New LAMMPS version of 2004 Mishin Ni-Al (2004--Mishin-Y--Ni-Al--LAMMPS--ipr2)

Background

Benedikt Eggle-Sievers (Friedrich-Alexander-Universität Erlangen-Nürnberg) noticed that the cohesive energies for the LAMMPS implementation of the Mishin 2004 Al-Ni (2004--Mishin-Y--Ni-Al--LAMMPS—ipr1) are not technically correct as the energy of the isolated atoms is non-zero. While the potential energies of various structures agree between the LAMMPS and SOLD implementations of the potential, their *cohesive* energies disagree because of the non-zero isolated atom energies of the LAMMPS version. The original plt tables were investigated and Yuri Mishin was contacted, and it was verified that the SOLD version of the potential gives individual isolated atoms an energy of 0. The new version presented here addresses and corrects this issue.

Implementation details

A new LAMMPS implementation was constructed by fitting cubic spline interpolations to the original plt files provided by Yuri Mishin (2004--Mishin-Y--Ni-Al--table—ipr1). Prior to fitting, a row was appended at the beginning of the embedding energy tables to explicitly set $F(\rho=0) = 0.0$. This modification removes the isolated atom energy. Additionally, the other plt tables were modified to explicitly set the final tabulated values (those at each function's cutoff) to be 0.0. New tables were then constructed with 10001 points for both ρ and r.

Compared to the original LAMMPS implementation, the new tables have the same $\Delta\rho$, Δr, and r cutoff values, but one extra evaluation point. As the tables start at values for $\rho,r = 0$, the extra point ensures that the final point at the cutoff distance is included in the tables. Plots of the EAM functions and their derivatives match between the two LAMMPS versions except for F at rho=0, F for Ni at large rho, and phi and rho for small values of r. The first difference is associated with the correction that the new LAMMPS version addresses. The other differences correspond to slightly different extrapolations to rho/r values not included in the plt files. The different extrapolations only affect small r values ($r < 1.5$ Angstrom) and are beyond the scope of what the original potential was designed to represent.

