BULK MANUAL

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I. DESCRIPTION

Program BULK was made for validation and comparison of semi-empirical EAM potentials. It works with cluster of 256 atoms and computes some basic parameters for FCC, BCC and HCP structure in one minute. Specifically lattice parameter, bulk modulus, cohesive energy, free surface energy (001), vacancy formation energy and elastic constants (only for BCC and HCP) c_{11}, c_{12}, c_{44}, tetragonal shear constant C'. Program BULK can read EAM potentials in dynamo/funcfl file format used by LAMMPS and tabulated file format, where three files with embedded, density and pair interaction function are given. Moreover program also perform deformation from FCC to BCC structure along [010] direction (Animation of this transformation is available here http://atavaha.weebly.com/simulations.html). Program does not perform any relaxation, because relaxation techniques increasing computational time, so vacancy formation energy and free surface energy are not relaxed. Program is written in FORTRAN. More detailed description of this program and implemented computational methods in Slovak language are in my Master's thesis published here:
http://atavaha.weebly.com/uploads/1/6/6/7/16679152/ing_29_finale.pdf.

II. COMPILATION

1. Make Bulk directory.
2. Download files BULK.for, T1.for and T2.for from the site http://atavaha.weebly.com/simulations.html into your Bulk directory.
3. Compile the program. Use one of the FORTRAN compilers g77, gfortran, ifort etc.
   LINUX example: Open terminal, go to Bulk directory with downloaded files and write:
   `gfortran BULK.for T1.for T2.for -w -o bulk.x`
   WINDOWS example: Open command line, go to Bulk directory with downloaded files and write: `g77 BULK.for T1.for T2.for -w -o bulk.x`
4. You obtain executable file bulk.x in your Bulk directory after compilation.

III. INPUT and EXECUTION

Input file **bulk.dat** has to be prepared before execution. Prepare it in your Bulk directory. It contains from 4 to 8 lines depending on EAM potential's format (more information in sec. V).
First three lines are common:

1st line: Element
2nd line: Start lattice parameters for bcc, fcc and hcp structure.
3rd line: EAM potential's format.

Program will compute energies for lattice parameters from start parameters set by you to start parameters plus 0.04 Å.
Lines 4 to 8 changes with EAM potential's format. There are three potential's formats: "dynamo"," tabulated" and "bulk".

If you use “dynamo” format:

4th line: File with potential.

If you use “tabulated” format:

4th line: File with embedding function.

5th line: File with pair interaction function.

6th line: File with electron density function.

7th line: Number of potential’s data (max. 10000).

If you use “bulk” format:

4th line: File with embedding function.

5th line: File with pair interaction function.

6th line: File with electron density function.

7th line: Number of potential’s data (max.10000), cutoff of the potential.

Example: “dynamo” format

```
Fe
2.85 3.63 2.57
dynamo
in.eam
```

Example: “tabulated” format

```
Fe
2.85 3.63 2.57
tabulated
in.embed
in.pair
in.den
3000
```

Example: “bulk” format

```
Fe
2.85 3.63 2.57
tabulated
in.embed
in.pair
in.den
3000 5.6
```

All files with potential’s data have to be in the Bulk directory, where is the executable file bulk.x . If you have potentials in special directory, you have to add file path and quotation marks (max. 80 characters).

Example:

```
Fe
2.85 3.63 2.57
dynamo
'/home/mydirectory/potentials/in.eam'
```

When you have prepared input file bulk.dat, you can execute the program bulk.x.

LINUX: Open terminal, go to your Bulk directory and type: `./bulk.x`
WINDOWS: Open command line, go to your Bulk directory and type: `.\bulk.x`

IV. OUTPUT

After termination, the program writes all results in terminal/command line. It also creates 14 output files. All results printed in terminal are in file results.dat. Here is an example:

```
Fe

  COMPUTED PARAMETER      BCC       FCC       HCP      UNIT
   lattice parameter     2.867     3.603     2.553       A
     cohesive energy    -4.300    -4.250    -4.242      eV
        bulk modulus    89.088    85.620    73.581     GPa
non.rel.vac.form.en.     1.836     1.784     1.779      eV
free surf. en. (100)     1.568     1.540     1.395   J/m^2

       delta Ec [eV]
          BCC-FCC       -0.050
          BCC-HCP       -0.058
          FCC-HCP       -0.007

ELASTIC PARAMETER     BCC       FCC      UNIT
       c11          123.693    63.779     GPa
       c12           71.933    93.700     GPa
       c44           60.683    81.917     GPa
        C'           25.880   -14.961     GPa
```

