NiAl.eam.alloy release notes, 7 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 (Ni3Al) files in the x,y plt format to the setfl format (NiAl.eam.alloy, conversion 7 Jan. 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 periodic boundary conditions and 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, "Atomistic modeling of the γ and γ'-phases of the Ni-Al system," Acta Mat. 52, 1451 (2004).

To use the file NiAl.eam.alloy with LAMMPS, the following should be included in the input file:

```
units          metal
atom_style     atomic
pair_style     eam/alloy
pair_coeff     * * NiAl.eam.alloy Ni Al
```

Calculated minimum energies

Alloy	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
Al	4.05	-0.134400000903E+02	-13.4400000903	= -3.360000022575 eV/atom
Ni	3.52	-0.177999999407E+02	-17.7999999407	= -4.449999985175 eV/atom
Ni3Al-L12	3.571	-0.185008771216E+02	-18.5008771217	= -4.625219280425 eV/atom (LAMMPS), -4.625219280400 eV/atom (SOLD)
Ni3Al-L12	3.5713	-0.185008794764E+02	-18.5008794764	
Ni3Al-L12	3.57135	-0.185008795501E+02	-18.5008795501	= -4.625219887525 eV/atom
Ni3Al-L12	3.5714	-0.185008795327E+02	-18.5008795327	

formation energy: (3*4.450+3.36)/4-4.625219280425 = -.447719280425 eV/atom
formation energy: (3*4.450+3.36)/4-4.625219887525 = -.447719887525 eV/atom
Note that both of these formation energies differ from the 2004 Acta Mat paper, where the L12 formation energy is -0.4486 eV/atom in Table 7, and where E0=-4.626 eV/atom at a=0.3571 nm in Table 5.

NiAl-L10	3.660	-0.176755604947E+02	-17.6755604947	
NiAl-L10	3.661	-0.176755881497E+02	-17.6755881497	= -4.418897037425 eV/atom
NiAl-L10	3.662	-0.176755828916E+02	-17.6755828917	

formation energy: (4.45+3.36)/2-4.418897037425 = -.513897037425 eV/tom

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EAM Function values from SOLD and LAMMPS

Al a=4.05 A

r^2	rho(SOLD)	rho(LAMMPS)	phi(SOLD)	phi(LAMMPS)
8.201250	0.053763961146261	0.053763961146285	-0.084613917657335	-0.084613917657304
16.402500	0.024999634754273	0.024999634754329	-0.008658685490427	-0.008658685490476
24.603750	0.006302044629806	0.006302044629847	0.012926685428692	0.012926685428644
32.805000	0.000689719907887	0.000689719907897	0.007417203930628	0.007417203930701
41.006250	0.000007470331783	0.000007470331784	0.000162983445444	0.000162983445452

rho(SOLD)	F(SOLD)	rho(LAMMPS)	F(LAMMPS)
0.954870340253536	-2.695839397901082	0.954870340255289	-2.695839397900988
0.954870340253537	-2.695839397901082	0.954870340255290	-2.695839397900988

Ni a=3.52 A

r^2	rho(SOLD)	rho(LAMMPS)	phi(SOLD)	phi(LAMMPS)
6.195200	0.073688253891477	0.073688253891216	-0.090055636605920	-0.090055636606581
6.195200	0.073688253891478	.	-0.090055636605920	.
12.390400	0.014561052185085	0.014561052184803	-0.025906718559590	-0.025906718559467
18.585600	0.001180718486126	0.001180718486054	-0.014289491913605	-0.014289491913245
24.780800	0.000003122384936	0.000003122384935	-0.000102151341610	-0.000102151341580

rho(SOLD)	F(SOLD)	rho(LAMMPS)	F(LAMMPS)
1.000000072094484	-2.869718412519696	1.000000072087921	-2.869718412518009
1.000000072094483	-2.869718412519696	.	.

Ni3Al a=3.57135 A

r^2	rho(SOLD)	rho(LAMMPS)	phi(SOLD)	phi(LAMMPS)
6.377270	0.070994076333054	0.070994076332703	-0.094033891755614	-0.094033891755703
6.377270	0.059640669644022	0.059640669644038	-0.174828024356864	-0.174828024356689
12.754541	0.012940401915607	0.012940401915388	-0.025852410663429	-0.025852410663546
12.754541	0.037585709909852	0.037585709909900	-0.027050045671377	-0.027050045671518
19.131811	0.000876888271704	0.000876888271650	-0.004724095840972	-0.004724095840645
19.131811	0.017021549059912	0.017021549059981	-0.011950887755432	-0.011950887754981
25.509082	0.005181722771404	0.005181722771441	0.014140872281463	0.014140872281431
25.509082	0.000000461323914	0.000000461323913	-0.000016333330638	-0.000016333330628
31.886352	0.000939122230617	0.000939122230629	0.009595150705734	0.009595150705800
38.263622	0.000059252460492	0.000059252460494	0.001074870872071	0.001074870872100
44.640893	0.000000002508368	0.000000002508368	0.000000073430775	0.000000073430773

rho(SOLD)	F(SOLD)	rho(LAMMPS)	F(LAMMPS)
1.161143186917430	-2.652414891358375	1.161143186912668	-2.652414891360225
1.041878859426508	-2.868670503708388	1.041878859422225	-2.868670503708212
1.041878859426509	-2.868670503708388	1.041878859422226	-2.868670503708212

NiAl-L10 a=3.661 A

r^2	rho(SOLD)	rho(LAMMPS)	phi(SOLD)	phi(LAMMPS)
6.701461	0.058635317589810	0.058635317589839	-0.044617862731586	-0.044617862731278
6.701461	0.066327869256667	0.066327869256308	-0.096909053060347	-0.096909053060203
6.701461	.	.	-0.175849938305069	-0.175849938304210
13.402921	0.035253623413708	0.035253623413779	-0.021124902807659	-0.021124902807771
13.402921	0.010414924054350	0.010414924054091	-0.026077591584673	-0.026077591584689
20.104382	0.014588412327843	0.014588412327901	0.000358470737401	0.000358470737326
20.104382	0.000489950524964	0.000489950524926	-0.001351844724583	-0.001351844724629
20.104382	.	.	-0.008100477900861	-0.008100477900476
26.805842	0.003847024630076	0.003847024630108	0.014806522094603	0.014806522094603
33.507303	0.000536770298526	0.000536770298534	0.007014787045814	0.007014787045885
33.507303	.	.	0.006270058681718	0.006270058681793
40.208763	0.000015224525242	0.000015224525243	0.000316073718879	0.000316073718893

rho(SOLD)	F(SOLD)	rho(LAMMPS)	F(LAMMPS)
1.151812726068049	-2.655894478938070	1.151812726066024	-2.655894478938431
1.042806088292858	-2.868623374839173	1.042806088290853	-2.868623374837526

Revision note: this version of the release notes (090207) corrects “4 unit cells” to be “1 unit cell” (4 atoms) from version 090202, adds more introductory material, and changes a bit of the formatting. No results were changed.