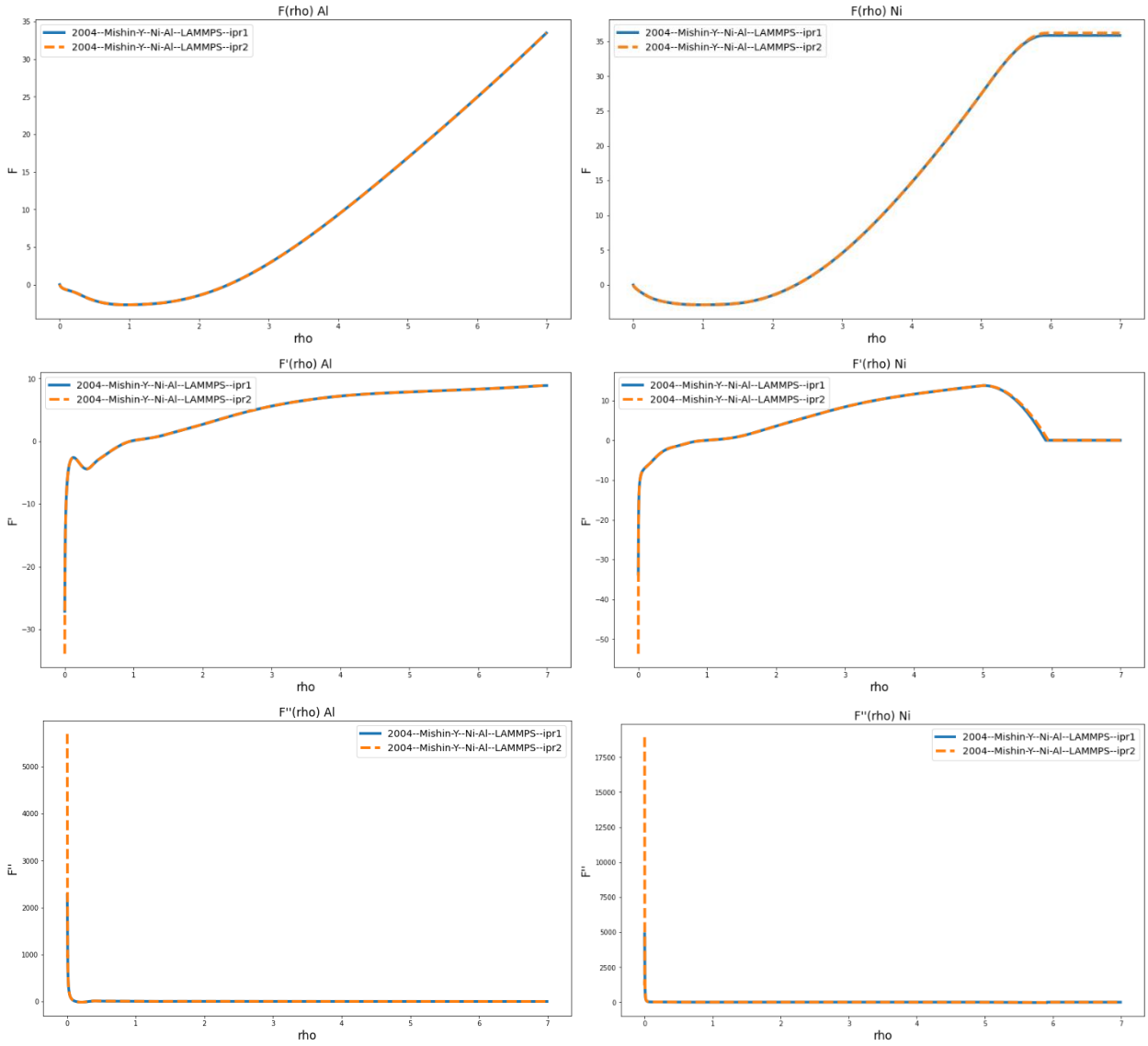


Figure 1: F(rho) functions and their derivatives

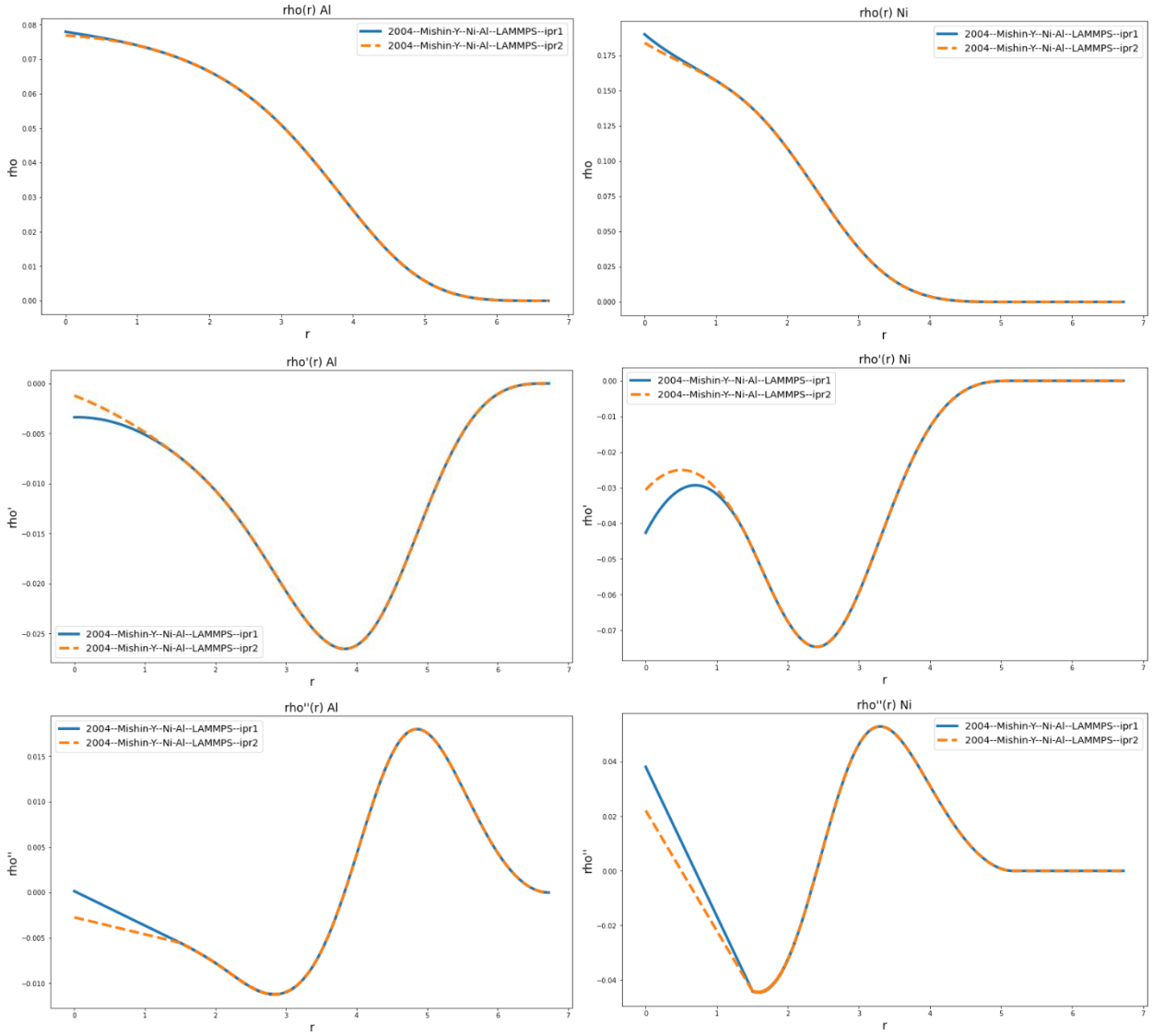


Figure 2: rho(r) functions and their derivatives

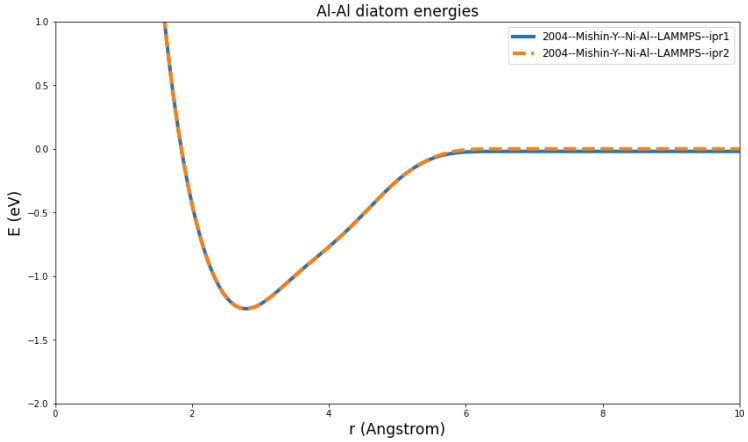
Plots of r*phi(r) not included as they are nearly visually indistinguishable for the two versions.

