NiAl02.eam.alloy release notes, 15 February 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 Ni-Al (B2) files in the x,y plt format to the setfl format (NiAl02.eam.alloy, conversion 14 February 2009 by C.A. Becker). The conversion was done by interpolating the plt files using cubic splines, ensuring the 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: Y. Mishin, M.J. Mehl and D.A. Papaconstantopoulos, "Embedded-atom potential for B2-NiAl," Phys. Rev. B 65, 224114 (2002).

To use the file NiAl02.eam.alloy with LAMMPS, the following should be included in the input file:
```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * NiAl02.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	-0.134482192421E+02	-13.4482192421	
	4.05	-0.134486826112E+02	-13.4486826112	= -3.3621706528 eV/atom
	4.055	-0.134485718665E+02	-13.4485718665	
fcc Ni	3.452	-0.180053318287E+02	-18.0053318287	
	3.45249	-0.180053406289E+02	-18.0053406289	= -4.501335157225 eV/atom
	3.4525	-0.180053406037E+02	-18.0053406037	
	3.45251	-0.180053405703E+02	-18.0053405703	
	3.4526	-0.180053399012E+02	-18.0053399012	
L12 Ni3Al	3.524	-0.183999352664E+02	-18.3999352664	
	3.525	-0.183999858047E+02	-18.3999858047	
	3.526	-0.183999871894E+02	-18.3999871894	= -4.59999679735 eV/atom
	3.527	-0.183999397664E+02	-18.3999397664	
L10 NiAl	3.661	-0.171721132385E+02	-17.1721132385	
	3.662	-0.171721461844E+02	-17.1721461844	= -4.29303654610 eV/atom
	3.663	-0.171721402557E+02	-17.1721402557	
B2 NiAl	2.850	-0.892952307615E+01	-8.92952307615	
	2.859	-0.893049356847E+01	-8.93049356847	= -4.465246784235 eV/atom
	2.870	-0.892886524539E+01	-8.92886524539	
L12 NiAl3	3.8200	-0.152188309315E+02	-15.2188309315	
	3.8290	-0.152198509006E+02	-15.2198509005	= -3.804962725 eV/atom
	3.8400	-0.152183719760E+02	-15.218371976	

EAM function values from SOLD and LAMMPS

Al a=4.05 A

r^2	rho(SOLD)	rho(LAMMPS)
8.201250	0.043946108409475	0.043946108409466

r^2		
16.402500	0.017573384482599	0.017573384482599
24.603750	0.008346570436699	0.008346570436697
32.805000	0.000225909397442	0.000225909397438

r^2	phi(SOLD)	phi(LAMMPS)
8.201250	-0.111811344118166	-0.111811344118145
16.402500	-0.038059091370072	-0.038059091370072
16.402500	-0.038059091370073	.
24.603750	-0.007330360307942	-0.007330360307932
32.805000	0.000123471982732	0.000123471982726

rho(SOLD)	F(SOLD)
0.835822211059370	-1.617632991561796
rho(LAMMPS)	F(LAMMPS)
0.835822211059183	-1.617632991561717
0.835822211059184	-1.617632991561717

Ni a=3.45249 A

r^2	rho(SOLD)	rho(LAMMPS)
5.959844	0.052696529032081	0.052696529032080
11.919687	0.016378251744889	0.016378251744871
17.879531	0.005637388183983	0.005637388183982
23.839374	0.001911880852584	0.001911880852586
29.799218	0.000291036595249	0.000291036595249

r^2	phi(SOLD)	phi(LAMMPS)
5.959844	-0.016832821854653	-0.016832821854681
11.919687	0.045536808285913	0.045536808285939
17.879531	0.020978568043810	0.020978568043813
23.839374	-0.000296171310189	-0.000296171310189
29.799218	-0.005662884450409	-0.005662884450418

rho(SOLD)	F(SOLD)
0.895852623786865	-4.936584495211010
0.895852623786866	-4.936584495211010
rho(LAMMPS)	F(SOLD)
0.895852623786757	-4.936584495211537

Ni3Al a=3.526 A

r^2	rho(SOLD)	rho(LAMMPS)
6.216338	0.049977591707164	0.049977591707161
6.216338	0.056161094091044	0.056161094091029
12.432676	0.014897460456436	0.014897460456432
12.432676	0.026710057001230	0.026710057001229
18.649014	0.004925961138323	0.004925961138322
18.649014	0.014168142157274	0.014168142157269
24.865352	0.001549270495666	0.001549270495666
24.865352	0.008141274167315	0.008141274167315
31.081690	0.000104833484002	0.000104833484002
31.081690	0.001502349365906	0.001502349365905

r^2	phi(SOLD)	phi(LAMMPS)
6.216338	-0.015338490989909	-0.015338490989909
6.216338	-0.121061835598938	-0.121061835598933
12.432676	0.044653776174558	0.044653776174558
12.432676	-0.072684445730627	-0.072684445730632
18.649014	0.007543779534717	0.007543779534722
18.649014	0.017536656675373	0.017536656675374
24.865352	-0.002655449868744	-0.002655449868745

24.865352	-0.006785750057125	-0.006785750057122
31.081690	0.002179995715665	0.002179995715664
31.081690	-0.003246870775648	-0.003246870775647

rho(SOLD)	F(SOLD)
0.938297764850755	-4.969259854489311
0.938297764850756	-4.969259854489311
0.978425803436937	-1.561886823809835
rho(LAMMPS)	F(LAMMPS)
0.938297764850571	-4.969259854489203
0.978425803436874	-1.561886823809775

NiAl (L10) a=3.662 A

r^2	rho(SOLD)	rho(LAMMPS)
6.705122	0.045204425086512	0.045204425086510
6.705122	0.052866334067597	0.052866334067601
13.410244	0.012461253385578	0.012461253385578
13.410244	0.023982817162942	0.023982817162942
20.115366	0.003804799181530	0.003804799181530
20.115366	0.012401333286619	0.012401333286613
26.820488	0.006541038882621	0.006541038882622
26.820488	0.000972312174681	0.000972312174681
33.525610	0.000061945570325	0.000061945570328
33.525610	0.000001963646295	0.000001963646295

r^2	phi(SOLD)	phi(LAMMPS)
6.705122	-0.008059548259796	-0.008059548259791
6.705122	-0.008059548259797	.
