Interatomic Potentials for the Simulation of Defects, Plasticity and Phase Transformations in Titanium

M.I. Mendelev[1*], T.L. Underwood[2] and G.J. Ackland[3]

[1]*Division of Materials Sciences and Engineering, Ames Laboratory, Ames, IA, 50011, USA*
[2] *Department of Physics, University of Bath, Bath, BA2 7AY, UK*
[3]*Centre for Science at Extreme Conditions, School of Physics, University of Edinburgh, Edinburgh EH9 3JZ, Scotland, UK*

New interatomic potentials describing defects, plasticity and high temperature phase transitions for Ti are presented. Fitting the martensitic hcp-bcc phase transformation temperature requires an efficient and accurate method to determine it. We apply a molecular dynamics (MD) method based on determination of the melting temperature of competing solid phases, and Gibbs-Helmholtz integration, and a lattice-switch Monte Carlo method (LSMC): these agree on the hcp-bcc transformation temperatures to within 2 K. We were able to develop embedded atom potentials which give a good fit to either low or high temperature data, but not both. The first developed potential (Ti1) reproduces the hcp-bcc transformation and melting temperatures and is suitable for the simulation of phase transitions and bcc Ti. Two other potentials (Ti2 and Ti3) correctly describe defect properties, and can be used to simulate plasticity or radiation damage in hcp Ti.

[*] Corresponding author; email address: mendelev@ameslab.gov

Table I. Properties of crystal phases at T=0[¥].

Property	Target value	Ti1	Ti2	Ti3
a (hcp) (Å)	2.951	**2.947**	**2.949**	**2.951**
c/a (hcp)	1.588	**1.597**	**1.593**	**1.589**
E_{coh} (eV/atom)	4.85	**5.346**	**5.247**	**5.402**
C_{11} (hcp, GPa)	176.1 [1]	**161**	**160**	**165**
C_{12} (hcp, GPa)	86.9 [1]	**80**	**70**	**88**
C_{44} (hcp, GPa)	50.8 [1]	**53**	**54**	**58**
C_{13} (hcp, GPa)	68.3 [1]	**86**	**70**	**83**
C_{33} (hcp, GPa)	172.5 [1]	**169**	**165**	**166**
C_{66} (hcp, GPa)	44.6 [1]	**40**	**45**	**39**
$\Delta E_{hcp\rightarrow\omega}$ (eV/atom)	0.005 [2]	0.005	0.007	0.016
a (fcc) (Å)	4.115 [2]	4.182	4.213	4.131
$\Delta E_{hcp\rightarrow fcc}$ (eV/atom)	0.059 [2]	0.059	0.052	0.053
a (bcc) (Å)	3.26 [2]	3.251	3.256	3.242
$\Delta E_{hcp\rightarrow bcc}$ (eV/atom)	0.099 [2]	0.029	0.074	0.089

[¥] The properties used in the fitting procedure are printed in bold.

Table II. Formation energies (eV) of point defects in hcp Ti at T=0[¥].

Property	Target value [3]	Ti1	Ti2	Ti3
E_f^v	1.97	**2.74**	**1.78**	**1.73**
E_f^O	2.13	**2.30**	**2.17**	**2.23**
E_f^{BO}	2.25	**2.30**	**2.28**	**2.29**
E_f^{BS}	2.45	**2.36**	**2.37**	**2.35**
E_f^S	2.48	3.15	2.79	3.01

[¥] The properties used in the fitting procedure are printed in bold.

Table III. Formation energies (mJ/m^2) of planar defects in hcp Ti at T=0[¥].

Defect	Target value [4]	Ti1	Ti2	Ti3
I_1 basal stacking fault defect energy	148	**130**	**119**	**118**
I_2 basal stacking fault defect energy	259	**257**	**236**	**236**
E basal stacking fault defect energy	353	**383**	**351**	**352**
Prism stacking fault defect energy	250	**208**	**257**	**255**
[0001] free surface energy	124	**86**	**120**	**141**

[¥] The properties used in the fitting procedure are printed in bold.

Table IV. Phase transformation data[¥]. For the hcp-bcc transformation temperatures, the top value is obtained from MD simulation and the bottom values are obtained from the LSMC.

