

**Zope-Ti-Al-2003.eam.alloy** release notes, 2 Dec. 2009. This file and the interatomic potential can be found at <http://www.ctcms.nist.gov/potentials/>.

These are the results of tests done to assess the accuracy of the conversion from R.R. Zope and Y. Mishin's 2003 Ti-Al files in the x,y plt format to the setfl format (Zope-Ti-Al-2003.eam.alloy, conversion 26 Sept. 2009 by C.A. Becker). The conversion was done by interpolating the plt files using cubic splines, ensuring  $\rho(r)$  and  $\phi(r)$  started at  $r = 0$ . The converter is adapted from Yuri Mishin's SOLD (Simulator of Lattice Defects) program in order to be as consistent as possible with previous results. For all tests, the simulation contained 1 unit cell with atoms in their ideal positions (four atoms for fcc-based phases, two atoms for bcc). Conjugate gradient energy minimization was used to minimize the total energy. The SOLD program was kindly provided by Yuri Mishin.

The original reference for this potential is: R.R. Zope and Y. Mishin, "Interatomic potentials for atomistic simulations of the Ti-Al system," Phys. Rev. B 68, 024102 (2003).

To use the file Zope-Ti-Al-2003.eam.alloy with LAMMPS, the following should be included in the input file:

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units metal
atom_style atomic
pair_style eam/alloy
pair_coeff * * Zope-Ti-Al-2003.eam.alloy Ti Al
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Comparison of minimum energies from SOLD and LAMMPS:

Alloy	a (Å)	c (Å)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Al	4.045		-13.4397745563	-13.4397745563	= -3.3600000286 eV/atom
	4.05		-13.4400001143	-13.4400001144	
	4.055		-13.4397762944	-13.4397762944	
hcp Ti	2.952	4.68	-19.4000339596	-19.4000340228	= -4.8500111 eV/atom
	2.952	4.6825	-19.4000389587	-19.4000389739	
	2.9525	4.68	-19.4000424069	-19.4000424375	
	2.9525	4.6825	-19.4000412472	-19.4000412464	
	2.953	4.68	-19.4000443787	-19.4000443862	
	2.953	4.6825	-19.4000370534	-19.4000370457	
L12 Ti3Al	4.088		-19.0600159959	-19.0600159628	= -4.765009 eV/atom
	4.089		-19.0600362232	-19.0600361946	
	4.090		-19.0600289674	-19.0600289854	

Alloy	a (Å)	c (Å)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
L10	3.992	4.19160	-18.0340329395	-18.034032892	
TiAl ( $\gamma$ )	3.993	4.19265	-18.0340905501	-18.0340905376	
	3.994	4.19370	-18.0341145962	-18.0341145898	
	3.995	4.19475	-18.0341051941	-18.0341051699	
	3.996	4.19580	-18.0340624813	-18.0340624855	
	3.999	4.178955	-18.0340940440	-18.0340940461	
	4.001	4.181045	-18.0341484449	-18.0341484247	= -4.5085371 eV/atom
	4.002	4.182090	-18.0341258523	-18.0341258384	
	4.003	4.183135	-18.0340702051	-18.0340701993	
	4	4.180	-18.0341378785	-18.0341378857	
	B2	3.277		-8.78153078882	-8.78153078995
TiAl	3.278		-8.78154772811	-8.7815477255	= -4.390773865 eV/atom
	3.279		-8.78154485255	-8.78154484153	
	3.280		-8.78152216632	-8.78152216452	
L12	4.049		-16.1437734681	-16.1437734506	
TiAl3	4.05		-16.1437985552	-16.1437985475	= -4.0359496 eV/atom
	4.051		-16.1437955663	-16.1437955655	

EAM function values from SOLD and LAMMPS:

Al a=4.05 Å

$r^2$	$\rho$ (SOLD)	$\rho$ (LAMMPS)
8.201250	0.053548222950895	0.053548222951017
16.402500	0.024899318931259	0.024899318931210
24.603750	0.006276756467770	0.006276756467765
32.805000	0.000686952274612	0.000686952274609
41.006250	0.000007440355646	0.000007440355646

