Mishin-Ni-Al-2009.eam.alloy release notes, 19 August 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 Yuri Mishin's 2009 Ni-Al (B2) files in the x,y plt format to the setfl format (Mishin-Ni-Al-2009.eam.alloy, conversion 13 August 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. 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: G.P. Purja Pun and Y. Mishin, "Development of an interatomic potential for the Ni-Al system," Phil. Mag., in press (2009).

To use the file Mishin-Ni-Al-2009.eam.alloy with LAMMPS, the following should be included in the input file:

```
units metal
atom_style atomic
pair_style eam/alloy
pair_coeff * * Mishin-Ni-Al-2009.eam.alloy Ni Al
```

Comparison of minimum energies from SOLD and LAMMPS:

Alloy	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Al	4.045	-0.134397756745E+02	-13.4397756743	
	4.05	-0.134399999516E+02	-13.4399999514	= -3.359999988 eV/atom
	4.055	-0.134397757919E+02	-13.4397757921	
fcc Ni	3.519	-0.177999820298E+02	-17.7999820299	
	3.52	-0.177999999432E+02	-17.799999943	= -4.449999986 eV/atom
	3.521	-0.177999820682E+02	-17.7999820682	
L12 Ni3Al	3.532	-0.185258859907E+02	-18.5258859916	
	3.533	-0.185259112893E+02	-18.5259112895	= -4.631477822 eV/atom
	3.534	-0.185258988109E+02	-18.5258988111	
L10 NiAl	3.625	-0.175439268133E+02	-17.5439268138	
	3.630	-0.175445438608E+02	-17.5445438608	= -4.3861359652 eV/atom
	3.635	-0.175442706557E+02	-17.5442706554	
B2 NiAl	2.820	-0.901988823544E+01	-9.0198882355	
	2.830	-0.902169181012E+01	-9.0216918095	= -4.510845905 eV/atom
	2.840	-0.902094269088E+01	-9.02094269103	
L12 NiAl3	3.7900	-0.155703519696E+02	-15.5703519696	
	3.8000	-0.155724044383E+02	-15.5724044386	= -3.893101110 eV/atom
	3.8100	-0.155713317233E+02	-15.5713317243	

EAM function values from SOLD and LAMMPS:

Al a=4.05 A

r^2	ρ(SOLD)	ρ(LAMMPS)
8.201250	0.095012346269134	0.095012346269451
16.402500	0.010278087363631	0.010278087363738
24.603750	0.002934125893647	0.002934125893662
32.805000	0.000805364633604	0.000805364633606

r^2	ϕ(SOLD)	ϕ(LAMMPS)
8.201250	0.003021015687258	0.003021015687296
16.402500	-0.024843572779205	-0.024843572779268
24.603750	-0.009452555071469	-0.009452555071459
32.805000	0.002059415665899	0.002059415665861

ρ(SOLD)	F(SOLD)
1.281900076462172	-3.045042405755795
1.281900076462173	-3.045042405755795
1.281900076462174	-3.045042405755795
ρ(LAMMPS)	F(LAMMPS)
1.281900076466997	-3.045042405697896

Ni a=3.52A

r^2	ρ(SOLD)	ρ(LAMMPS)
6.195200	0.073688253896076	0.073688253896035
12.390400	0.014561052186354	0.014561052186232
18.585600	0.001180718486776	0.001180718486747
24.780800	0.000003122384944	0.000003122384944

r^2	ϕ(SOLD)	ϕ(LAMMPS)
6.195200	-0.112571381127819	-0.112571381126468
12.390400	-0.030355907048780	-0.030355907048621
18.585600	-0.014650265237694	-0.014650265237707
24.780800	-0.000103105399284	-0.000103105399281

ρ(SOLD)	F(SOLD)
1.000000072172976	-2.564164339477435
1.000000072172977	-2.564164339477435
ρ(LAMMPS)	F(SOLD)
1.000000072171081	-2.564164339431999
1.000000072171082	-2.564164339431999

Ni3Al a=3.533 A

r^2	ρ(SOLD)	ρ(LAMMPS)
6.241045	0.073005057141230	0.073005057141415
6.241045	0.108995483947539	0.108995483946264
12.482089	0.014138455656304	0.014138455656097
12.482089	0.033446551884762	0.033446551884614
18.723134	0.001097425590302	0.001097425590348
18.723134	0.006084948244929	0.006084948244962
24.964178	0.000002085072347	0.000002085072347
24.964178	0.002856275714075	0.002856275714105
31.205223	0.001307483750806	0.001307483750793
37.446267	0.000004676698321	0.000004676698321

r^2	ϕ(SOLD)	ϕ(LAMMPS)
6.241045	-0.110253680090281	-0.110253680090229
6.241045	-0.113547560396814	-0.113547560396325
12.482089	-0.019418290634449	-0.019418290634214
12.482089	-0.030192304350768	-0.030192304350467
18.723134	-0.014030176104746	-0.014030176104474
18.723134	-0.026513477113150	-0.026513477112948
24.964178	-0.000070260836842	-0.000070260836842
24.964178	-0.008158976726245	-0.008158976726229
31.205223	-0.000014307495552	-0.000014307495554
37.446267	-0.000026608991175	-0.000026608991176

