

The NIST Interatomic Potentials Repository

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What is an interatomic potential?

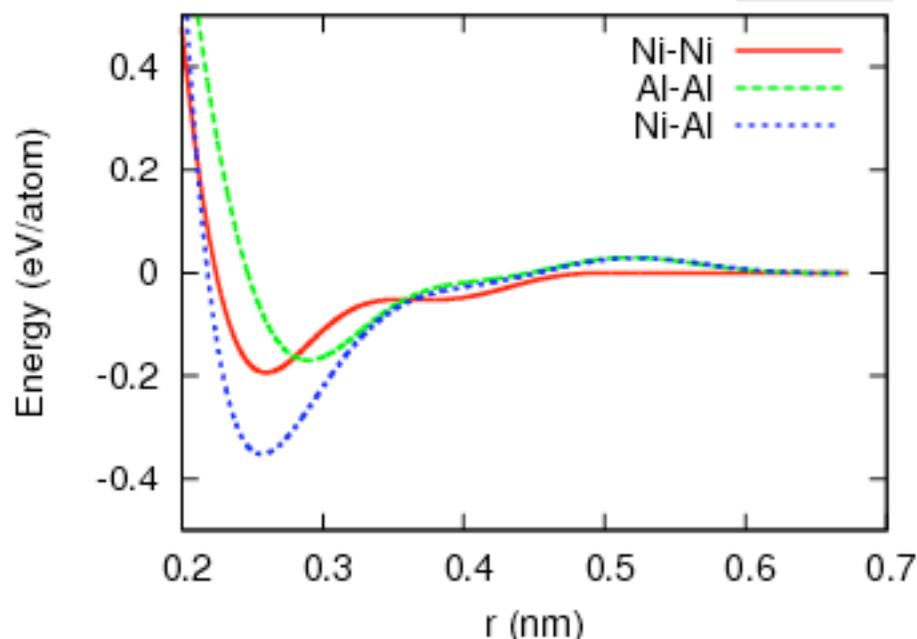
- ▶ Description of the interactions between atoms
- ▶ aka “forcefields”
- ▶ Can be analytical or non-analytical
- ▶ Models can include different physics (e.g. metallic vs. covalent bonds, charge)
- ▶ Files can be various formats

$$E_{tot} = \frac{1}{2} \sum_{ij} \phi(r_{ij}) + \sum_i F(\bar{\rho}_i)$$
$$\bar{\rho}_i = \sum_{j \neq i} \rho(r_{ij})$$

Pair interactions

Embedding energy

Host electron density



NiAl (L12) EAM from Y. Mishin, Acta Mat. 52, 1451-1467 (2004).

LAMMPS setfl format. Conversion by C. A. Becker from Y. Mishin files.

