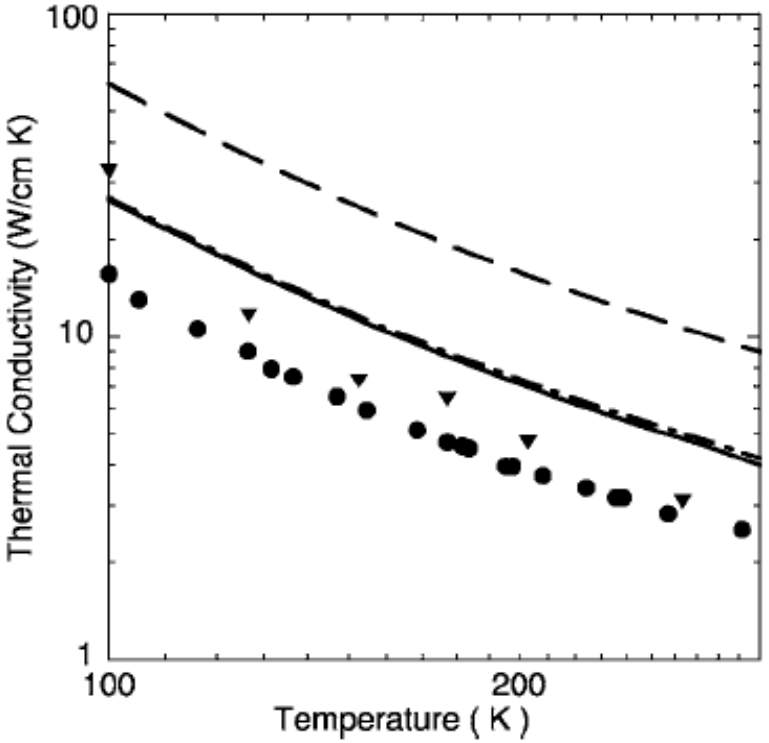


FIG. 5. Calculated lattice thermal conductivity for isotopically enriched Si using SW (dashed line), Tersoff (dashed-dotted line) and ED (solid line) models in the temperature range between 100 K and 300 K compared to measured values.

Broido et al, *Physical Review B* **72** (2005) 014308.

None of the commonly used potentials for silicon does a good job of predicting its thermal conductivity.

Embedded Atom Method Potential for Copper

Mishin et al., "Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations." *Physical Review B* **63** (2001) 224106.

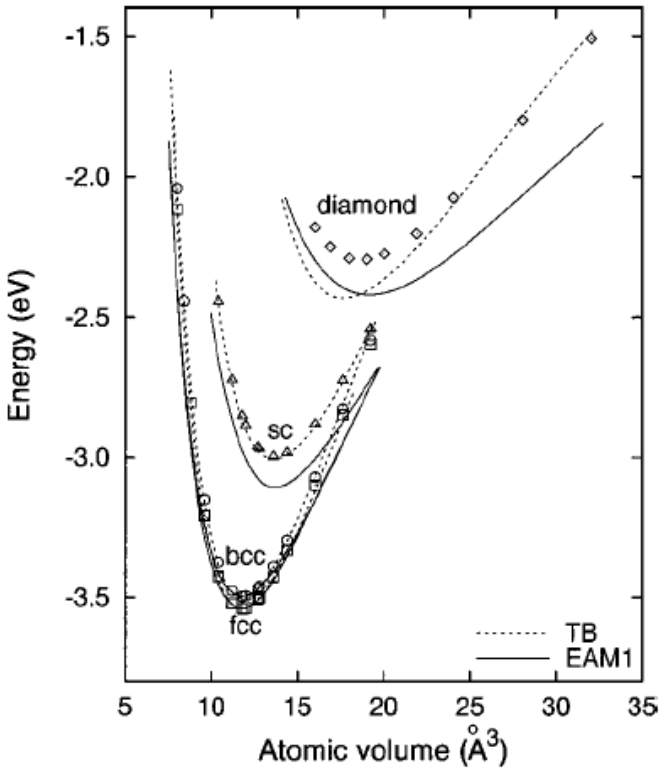


FIG. 7. Comparison of *ab initio* (LDA), TB, and EAM-calculated equations of state of the fcc (□), bcc (○), sc (△), and diamond (◇) structures of Cu around equilibrium.

TABLE VII. Bond length (R_d, in Å) and bond strength (E_d, in eV) of a Cu dimer predicted by the EAM potentials in comparison with experimental data and *ab initio* (GGA) calculations.