Here is list of remaining 13 output files:
bcc-i.dat (Initial dependence of energy in eV on lattice parameter in Å for bcc structure.)
bcc-r.dat (Refined dependence of energy in eV on lattice parameter in Å for bcc structure.)
fcc-i.dat (Initial dependence of energy in eV on lattice parameter in Å for fcc structure.)
fcc-r.dat (Refined dependence of energy in eV on lattice parameter in Å for fcc structure.)
hcp-i.dat (Initial dependence of energy in eV on lattice parameter in Å for hcp structure.)
hcp-r.dat (Refined dependence of energy in eV on lattice parameter in Å for hcp structure.)
c11bcc.dat (Dependence of energy in eV on c_{11} dilatation for bcc structure.)
c11fcc.dat (Dependence of energy in eV on c_{11} dilatation for fcc structure.)
c12bcc.dat (Dependence of energy in eV on c_{12} dilatation for bcc structure.)
c12fcc.dat (Dependence of energy in eV on c_{12} dilatation for fcc structure.)
c44bcc.dat (Dependence of energy in eV on c_{44} dilatation for bcc structure.)
c44fcc.dat (Dependence of energy in eV on c_{44} dilatation for fcc structure.)
fcctobcc.dat (Transformation from fcc to bcc structure. 1st column is energy in eV, 2nd column is lattice parameter in y direction.)

In is always good to check files bcc-r.dat, fcc-r.dat and hcp-r.dat and make sure, that simulation is near minimum. If there is no minimum, please change starts lattice parameters.

V. POTENTIALS

Program Bulk requires three files to compute energy: one with embedding function and its differentiation, one with density function and its differentiation and one with pair function and its differentiation. Example is shown below. This is referred as “bulk” format.

Example of “bulk” format:

```
    1.50118494          0.13502988E+00          0.85358223E-01
    1.50236989          0.13501941E+00         -0.17071645E+00
    1.50355483          0.13500877E+00         -0.10202069E+00
    1.50473977          0.13499797E+00         -0.12072905E+00
...

    0.00161583         -0.15721367E+00         -0.47316018E+04
    0.00323166         -0.25833427E+00          0.94632037E+04
    0.00484750         -0.34406320E+00          0.22495557E+04
    0.00646333         -0.42056034E+00          0.27536824E+04
...

    1.50118494          0.81825930E+02         -0.26332703E+04
    1.50236989          0.81189511E+02          0.52665405E+04
    1.50355483          0.80558134E+02          0.31114243E+04
    1.50473977          0.79931756E+02          0.36508508E+04
...
```

The most common formats, which can be found on internet are dynamo/funcfl file format and tabulated file format. Subroutines T1 and T2 convert these two formats into bulk format. Examples are showed below.

Example of “dynamo” format:

```
Sourse: Potential #2 from [M.I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun and M. Asta, Phil. Mag. A, 83
Contact information: mendelev@ameslab.gov
Sunday, Feb 22, 2009  The potential was taken from v9_4_bcc (in C:\SIMULATION.MD\Fe\Results\ab_initio+Interstitials)
1  Fe
10000   3.00000000000000E-0002  10000   5.30000000000000E-0004   5.30000000000000E+0000
26   5.58500000000000E+0001   2.85531200000000E+0000  bcc
0  -1.73205399240757E-0001  -2.44950248213795E-0001  -3.00002866354823E-0001  -3.46415257255683E-0001
-3.87306296717472E-0001  -4.24275534131220E-0001  -4.58273175205176E-0001  -4.89918331524266E-0001  -5.19641039464070E-0001
-5.47754405892088E-0001  -5.74494801201978E-0001  -6.00045861677168E-0001  -6.24553623613738E-0001  -6.48136492679153E-0001
-6.70892052120511E-0001  -6.92901854898071E-0001  -7.14234884692489E-0001  -7.34950111608580E-0001  -7.55098416203863E-0001
-7.74724062789171E-0001  -7.93865844705703E-0001  -8.12557986656298E-0001  -8.30830864258625E-0001  -8.48711584132527E-0001
-8.66224456202701E-0001  -8.83391381728377E-0001  -9.00232174740661E-0001  -9.16764830344636E-0001  -9.33005750242895E-0001
-9.48969933532811E-0001  -9.64671139097615E-0001  -9.80122024595352E-0001  -9.95334266040200E-0001  -1.01031866118903E+0000
-1.02508521933575E+0000  -1.03964323963583E+0000  -1.05400137970224E+0000  -1.06816771591028E+0000  -1.08214979660428E+0000
-1.09595468920108E+0000  -1.10958902202510E+0000  -1.12305902157749E+0000  -1.13637054583424E+0000  -1.14952911407841E+0000
-1.16253993369739E+0000  -1.17540792431434E+0000  -1.18813773957090E+0000  -1.20073378683468E+0000  -1.21320024506821E+0000
-1.22554108106464E+0000  -1.23776006422914E+0000  -1.24986078006205E+0000  -1.26184664248049E+0000  -1.27372090509843E+0000
-1.28548667157090E+0000  -1.29714690509544E+0000  -1.30870443715330E+0000  -1.32016197556335E+0000  -1.33152211191376E+0000
-1.34278732842906E+0000  -1.35396000432423E+0000  -1.36504242169186E+0000  -1.37603677096368E+0000  -1.38694515598342E+0000
-1.39776959872435E+0000  -1.40851204368135E+0000  -1.41917436196471E+0000  -1.42975835511984E+0000  -1.44026575869517E+0000
-1.45069824557812E+0000  -1.46105742911738E+0000  -1.47134486604794E+0000  -1.48156205923394E+0000  -1.49171046024298E+0000
...
```