Property	Target value [5]	Ti1	Ti2	Ti3
$T_{\alpha\rightarrow\beta}$ (K)	1155	**1150** **1152**	**1148** **1150** **1151**	**1148** **1149**
$\Delta H_{\alpha\rightarrow\beta}$ (eV/atom)	0.0435	**0.022**	**0.032**	**0.041**
$\Delta V_{\alpha\rightarrow\beta}/V_{\alpha}$ (%)		-0.70	-0.03	0.71
T_m (hcp, K)		1765	1277	1189
ΔH_m (hcp, eV/atom)		0.143	0.124	0.122
T_m (bcc, K)	1941	**1918**	1322	1210
ΔH_m (bcc, eV/atom)	0.157	**0.130**	0.097	0.083

Table V. Activation energies for self-diffusion (eV/atom) in the vacancy (v) and self-interstitial mechanisms (i). For hcp Ti the point defect formation energies at T=1100 K were used and for the bcc the point defect formation energies at T=1500 K, T=1200 K and T=1100 K were used for potentials Ti1, Ti2 and Ti3, respectively.

Phase	Experiment	*Ab initio*	Ti1	Ti2	Ti3
hcp	2.00 [6] 3.14 [7]	v: 2.39 [8] v: 2.61 [9]	v: 3.61 i: 2.39	v: 2.70 i: 2.00	v: 2.51 i: 1.98
bcc	1.58 [10] 1.35-2.60 [11]		v: 2.86 i: 1.51	v: 1.76 i: 0.84	v: 1.25 i: 0.70

Table VI. Point defect migration energies (eV/atom) obtained from MD simulation.

Phase	Point defect	Ti1	Ti2	Ti3
hcp	vacancy	0.72	0.49	0.41
	interstitial	0.07	0.08	0.11
bcc	vacancy	0.30	0.24	0.24
	interstitial	0.11	0.10	0.13

[¥] The properties used in the fitting procedure are printed in bold.