7 January 2009. <http://www.ctcms.nist.gov/potentials>

2 Ni Al

10000 0.6995103513405870E-03 10000 0.6724883999724820E-03 0.6724883999724820E+01

28 0.5871000000E+02 0.3520000000E+01 fcc

-0.2254965015409191E-01

-0.4608461404747549E-01

-0.6722644273232049E-01

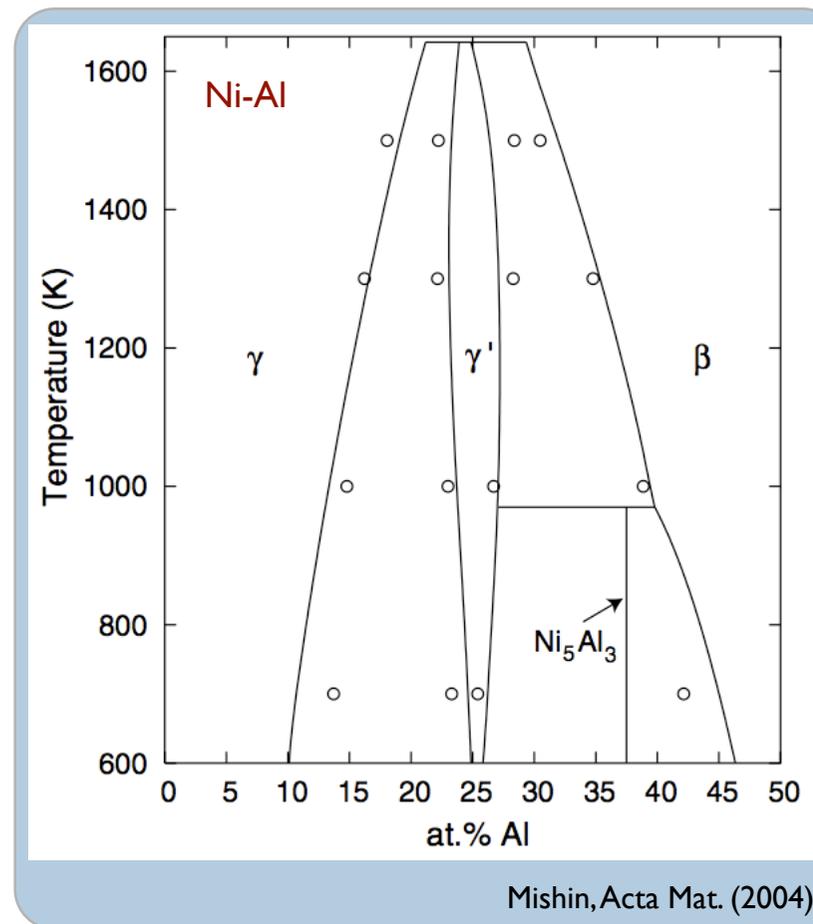
0.8623912617422493E-01

Why isn't everyone using them?

- ▶ accuracy of interatomic models
- ▶ multicomponent systems
- ▶ transferability - behavior outside the fitted region
- ▶ calculation speed, tractable system sizes
- ▶ finding, evaluating, and comparing models
- ▶ incompatible file formats for software
- ▶ version control: files may be corrupt, incorrect user implementation, multiple versions, websites out of date

reference? →

```
Ag functions (universal 3)
 47   107.87   4.0900   FCC
 500 5.0100200400801306e-04 500 1.121212121212229e-02 5.550000
 0. -5.3437496524125194e-01 -7.9903970176950523
-1.3414582590500288e+00 -1.4853604249917538e+00 -1.6189116822476493
-1.9760965580129337e+00 -2.0844912853647344e+00 -2.1888075291300311
-2.4820202718935036e+00 -2.5743582262663978e+00 -2.6644475069132341
-2.9231988641276132e+00 -3.0061444187879260e+00 -3.0876567146272293
```



Project overview and goals

- ▶ Provide a **public repository of interatomic potentials** from *known sources* with *reference data and tools* to facilitate comparison.
- ▶ Not to declare “The Best” since that depends on application
- ▶ One-stop shop for interatomic potentials with references
 - work with developers to make potentials available
 - find out references and version information of existing files
 - multiple formats and materials
- ▶ Conversions between formats. Standardization.
- ▶ Develop standard property evaluation metrics and methods
- ▶ Reference data from experiment and/or first-principles

NIST Interatomic Potentials Repository

www.ctcms.nist.gov/potentials/

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Center for Theoretical and Computational Materials Science

Interatomic Potentials Repository Project

Overview

This repository represents the first step in a project to facilitate the use of atomistic simulations by providing a source for interatomic potentials (force fields), evaluation tools, and reference data (experimental and/or *ab-initio*) to allow researchers to judge the quality of an interatomic model for their needs. It allows users to download interatomic potentials which were submitted or vetted by their developers and provides the appropriate references. Please note that, due to the wide range of interatomic potential functions and formats, it is the user's responsibility to check that the interatomic potentials produce expected results. More information can be found in the [FAQ](#).

Please send feedback and contributions to: Chandler.Becker@nist.gov

Project Home

- [FAQ](#)
- [Credits](#)
- [Privacy / Security / Accessibility](#)

Working Group

- [Chandler Becker](#)

NIST

www.ctcms.nist.gov/potentials/

NIST Interatomic Potentials Repository

Interatomic Potentials

Elements	Multi-component
Ag	Ag-Cu
	Al-Cu
Al	Al-Fe
	Al-Mg
	Al-Ni
Au	
	Cu-Ag
	Cu-Al
Cu	Cu-Ni
	Cu-Pb
	Cu-Zr
	Fe-Al
Fe	Fe-Ni
	Fe-P
	Fe-V
Mg	Mg-Al
Mo	
	Ni-Al
Ni	Ni-Cu
	Ni-Fe
P	P-Fe
Pb	Pb-Cu
Pd	
Pt	
Ru	
V	V-Fe
Zr	Zr-Cu

www.ctcms.nist.gov/potentials/

Various elements and alloys are available for download.

All have been vetted by their developers (authors of the files).

Many are compatible with the LAMMPS MD package (lammmps.sandia.gov) and other open source software.

No particular format is required, but formatting information is.