	Experiment	*ab initio*	EAM1	EAM2
R_d	2.2[a]	2.32	2.18	2.24
E_d	−2.05[a]	−1.80	−1.93	−2.07

TABLE IV. Properties of point defects in Cu predicted by the EAM potentials in comparison with experimental data. k_B is the Boltzmann constant; other notations are explained in Sec. IV C.

	Experiment	EAM1	EAM2
Vacancy:			
E_f (eV)	1.27[a], 1.28[b]	1.272	1.258
Ω_f/Ω_0	0.78[c]	0.701	0.743
S_f/k_B	2.35[b]	1.404	1.245
E_m (eV)	0.71[b]	0.689	0.690
Ω_m/Ω_0	0.12[d]	0.107	0.166
ν_0 (THz)		7.69	16.22
Interstitial:			
E_f (eV)	2.8-4.2[e]	3.063	3.229
Ω_f/Ω_0	0.55± 0.20[e]	0.834	1.061
S_f/k_B		7.429	11.00
E_m (eV)	0.12[f]	0.098	0.083
Ω_m/Ω_0		0.041	0.038
ν_0 (THz)		1.20	1.36

More on the Mishin EAM Potential for Copper

TABLE III. Lattice properties of Cu predicted by the EAM potentials in comparison with experimental data. * data not included in the fit.

	Experiment	EAM1	EAM2
a_0 (Å)	3.615[a]	3.615	3.615
E_0 (eV/atom)	−3.54[b]	−3.54	−3.54
B (10^{11} Pa)	1.383[c]	1.383	1.419
c_{11} (10^{11} Pa)	1.700[c]	1.699	1.793
c_{12} (10^{11} Pa)	1.225[c]	1.226	1.232
c_{44} (10^{11} Pa)	0.758[c]	0.762	0.810
$\nu_L(X)$ (THz)	7.38[d]	7.82	7.94*
$\nu_T(X)$ (THz)	5.16[d]	5.20	5.22*
$\nu_L(L)$ (THz)	7.44[d]	7.78*	7.93*
$\nu_T(L)$ (THz)	3.41[d]	3.32*	3.36*
$\nu_L(K)$ (THz)	5.90[d]	6.22*	6.37*
$\nu_{T_1}(K)$ (THz)	4.60[d]	4.65*	4.71*
$\nu_{T_2}(K)$ (THz)	6.70[d]	7.17*	7.30*

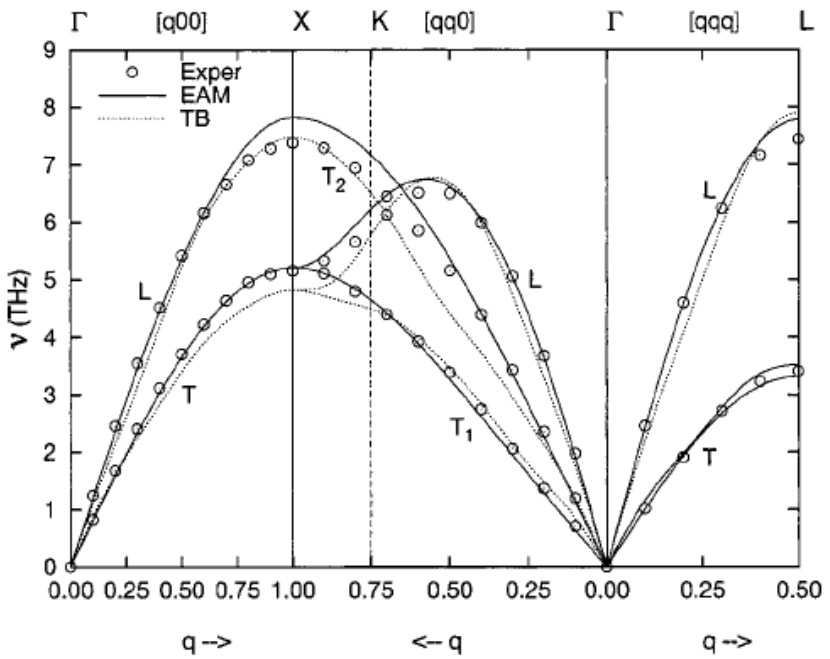


FIG. 2. Phonon dispersion curves calculated with the EAM1 potential and by the TB method. Experimental points (○) measured by neutron diffraction at temperature 80 K are shown for comparison (Ref. 57).