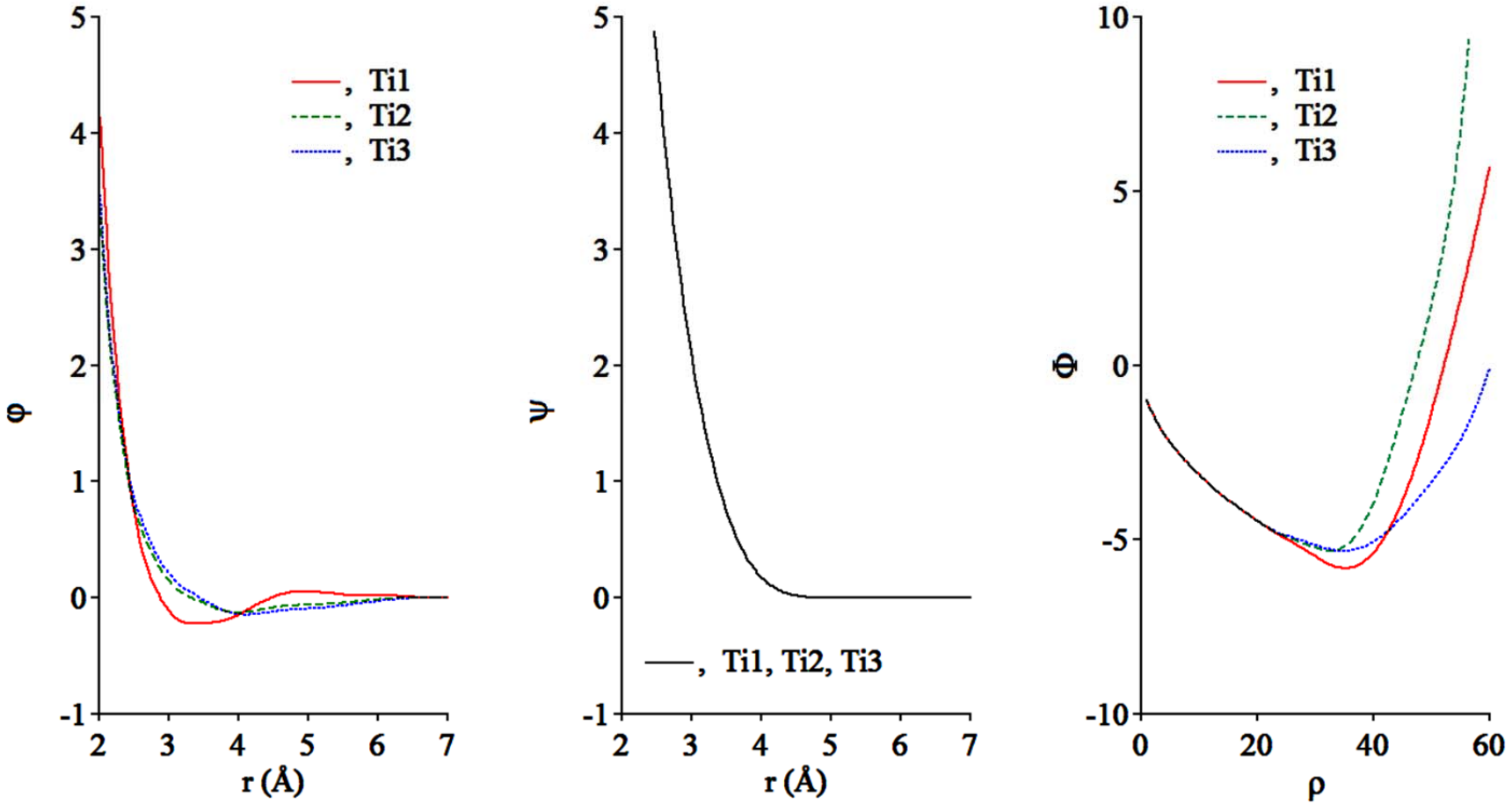

Figure 1. Potential functions.