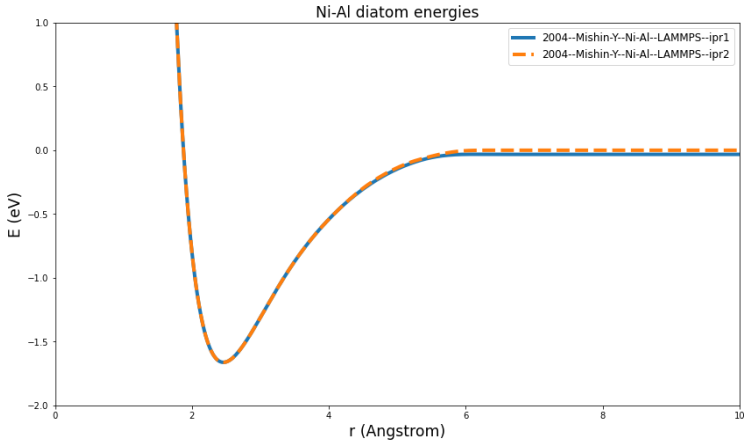
Computed properties

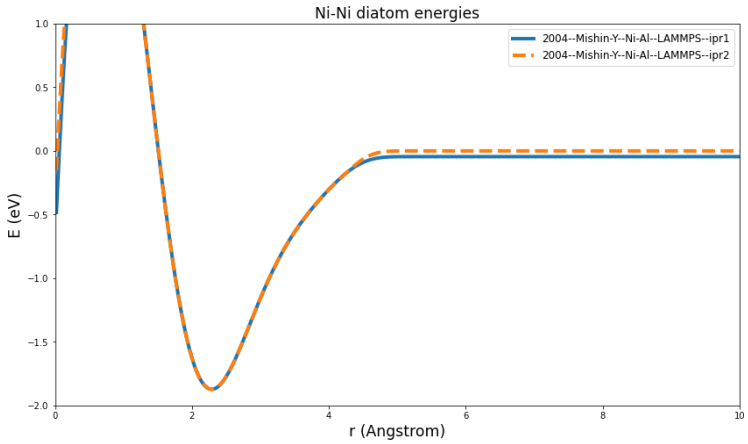
Isolated energies in eV

	2004--Mishin-Y--Ni-Al—LAMMPS--ipr1	2004--Mishin-Y--Ni-Al—LAMMPS--ipr2
Ni	-0.022549650154092004	0.0
Al	-0.0098690015330354	0.0