$r^2$	$\phi$ (SOLD)	$\phi$ (LAMMPS)
8.201250	-0.153237026567445	-0.153237026567273
16.402500	-0.040567656105673	-0.040567656106000
24.603750	0.004882897654908	0.004882897654882
32.805000	0.006536860934147	0.006536860934180
41.006250	0.000153448477333	0.000153448477334

$\rho$ (SOLD)	F(SOLD)
0.951038740055635	-1.477064411514435
0.951038740055636	-1.477064411514434

$\rho$ (LAMMPS)	F(LAMMPS)
0.951038740056642	-1.477064411531952
0.951038740056643	-1.477064411531952

Ti a=2.953 Å, c=4.68 Å

$r^2$	$\rho(\text{SOLD})$	$\rho(\text{LAMMPS})$
8.382336	0.077993932478011	0.077993932494381
8.720209	0.072878989684641	0.072878989674376
8.720209	0.072878989684641	0.072878989674377
17.102545	0.015074778424383	0.015074778413629
21.902400	0.002198389994279	0.002198389990021
25.822754	0.000003951585165	0.000003951584164
26.160627	0.000000935412833	0.000000935412705

$r^2$	$\phi(\text{SOLD})$	$\phi(\text{LAMMPS})$
8.382336	-0.504769244469236	-0.504769244506904
8.720209	-0.483071385713732	-0.483071385675987
8.720209	-0.483071385713733	.
17.102545	-0.113754845750639	-0.113754845678595
21.902400	-0.019570779636508	-0.019570779601121
25.822754	-0.000043894516520	-0.000043894505591
26.160627	-0.000010624828922	-0.000010624827485

$\rho(\text{SOLD})$	F(SOLD)
1.000136015009747	1.799293803364773
1.000136015009748	1.799293803364774

$\rho(\text{LAMMPS})$	F(LAMMPS)
1.000136014960556	1.799293800851622
1.000136014960556	1.799293800851623
1.000136014960557	1.799293800851625

Ti3Al a=4.089 A

$r^2$	$\rho(\text{SOLD})$	$\rho(\text{LAMMPS})$
8.359961	0.053015433408027	0.053015433407783
8.359961	0.078347813960427	0.078347814008026
16.719921	0.016348980442366	0.016348980434649
16.719921	0.023896512951710	0.023896512951482
25.079882	0.000032539122022	0.000032539121936
25.079882	0.005669599519277	0.005669599519295
33.439842	0.000547976900157	0.000547976900155
41.799803	0.000003171684309	0.000003171684309

$r^2$	$\phi(\text{SOLD})$	$\phi(\text{LAMMPS})$
8.359961	-0.326976325430722	-0.326976325091837
8.359961	-0.506150077154965	-0.506150077378305
16.719921	-0.038628873604745	-0.038628873604539
16.719921	-0.122400704716078	-0.122400704666007
25.079882	-0.000344741774732	-0.000344741773846
25.079882	-0.011518627489789	-0.011518627263213
33.439842	0.005675186775722	0.005675186775758
41.799803	0.000000000000000	0.000000000000000

$\rho(\text{SOLD})$	F(SOLD)
0.982840923550754	1.715811005123697
1.090909506965781	-1.276110166576228

$\rho(\text{LAMMPS})$	F(LAMMPS)
0.982840923883050	1.715811009477530
0.982840923883050	1.715811009477531
1.090909507533538	-1.276110165688090

TiAl (L10) a=4.001 Å, c=4.181045 Å

$r^2$	$\rho(\text{SOLD})$	$\rho(\text{LAMMPS})$
8.004000	0.054205591655335	0.054205591654916
8.004001	0.084245980422628	0.084245980421391
8.372285	0.052973921244416	0.052973921244184
8.372285	0.078152663294110	0.078152663249015
16.008001	0.018859747925919	0.018859747925465
16.008001	0.026170668913723	0.026170668913905
17.481137	0.013856099936548	0.013856099930796
17.481137	0.021570698699873	0.021570698700080
24.380286	0.000126936179336	0.000126936181535
24.380286	0.006577775154540	0.006577775154562
25.485138	0.000011656546466	0.000011656543594
25.485138	0.005188367908258	0.005188367908285
32.016002	0.000896583740148	0.000896583740145
33.489138	0.000538188443496	0.000538188443493
40.020003	0.000017659318402	0.000017659318403
40.388287	0.000013049167196	0.000013049167195
43.334559	0.000000283670397	0.000000283670397