ρ(SOLD)	F(SOLD)
1.137390933326043	-2.984357953980942
1.181576413136688	-2.487640081492315
1.181576413136689	-2.487640081492315

ρ(LAMMPS)	F(LAMMPS)
1.137390933328845	-2.984357953907380
1.181576413132721	-2.487640081598588

NiAl (L10) a=3.630 A

r^2	ρ(SOLD)	ρ(LAMMPS)
6.588450	0.108013740065148	0.067934912475959
6.588450	0.067934912475745	0.067934912475959
13.176900	0.011245545098604	0.011245545098042
13.176900	0.026817613620918	0.026817613620904
19.765350	0.000605281722629	0.000605281722630
19.765350	0.005014815454141	0.005014815454171
26.353800	0.002549677682835	0.002549677682805
32.942250	0.000761488818573	0.000761488818572

r^2	ϕ(SOLD)	ϕ(LAMMPS)
6.588450	0.081601556923343	0.081601556923653
6.588450	-0.116449068226131	-0.116449068225733
6.588450	-0.117204541686610	-0.117204541685705
13.176900	-0.019163663943906	-0.019163663943725
13.176900	-0.029414311308588	-0.029414311308263
19.765350	-0.009564006911081	-0.009564006911047
19.765350	-0.023253719065688	-0.023253719065980
19.765350	-0.023922289812956	-0.023922289812901
26.353800	-0.003648248914402	-0.003648248914381
32.942250	0.000000000000000	0.000000000000000
32.942250	0.001962364885558	0.001962364885536

ρ(SOLD)	F(SOLD)
1.222931015729853	-3.025871489710112
1.222931015729854	-3.025871489710112
1.300586005611142	-2.409244457873587

ρ(LAMMPS)	F(LAMMPS)
1.222931015743197	-3.025871489644225
1.300586005632739	-2.409244457954034
1.300586005632740	-2.409244457954033

NiAl (B2) a=2.830 A

r^2	ρ(SOLD)	ρ(LAMMPS)
6.006675	0.076530737651828	0.076530737651892
6.006675	0.109324281961265	0.109324281962944
8.008900	0.097309997868845	0.097309997868980
8.008900	0.049376097044988	0.049376097044603
16.017800	0.011386816645887	0.011386816645602
16.017800	0.003901531025568	0.003901531025548
22.024475	0.000116887902962	0.000116887902958
22.024475	0.003655426544560	0.003655426544550
24.026700	0.000011903898884	0.000011903898884
24.026700	0.003062294130700	0.003062294130692
32.035600	0.001051192819874	0.001051192819865
38.042275	0.000000792834243	0.000000792834244

r^2	ϕ(SOLD)	ϕ(LAMMPS)
6.006675	-0.102323752861595	-0.102323752861899
8.008900	0.007674646694968	0.007674646694976
8.008900	-0.093365586940797	-0.093365586940092
16.017800	-0.024249758358247	-0.024249758357835
16.017800	-0.025173373358654	-0.025173373359001
22.024475	-0.015233745074511	-0.015233745074431
24.026700	-0.000360196990495	-0.000360196990491
24.026700	-0.011576291225339	-0.011576291224749
32.035600	0.002501538849733	0.002501538849726
38.042275	0.000000000000000	0.000000000000000

ρ(SOLD)	F(SOLD)
1.305513706549218	-2.405389922321818
1.366358507814260	-3.060196183728233

ρ(LAMMPS)	F(LAMMPS)
1.305513706559849	-2.405389921749509
1.366358507811938	-3.060196183687272

NiAl3 a=3.800 A

r^2	ρ(SOLD)	ρ(LAMMPS)
7.220000	0.059235192050682	0.059235192050512
7.220000	0.104625762051193	0.104625762053465
14.440000	0.007212353782054	0.007212353782015
14.440000	0.018046285208120	0.018046285208394
21.660000	0.000159428090849	0.000159428090852
21.660000	0.003809354425202	0.003809354425247
28.880000	0.001948023172393	0.001948023172424
36.100000	0.000057267877297	0.000057267877297

r^2	ϕ(SOLD)	ϕ(LAMMPS)
7.220000	0.036996355725751	0.036996355726045
7.220000	-0.115939522714876	-0.115939522714970
14.440000	-0.020567361068403	-0.020567361068789
14.440000	-0.028446858918770	-0.028446858918890
21.660000	-0.016495190659379	-0.016495190659618
21.660000	-0.019745311462672	-0.019745311462505
28.880000	0.001475053462899	0.001475053462860
36.100000	0.000000000000000	0.000000000000000
36.100000	0.000050609961253	0.000050609961252

ρ(SOLD)	F(SOLD)
1.268742235496480	-3.041452573270912
1.268742235496481	-3.041452573270912
1.268742235496481	-3.041452573270913
1.391582202566611	-2.328504158927436

ρ(LAMMPS)	F(LAMMPS)
1.268742235516733	-3.041452573321823
1.391582202594718	-2.328504159118253