We are expanding to include more potentials and different types.

Download Potentials

NIST

Materials Science and Engineering Laboratory

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Center for Theoretical and Computational Materials Science

Interatomic Potentials Repository

Al ← Element Reference

M.I. Mendeleev, M.J. Kramer, C.A. Becker, and M. Asta, "Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu," *Phil. Mag.* **88**, 1723-1750 (2008). DOI: 10.1080/14786430802206482.

Al1.eam.fs EAM/FS setfl ← File format

Note: These files were provided by Mikhail Mendeleev. ← Submitter

X.-Y. Liu, F. Ercolessi, and J.B. Adams, "Aluminium interatomic potential from density functional theory calculations with improved stacking fault energy," *Modelling Simul. Mater. Sci. Eng.* **12**, 665-670 (2004). DOI: 10.1088/0965-0393/12/4/007.

NEWAl.txt EAM
Al-LEA.eam.alloy EAM setfl

Note: NEWAl.txt was obtained from <http://enpub.fulton.asu.edu/cms/potentials/main/main.htm> and posted with the permission of J.B. Adams. Al-LEA.eam.alloy is a version of the same potential which has been formatted for use in LAMMPS ("D" was replaced by "e", "FCC" by "fcc", and "Al" was added on line 3). ← Additional Notes

Project Home

- FAQ
- Credits
- Privacy / Security / Accessibility

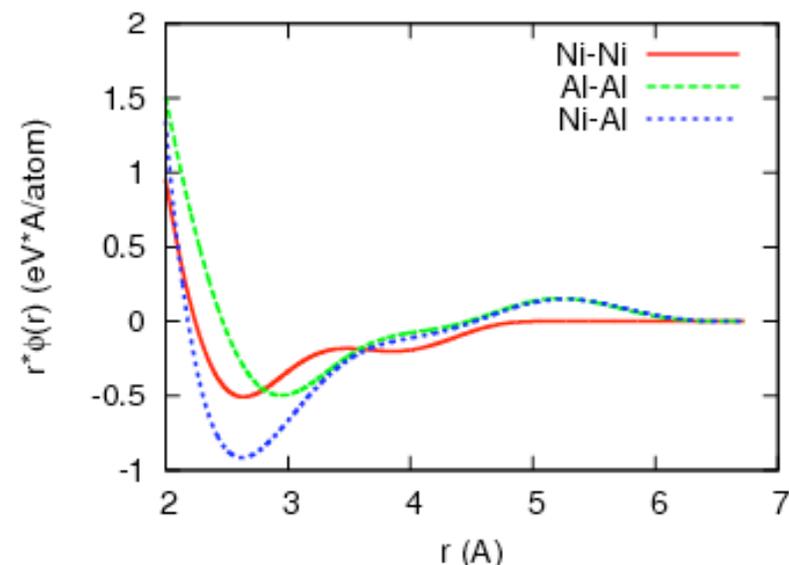
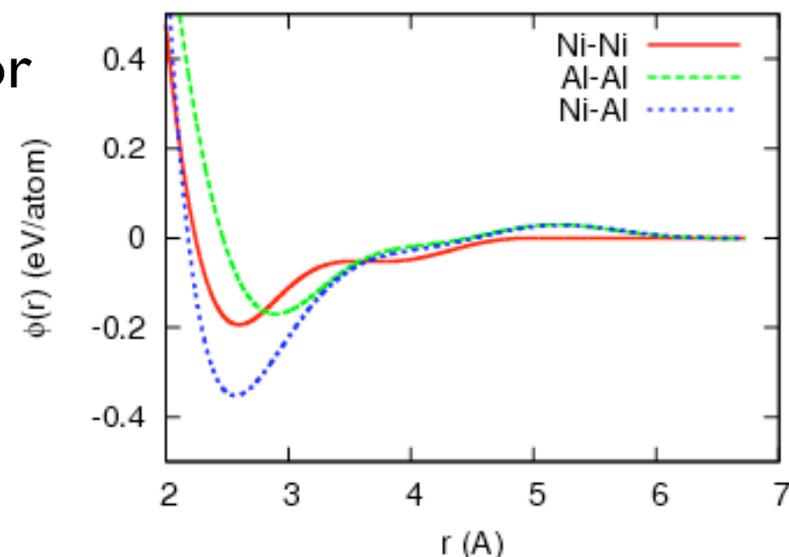
Working Group