$r^2$	$\phi(\text{SOLD})$	$\phi(\text{LAMMPS})$
8.004000	-0.152838354980357	.
8.004001	.	-0.152838354979688
8.004001	-0.526762871888997	-0.526762871884897
8.372285	-0.326833654759253	-0.326833654624253
16.008001	-0.043064043595308	-0.043064043595710
16.008001	-0.139419732808950	-0.139419732803602
16.008001	.	-0.139419732803603
17.481137	-0.034103702832233	-0.034103702832284
17.481137	-0.105457775422563	-0.105457775382281
24.380286	-0.015522577247653	-0.015522576969650
25.485138	-0.000126690051919	-0.000126690021397
25.485138	0.007467772205842	0.007467772205805
32.016002	0.007611031133211	0.007611031133203
33.489138	0.005609203556565	0.005609203556537
40.020003	0.000341003700850	0.000341003700850
40.388287	0.000000000000000	0.000000000000000
43.334559	0.000000000000000	0.000000000000000

$\rho(\text{SOLD})$	F(SOLD)
0.969370800767724	1.651109425610925
1.041438785220075	-1.351434170205382

$\rho(\text{LAMMPS})$	F(LAMMPS)
0.969370800724962	1.651109424828282
1.041438784894151	-1.351434170733075

TiAl (B2) a=3.278 Å

$r^2$	$\rho(\text{SOLD})$	$\rho(\text{LAMMPS})$
8.058963	0.054022964285386	0.054022964285147
8.058963	0.083302691944330	0.083302691926748
10.745284	0.044681092277725	0.044681092277698
10.745284	0.049384334971956	0.049384334647721
21.490568	0.011474449830716	0.011474449831014
21.490568	0.002949349116107	0.002949349134655
29.549531	0.001889584757241	0.001889584757265
32.235852	0.000833729738263	0.000833729738263
42.981136	0.000000567858517	0.000000567858517

$r^2$	$\phi(\text{SOLD})$	$\phi(\text{LAMMPS})$
8.058963	-0.328510454081027	-0.328510454090304
10.745284	-0.112838124250355	-0.112838124250509
10.745284	-0.349099330705826	-0.349099328566640
21.490568	-0.009900934805042	-0.009900934805068
21.490568	-0.025763158515536	-0.025763158666320
29.549531	0.000086147507834	0.000086147515289
32.235852	0.007314109197495	0.007314109197526
42.981136	0.000013169940748	0.000013169940748

$\rho(\text{SOLD})$	F(SOLD)
0.809231947681909	0.906284111067930
1.078874732246792	-1.294797697894381

$\rho(\text{LAMMPS})$	F(LAMMPS)
0.809231945957733	0.906284102687796
1.078874732109539	-1.294797698145194

TiAl3 a=4.05 A

$r^2$	$\rho(\text{SOLD})$	$\rho(\text{LAMMPS})$
8.201250	0.053548222950895	0.053548222951017
8.201250	0.080914845147963	0.080914845138743
16.402500	0.024899318931259	0.024899318931210
16.402500	0.017443841847804	0.017443841625047
24.603750	0.006276756467770	0.006276756467765
24.603750	0.000085745113656	0.000085745113701
32.805000	0.000686952274612	0.000686952274609
41.006250	0.000007440355646	0.000007440355646

$r^2$	$\phi(\text{SOLD})$	$\phi(\text{LAMMPS})$
8.201250	-0.153237026567445	-0.153237026567273
8.201250	-0.328282630136492	-0.328282630163534
16.402500	-0.040567656105673	-0.040567656106000
16.402500	-0.129820473949353	-0.129820472435009
24.603750	0.004882897654908	0.004882897654882
24.603750	.	0.004882897654883
24.603750	-0.014194866734730	-0.014194866674632
32.805000	0.006536860934147	0.006536860934180
41.006250	0.000153448477333	0.000153448477334

$\rho(\text{SOLD})$	F(SOLD)
0.898062450259557	1.313491331373675
1.010917615165827	-1.395798492272024
1.010917615165827	-1.395798492272025

$\rho(\text{LAMMPS})$	F(LAMMPS)
0.898062448924354	1.313491327837591
1.010917615129869	-1.395798492288835