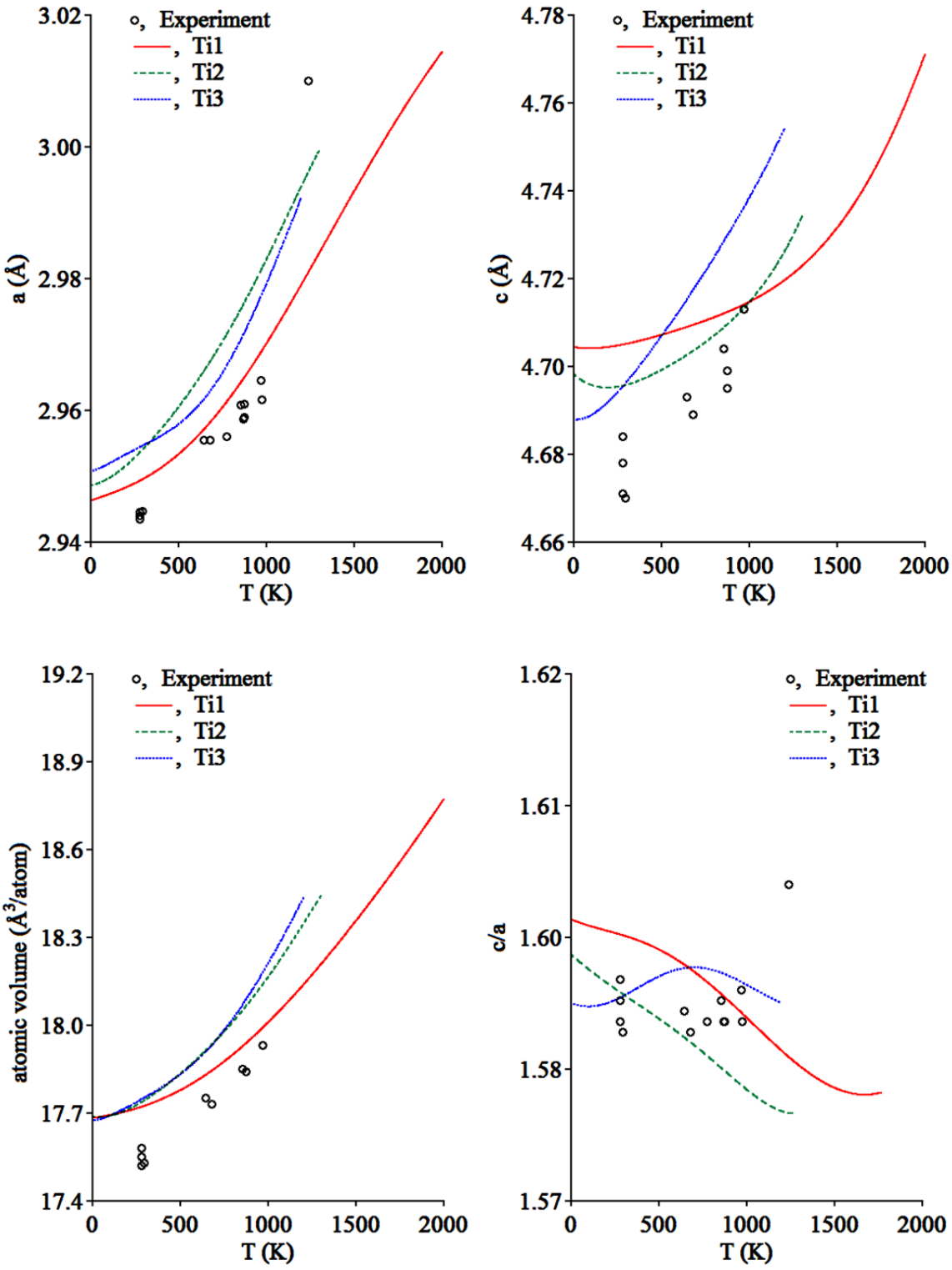

Figure 2. HCP lattice parameters as function of temperature. The experimental data are from [12].