6.705122	-0.027437193181508	-0.027437193181480
6.705122	-0.027437193181509	.
6.705122	-0.115160906037389	-0.115160906037394
13.410244	0.041675559185837	0.041675559185836
13.410244	-0.062114347455225	-0.062114347455223
20.115366	0.006863471253808	0.006863471253810
20.115366	0.011514770308719	0.011514770308722
20.115366	-0.019987332747115	-0.019987332747118
26.820488	-0.003234433767130	-0.003234433767130
26.820488	-0.005894011972231	-0.005894011972229
33.525610	0.000041322724035	0.000041322724032
33.525610	0.000116326220254	0.000116326220253
33.525610	-0.000176444772655	-0.000176444772654

rho(SOLD)	F(SOLD)
0.920050203630168	-4.957282667531691
0.956104542632348	-1.566546927107623
rho(LAMMPS)	F(LAMMPS)
0.920050203630129	-4.957282667531289
0.920050203630129	-4.957282667531290
0.956104542632316	-1.566546927107463
0.956104542632317	-1.566546927107463

NiAl (B2) a=2.859 A

r^2	rho(SOLD)	rho(LAMMPS)
6.130411	0.050871370399278	0.050871370399284
6.130411	0.056759573944192	0.056759573944197
8.173881	0.033609702736149	0.033609702736148
8.173881	0.044093956703371	0.044093956703367
16.347762	0.007377317979248	0.007377317979248
16.347762	0.017669175811745	0.017669175811717

22.478173	0.002481532862784	0.002481532862785
22.478173	0.010086980249931	0.010086980249939
24.521643	0.001665270473457	0.001665270473456
24.521643	0.008411081862180	0.008411081862183
32.695524	0.000265901570868	0.000265901570878
32.695524	0.000011716351718	0.000011716351718

r^2	phi(SOLD)	phi(LAMMPS)
6.130411	-0.120899044025914	-0.120899044025881
8.173881	0.020775827082729	0.020775827082733
8.173881	-0.111485019337917	-0.111485019337888
16.347762	0.028256924822905	0.028256924822866
16.347762	-0.038406126715367	-0.038406126715385
22.478173	0.006135252343991	0.006135252343991
24.521643	-0.001910237359988	-0.001910237359988
24.521643	-0.007504842365274	-0.007504842365259
32.695524	0.000140420507126	0.000140420507140
32.695524	-0.000696569860994	-0.000696569861034

rho(SOLD)	F(SOLD)
0.999742611617712	-4.986832861758329
1.012005666184867	-1.559065004641431

rho(LAMMPS)	F(LAMMPS)
0.999742611617931	-4.986832861758336
1.012005666184641	-1.559065004640355

NiAl3 a=3.829 A

r^2	rho(SOLD)	rho(LAMMPS)
7.330620	0.048925473579194	0.048925473579200
7.330621	0.039803995188809	0.039803995188812
14.661241	0.009948847806622	0.009948847806621
14.661241	0.020986879208441	0.020986879208426
21.991862	0.002714933152612	0.002714933152612
21.991862	0.010521043883246	0.010521043883235
29.322482	0.003810361219447	0.000382522595385
29.322482	0.000382522595385	0.003810361219438

r^2	phi(SOLD)	phi(LAMMPS)
7.330620	-0.098389984530717	-0.098389984530706
7.330621	-0.084613845312659	-0.084613845312446
14.661241	0.036376958311415	0.036376958311428
14.661241	-0.050676340715060	-0.050676340715061
21.991862	0.006237438275891	0.006237438275892
21.991862	-0.013821960314583	-0.013821960314580
29.322482	-0.000209531249018	-0.000209531249021
29.322482	-0.006271455092701	-0.006271455092666

rho(SOLD)	F(SOLD)
0.903894094132579	-4.944073933260764
0.912321546625625	-1.580971674704628

rho(LAMMPS)	F(LAMMPS)
0.903894094132370	-4.944073933259568
0.912321546625305	-1.580971674705626