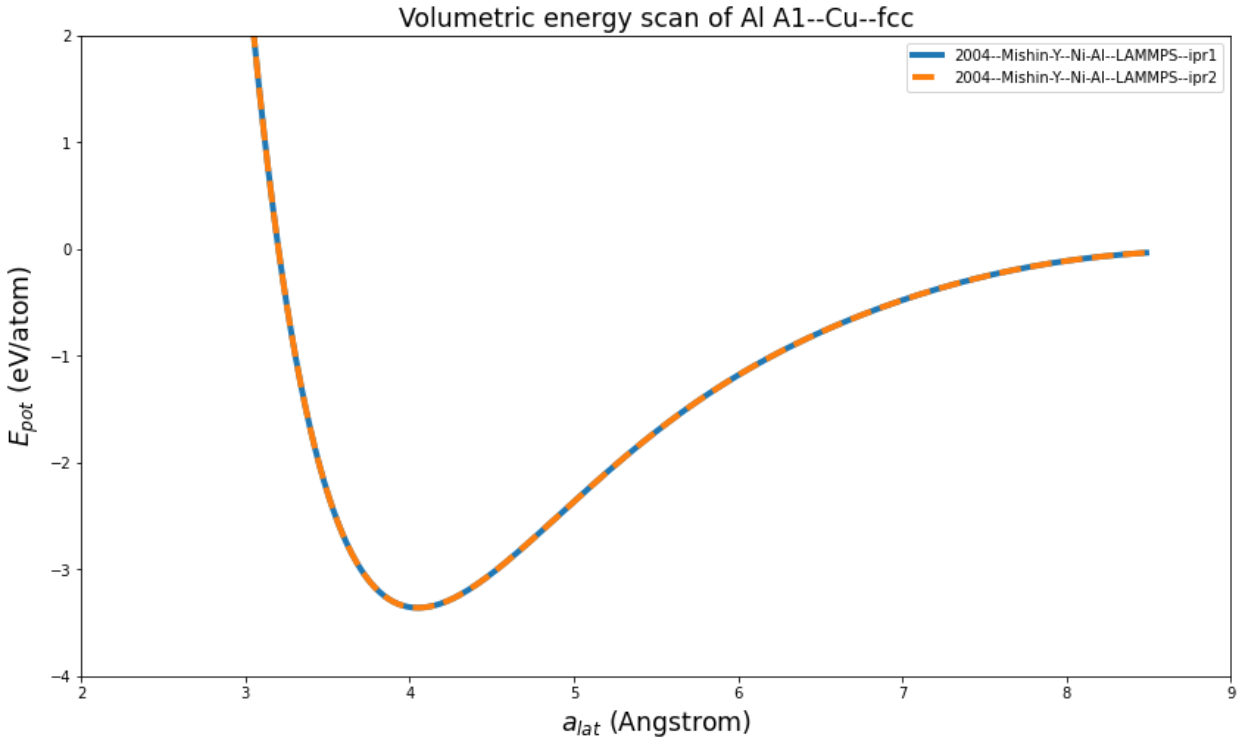
Diatom scans

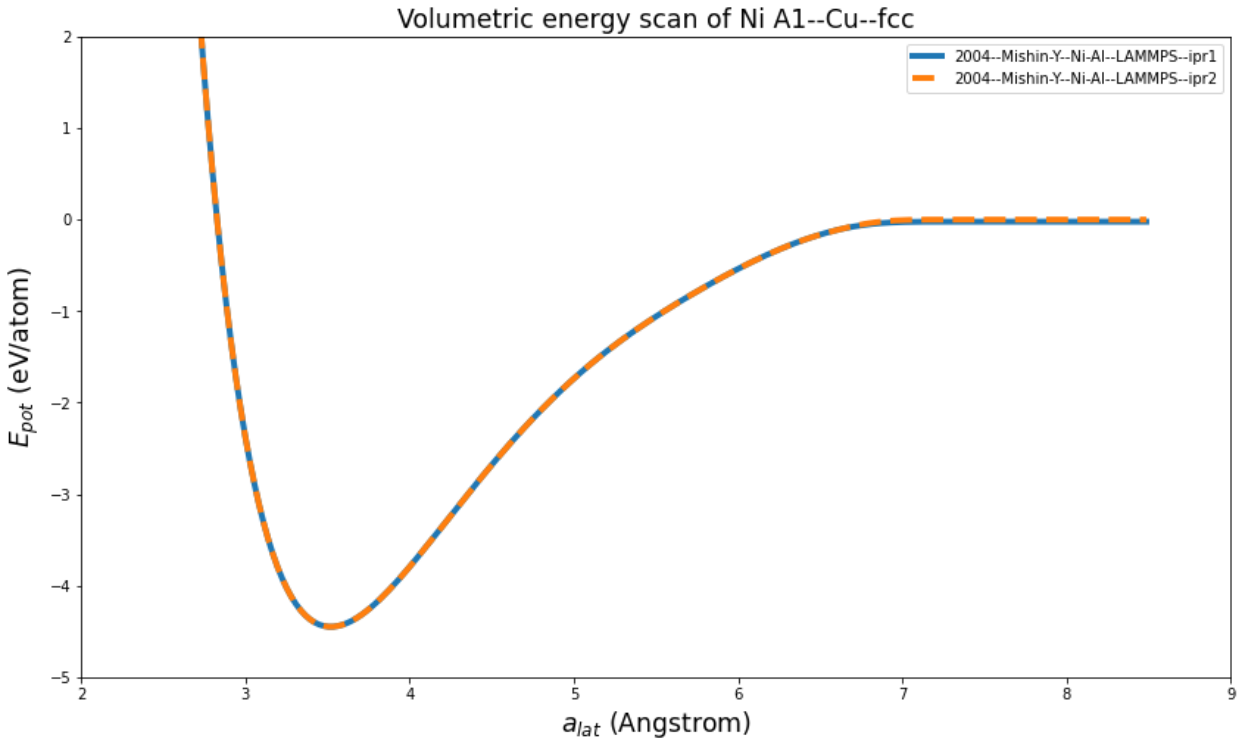






Volumetric scans of fcc structures





Notes on scans: the plotted energies are the measured potential energies, which agree between the two models except at low/high r/a values. Where they differ is in the *cohesive* energies as the reference isolated energies are not the same.