Example of “tabulated” format:

```
# Electron density of Fe
#  Distance (Angstr.)       Density
   1.50118494266664       0.135029877700000
   1.50236988533328       0.135019407000000
   1.50355482799992       0.135008772600000
   1.50473977066655       0.134997974500000
...
```

```
# Embedding function of Fe
#  Electron density       Energy (eV)
   1.61583175409239D-003 -0.157213669000000
   3.23166350818479D-003 -0.258334267800000
   4.84749526227718D-003 -0.344063204400000
   6.46332701636957D-003 -0.420560343100000
...
```

```
# Pair interaction Fe-Fe
#  Distance (Angstr.)       Energy (eV)
   1.50118494266664        81.8259297900000
   1.50236988533328        81.1895109900000
   1.50355482799992        80.5581338800000
   1.50473977066655        79.9317560500000
...
```

The headers of these files are very important. Program T2 transforms tabulated format. It skips first two lines of the files. If you have files without description in first two lines, please add some characters there. Program T1 transforms dynamo format. It skips first four lines, then read number of potentials data, steps for density and distance and cutoff. Finally it skips fifth line and then continues to read potential data. Sometimes the text in first four lines is missing. If this happens, please add some characters there.

VI. SUBROUTINES

Here is a list of subroutines and functions used in program BULK and their tasks**.**

Subroutine/function	**task**
T1.for	To transform DYNAMO/funcfl EAM file format into format used by program BULK.
T2.for	To transform tabulated EAM file format into format used by program BULK. Only the differentiation of the function is added.
DAREAD	To read embedding atom potential.
LATT_BCC	To generate coordinates of atoms for bcc lattice.
LATT_FCC	To generate coordinates of atoms for fcc lattice.
LATT_HCP	To generate coordinates of atoms for hcp lattice.
FCCtoBCC	To make deformation from fcc to bcc structure.
DIST	To calculate distance between i and j atom.
NEIGH	To find neighbors for each atom in a given radius.
FEI	To simulate energy of atom i.
MULTY	To make supercell of NAT*27 atoms. It multiplies bulk of NAT atoms 3 times in x-,y-,z-direction.
AMCB	To simulate total energy of a bulk by embedding atom potential.
C11	To make deformation of lattice for computation of parameter c_{11}.
c12	To make deformation of lattice for computation of parameter c_{12}.
c44	To make deformation of lattice for computation of parameter c_{44}.
SURFACE	To make free surface in crystal. It splits crystal in [001] direction.
ROTACIA	To rotate crystal.

Here is a list of downloaded subroutines used in program BULK which were written by different authors.

SPLINT	http://www.irb.hr/users/maks/v5/splint.for
POTFIT	BEVINGTON, PAGES 140-142.
DETERM	BEVINGTON, PAGE 294.

VII. ERRORS

In current state you can obtain two error messages:
`'Please check potential format in input file.'`
and
`'Periodical boundary condition not met.'`
The first one means, that you probably made typing mistake in input file bulk.dat and specified unknown potential format. The second one means that lattice parameter in one of the directions is too small, so the periodical boundary conditions are violated. There are two possible solutions: to increase start lattice parameters or to increase number of elementary cells in x, y, and z direction. The second possibility leads to change of the code and recompilation of the program.

VIII. CONCLUSION

Program BULK was created by Eva Vitkovská and Peter Ballo. Authors will gladly answer all your questions and appreciate any suggestions for improvement of program BULK. Do not hesitate to contact us.