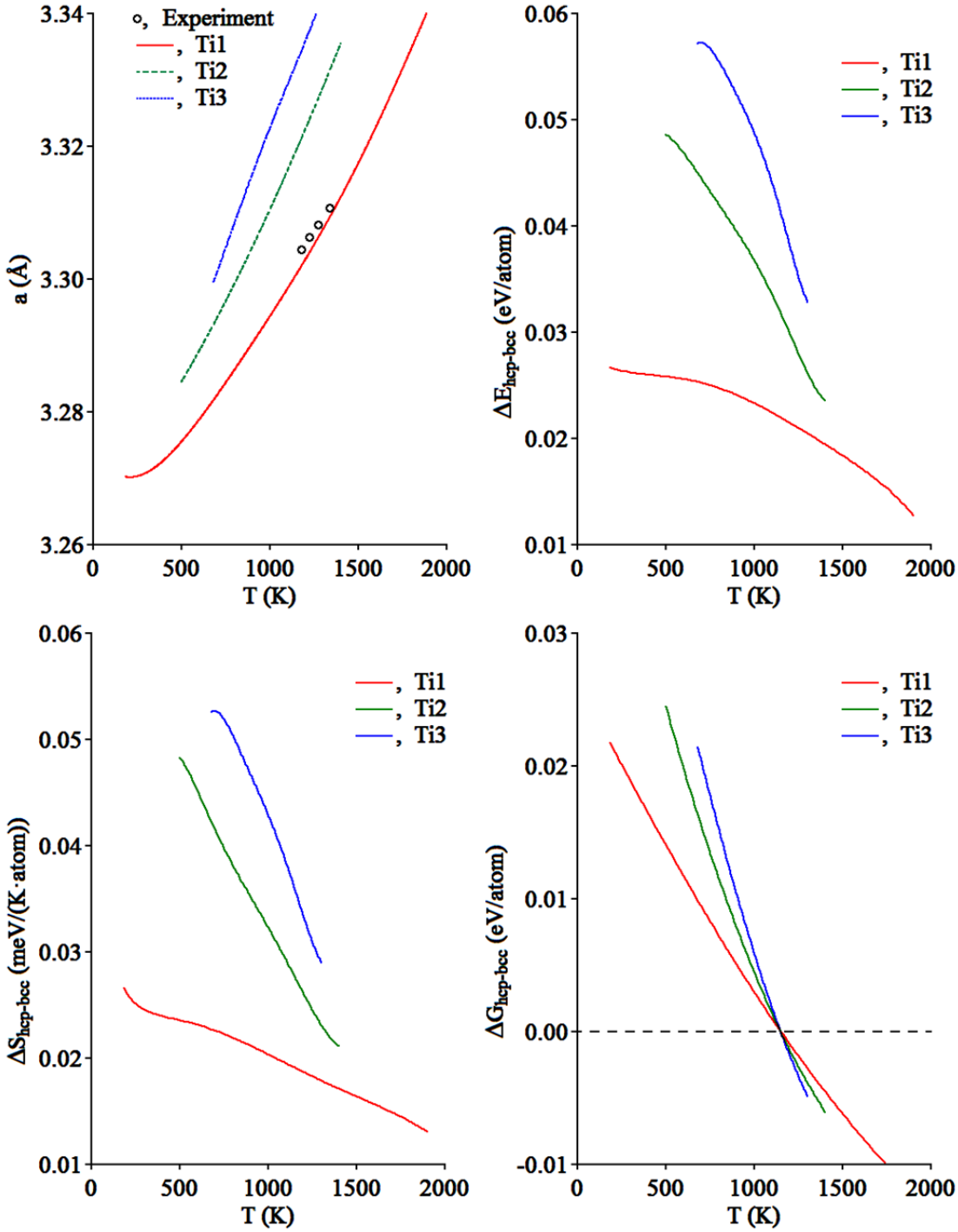

Figure 3. BCC lattice parameter, relative (to hcp) energy, entropy and free energy as functions of temperature. The experimental data are from [12].

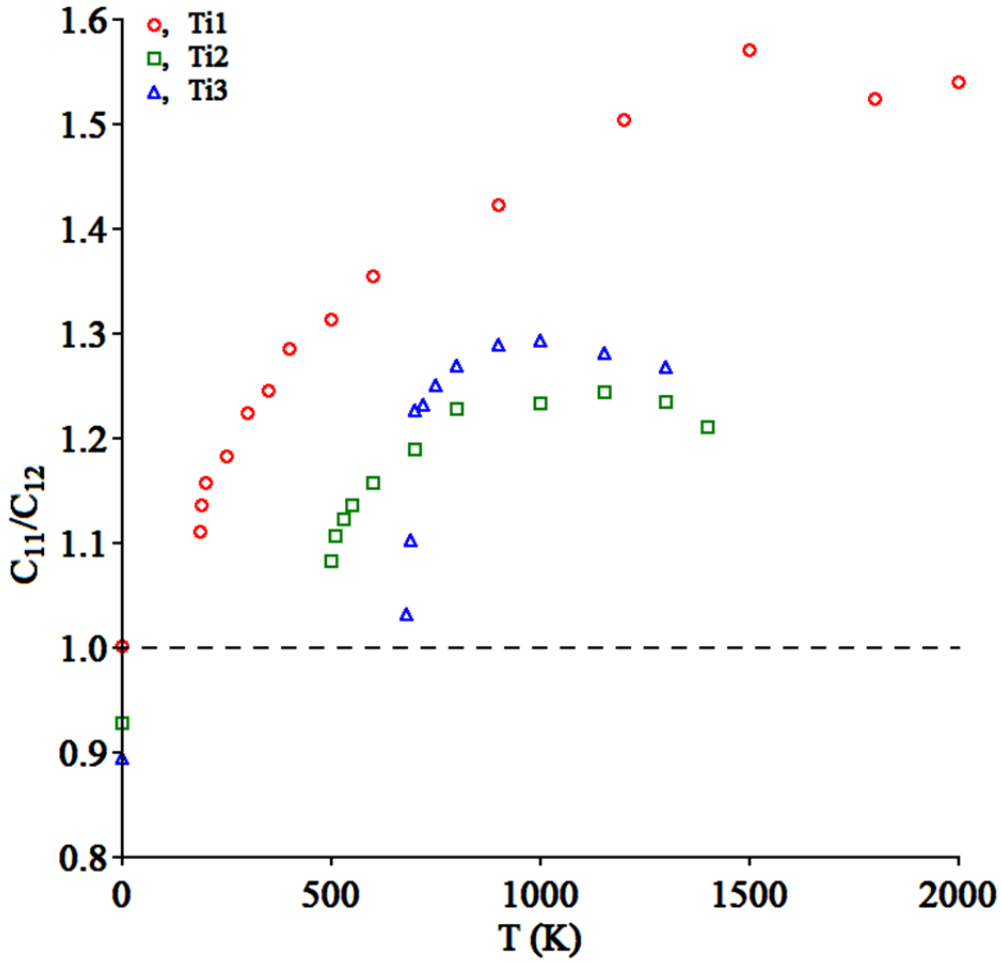

Figure 4. The C_{11}/C_{12} ratio for bcc Ti as function of temperature.

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