Bulk structure properties for FCC Al

	2004--Mishin-Y--Ni-Al—LAMMPS--ipr1	2004--Mishin-Y--Ni-Al—LAMMPS--ipr2	Published
a_{fcc} (Å)	4.049999839013269	4.049999839012033	4.05
E_{pot} (eV)	-3.36000002259075	-3.36000002259075	-3.36
E_{coh} (eV)	-3.3501310210577144	-3.36000002259075	-3.36
C_{11} (GPa)	116.80747014889499	116.80747014838	116.8
C_{12} (GPa)	60.11308925209276	60.11308925212451	60.1
C_{44} (GPa)	31.6566980163005	31.656698018923	31.7
ΔE_{bcc} (eV)	0.09261654945570008	0.09261654945575026	0.09
ΔE_{hcp} (eV)	0.02156946033424978	0.021569460331699375	0.03
ΔE_{sc} (eV)	0.29661095428215045	0.29661095428405027	0.30
ΔE_{dia} (eV)	0.8841709734133749	0.8841709734171252	0.88

Bulk structure properties for Ni – Dashes indicate structures that transformed during relaxation

	2004--Mishin-Y--Ni-Al—LAMMPS--ipr1	2004--Mishin-Y--Ni-Al—LAMMPS--ipr2	Published
a_{fcc} (Å)	3.5200000306764094	3.52000003065715	3.52
E_{pot} (eV)	-4.44999998517825	-4.449999985170001	-4.45
E_{coh} (eV)	-4.427450335024158	-4.449999985170001	-4.45
C_{11} (GPa)	241.34257190475998	241.34257302362502	241.3
C_{12} (GPa)	150.82443510343498	150.824435712275	150.8
C_{44} (GPa)	127.344652140085	127.34465270446502	127.3
ΔE_{bcc} (eV)	----	0.0672858484079013	0.07
ΔE_{hcp} (eV)	----	----	0.02
ΔE_{sc} (eV)	0.7235998443960505	0.7235998443870004	0.72
ΔE_{dia} (eV)	1.4164289733253757	1.4164289733138755	1.42

Bulk properties of $L1_2$ Ni_3Al in GPa

	2004--Mishin-Y--Ni-Al—LAMMPS--ipr1	2004--Mishin-Y--Ni-Al—LAMMPS--ipr2	Published
C11	236.00496602572997	236.004966829575	236
C12	154.3015602474975	154.30156074627502	154
C44	127.06346124902501	127.063461695675	127

Ni-Al formation energies in eV

	2004--Mishin-Y--Ni-Al—LAMMPS--ipr1	2004--Mishin-Y--Ni-Al—LAMMPS--ipr2	Published
Ni_3Al			
$L1_2$	-0.447719894081124	-0.4477198940831242	-0.4486
$D0_3$	-0.43562086571856184	-0.43562086573306225	-0.4356
NiAl			
B1	0.059576049502374495	0.05957604949562478	0.0596
B2	-0.5904200463290001	-0.5904200463394496	-0.5918
$L1_0$	----	----	-0.5139

Surface energies in mJ/m^2

	2004--Mishin-Y--Ni-Al—LAMMPS--ipr1	2004--Mishin-Y--Ni-Al—LAMMPS--ipr2	Published
Al (110)	792.6281192121613	792.628119216484	792
Al (100)	607.0608079981145	607.0608080017424	607
Al (111)	601.2014168517616	601.2014168145294	601
Ni (110)	2087.0767707057043	2087.076770764117	2087
Ni (100)	1936.0355765428644	1936.0355765640666	1936
Ni (111)	1759.0961604598424	1759.0961605330344	1759

In summary, the evaluated properties between the two versions agree extremely well with each other and with the published values except for the isolated atom energy and dependent cohesive energy.