- Chandler Becker

NIST

www.ctcms.nist.gov/potentials/

- ▶ Project information, including instructions for submitting potentials and crediting the site
- ▶ Descriptions of file formats
- ▶ “Why doesn’t it look like the figure in the paper?”
 - Different file formats
 - Different functions
 - Invariant transformations
 - Interatomic potentials which look very similar (different) may have properties that are very different (similar).
- ▶ Links to other software (e.g. LAMMPS)



Format Conversion

- ▶ Conversion from the *plt* (x,y) format to the *EAM/ally setfl* format:

Pair interactions Embedding energy

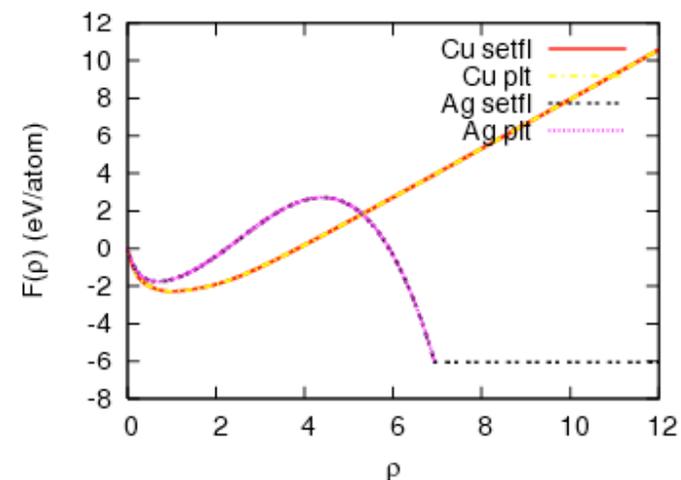
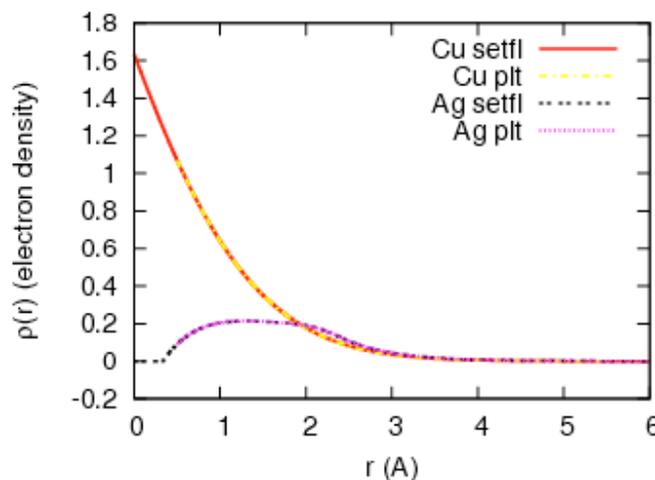
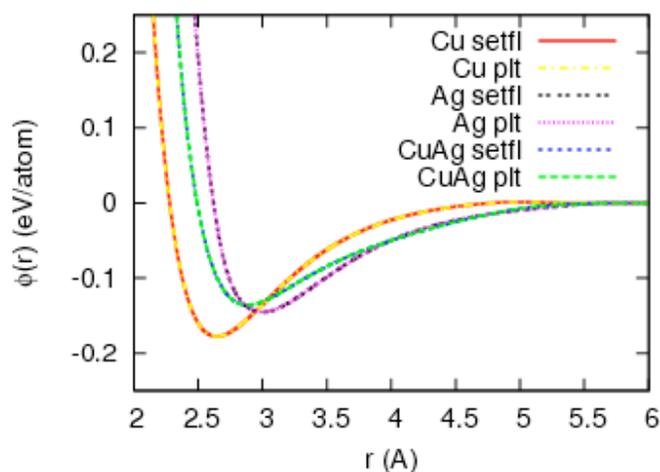
$$E_{tot} = \frac{1}{2} \sum_{ij} \phi(r_{ij}) + \sum_i F(\bar{\rho}_i)$$

$$\bar{\rho}_i = \sum_{j \neq i} \rho(r_{ij})$$

Host electron density

▶ Issues:

- splines
- need a common scale
- upper/lower bounds
- $r_{min}=0, r_{min}=dr, r_{min}=0.5 \text{ \AA}$
- different order of functions
- $\Phi(r)$ vs $r*\Phi(r)$



Conversion testing

- ▶ Calculated E_0 and EAM functions for *setfl* (LAMMPS) and *plt* (SOLD) for atoms in ideal fcc positions

- ▶ Differences between results are highlighted:

Pair interactions Embedding energy

$$E_{tot} = \frac{1}{2} \sum_{ij} \phi(r_{ij}) + \sum_i F(\bar{\rho}_i)$$

$$\bar{\rho}_i = \sum_{j \neq i} \rho(r_{ij})$$

Host electron density

Comparison of minimum energies from SOLD and LAMMPS

Alloy	a (Å)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Ag	4.085	-0.113996999978E+02	-11.3996999978	= -2.849999974725 eV/atom
	4.09	-0.113999998989E+02	-11.3999998989	
	4.095	-0.113997024609E+02	-11.3997024609	
fcc Cu	3.614	-0.141599858176E+02	-14.1599858176	= -3.539999968675 eV/atom
	3.615	-0.141599998746E+02	-14.1599998747	
	3.616	-0.141599858326E+02	-14.1599858326	
L12 Ag3Cu	3.9834	-0.117565455676E+02	-11.7565455676	= -2.939136398225 eV/atom
	3.9835	-0.117565455929E+02	-11.7565455929	
	3.9836	-0.117565453583E+02	-11.7565453583	
L10 CuAg	3.880	-0.123070560947E+02	-12.3070560948	= -3.07677012405 eV/atom
	3.881	-0.123070804962E+02	-12.3070804962	
	3.882	-0.123070738275E+02	-12.3070738275	
L12 Cu3Ag	3.757	-0.130877673407E+02	-13.0877673407	= -3.27194702375 eV/atom
	3.758	-0.130877880950E+02	-13.087788095	
	3.759	-0.130877780304E+02	-13.0877780304	

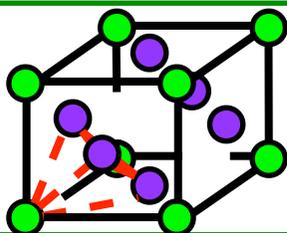
EAM function values from SOLD and LAMMPS

Cu3Ag a=3.758 Å

r ²	rho(SOLD)	rho(LAMMPS)
7.061282	0.062852970138718	0.062852970138713
7.061282	0.080422918188860	0.080422918188852
14.122564	0.007884125490181	0.007884125490182
14.122564	0.011022393370322	0.011022393370319
21.183846	0.001113794054072	0.001113794054071
21.183846	0.002301934021530	0.002301934021529
28.245128	0.000004416130543	0.000004416130543
28.245128	0.000444063188335	0.000444063188335
35.306410	0.00000017231091	0.00000017231090

r ²	phi(SOLD)	phi(LAMMPS)
7.061282	-0.051746694850591	-0.051746694850604
7.061282	-0.088898522362072	-0.088898522362017
14.122564	-0.019108034575602	-0.019108034575602
14.122564	-0.035264699809090	-0.035264699809092
21.183846	-0.001446381632289	-0.001446381632290
21.183846	-0.010516854510566	-0.010516854510556
28.245128	0.000052252751389	0.000052252751390
28.245128	-0.002236685226569	-0.002236685226569
35.306410	-0.000000042896298	-0.000000042896298

rho(SOLD)	F(SOLD)
0.852429817444297	-1.730440623420056
0.908109495258908	-2.275710973226181
0.908109495258909	-2.275710973226181
rho(LAMMPS)	F(LAMMPS)
0.852429817444197	-1.730440623413965
0.908109495258811	-2.275710973226475



L1₂

SOLD was kindly provided by Yuri Mishin

User community

- ▶ Working with users and developers
 - helping people use potentials; answering questions about formats, etc.
 - helping developers convert potentials, ensure they run, distribute the files
- ▶ Informal interactions with individuals in academia, government, and industry (what do you need? what can you provide?)
 - radiation potentials
- ▶ these workshops
- ▶ LAMMPS mailing list - users refer each other to the website
- ▶ word of mouth

Summary and Future

- ▶ NIST Interatomic Potentials Repository to provide a resource for obtaining and evaluating interatomic potentials (with references):
www.ctcms.nist.gov/potentials
- ▶ Conversions of interatomic potentials to common formats.
- ▶ Begun developing tools and methods to help users evaluate the suitability of an interatomic potential.
- ▶ **Future directions:**
 - **Other elements, multicomponent alloys, and other forms of interatomic interactions**, e.g. those used in polymers and ceramics
 - **Standardization** (with the help of the community); user forum
 - Collecting **reference data** for properties
 - **Property evaluations** -- systematically examine the significance of parameters like system size, relaxation times, run lengths, timesteps,....