

## AFLOW V 3.1.111

```
*****
*
*           Aflow STEFANO CURTAROLO - Duke University 2003-2013
*           High-Throughput ab-initio Materials Discovery
*
*****
```

Elastic properties calculated directly from stress-strain data.  
This implementation in AFLOW written by Cormac Toher and Stefano Curtarolo,  
and is described in the paper Scientific Data 2, 150009 (2015).  
Please cite the papers mentioned above in addition to the standard AFLOW papers  
if you use results obtained using the AFLOW AEL code.

The current version of AEL can calculate the Poisson ratio, bulk modulus, shear modulus, compliance tensor and stiffness tensor (elastic constants). The results are written in a variety of formats in different output files. For further details on the output files written, see points (8) and (9) below. Other results can be written and plotted by setting the appropriate values in the aflow.in file, as described in point (9) below.

AFLOW AEL expects a well relaxed structure on input. There is no additional relaxation of the cell shape and size inside the AFLOW AEL, only of the ion positions. So, you have to prepare such a structure by a separate AFLOW relaxation mode for energy and/or forces.

When AFLOW AEL is run, it will first check for the existence of the required DFT calculations. If these exist, then it will extract the required information and proceed to calculate the thermal properties. If these do not exist, then it will create the required directories and aflow.in files, and then stop. By running AFLOW with "--multi" flags, AFLOW will then automatically descend into these subdirectories and run the required electronic structure calculations, after which it will stop. The user will then have to rename or delete the LOCK file in the directory, and the run AFLOW again to calculate the thermal properties. This can all be performed within a subshell script as in the following example:

```
aflow --multi -D $pathname/ >> log.$PBS_JOBID
mv $pathname/LOCK $pathname/LOCK.old
aflow --multi -D $pathname/ >> log.$PBS_JOBID
```

This procedure is similar to that required to run AFLOW APL and AFLOW AGL.

1) To perform a AFLOW AEL calculation the following line has to be present in aflow.in:

```
[AFLOW_AEL]CALC
```

AFLOW checks for the existence of this line in aflow.in. If it does not exist, then the job is not an AFLOW AEL calculation and no other AEL settings are read.

AEL can also be run from within other parts of AFLOW, such as from AGL, in order to obtain properties such as Poisson ratio to be used within these other parts of AFLOW. In this case, AEL will run and the other AEL settings in the aflow.in file will be read, even if the "[AFLOW\_AEL]CALC" line is not present.

2) The AFLOW AEL method requires a set of stress vs. strain data, which are obtained from DFT calculations of a set of strained structures. There are two types of strains: normal strains and shear strains. For each strain type, there are up to three independent strain directions. The user has the possibility to set the number of strained structures in each direction, and the size of the strain step, for each type of strain. These parameters can be set by including the following lines in the aflow.in file:

```
[AFLOW_AEL]NNORMALSTRAINS=number
[AFLOW_AEL]NSHEARSTRAINS=number
[AFLOW_AEL]NORMALSTRAINSTEP=number
[AFLOW_AEL]SHEARSTRAINSTEP=number
```

The default setting is 4 strains in each direction and a step size of 0.005. The default is to apply both positive and negative strains, i.e. to both stretch and compress the lattice. This can be controlled by including the following line in the aflow.in file:

```
[AFLOW_AEL]NEGSTRAINS=option
```

A value of "ON" uses both positive and negative strains, while a value of "OFF" uses positive strains only.

- 3) The AFLOW AEL method can use the symmetry of the lattice to reduce the number of independent strains required for elasticity calculation. For example, for lattices with cubic, the three orthogonal directions are equivalent and there is only one independent strain direction for each type of strain. The number of strain directions can be set automatically by including the following line in the aflow.in file:

```
[AFLOW_AEL]STRAINSYMMETRY=option
```

The default is "OFF" so that all three directions are treated as independent for each strain type. The number of strain directions can also be set directly by the user by including the following line in the aflow.in file:

```
[AFLOW_AEL]NINDSTRAINS=number
```

The default value for the number of strain directions is three for each type of strain.

The lattice symmetry can also be used to check the elastic constant tensor calculated by AFLOW AEL. If the tensor does not have the correct symmetry, AFLOW AEL will issue a warning for the user. This can be controlled by including the following line in the aflow.in file:

```
[AFLOW_AEL]CHECKELASTICSYMMETRY=option
```

The default is "ON" so that the symmetry check is performed. The tolerance used for checking the symmetry can be set by including the following line in the aflow.in file:

```
[AFLOW_AEL]SYMTOLFRAC=number
```

The default value is 0.05, and refers to the fractional difference allowed between two values which should be equal.

- 4) The AFLOW AEL method allows to choose whether or not to calculate and/or fit the stress for the zero-strain system. The stress tensor for the zero-strain system can be calculated by including the following line in the aflow.in file:

```
[AFLOW_AEL]CALCSTRAINORIGIN=option
```

The default is "OFF" so that the zero-strain system is not calculated.

The zero-strain stress can be included in the fitting points used to obtain the elastic constants by including the following line in the aflow.in file:

```
[AFLOW_AEL]FITSTRAINORIGIN=option
```

The default is "OFF" so that the zero-strain system is not calculated. Note that if the zero-strain system is used and the stress is being explicitly calculated, AFLOW AEL will use values of 0.0 for all elements of the stress tensor. The system should be very well relaxed (including cell size and shape) prior to the AEL run in order to be valid.

The stress-strain data from a previous AFLOW relaxation can also be fitted by including the following line in the aflow.in file:

```
[AFLOW_AEL]FITRELAXEDSTRUCT=option
```

The default is "OFF" so that the previously relaxed system is not calculated. Note that this keyword requires a full AFLOW relaxation run be present in the directory in which the AEL calculation is being run. This keyword requires that a relaxation already exists, so that an additional point can be added to the stress-strain data for the fit with additional DFT calculations.

- 5) The PREC and ALGO settings for the VASP calculations for the strained systems are set to ACCURATE and NORMAL. These values are chosen as tests of the AFLOW AEL method has shown that these settings produce the most reliable results. To read the values for PREC and ALGO from the original aflow.in file, the following line should be included in the aflow.in file:

```
[AFLOW_AEL]PRECACALGONORM=option
```

The default is "OFF" so that the PREC and ALGO settings in the initial aflow.in file are ignored and the settings ACCURATE and ALGO=NORMAL are used.

- 6) The stress tensor for a particular deformed system as calculated with VASP can be read from either the OUTCAR or the OUTCAST file.

the vasprun.xml file. The stress tensor can be read from the vasprun.xml file by including the following line in the aflow.in file:

```
[AFLOW_AEL]VASPRUNXMLSTRESS=option
```

The default is "OFF" so that the stress tensor is read from the OUTCAR file.

- 7) The AFLOW AEL method allows the user to control what type of AFLOW runs are used to calculate the stress tensor for a given structure, independently of the [VASP\_RUN] setting contained in the original aflow.in file. The possible settings are RELAX\_STATIC=2, and STATIC, and can be set by including the following lines in the aflow.in file respectively:

```
[AFLOW_AEL]RELAX=option
[AFLOW_AEL]RELAX_STATIC=option
[AFLOW_AEL]STATIC=option
```

The default is RELAX\_STATIC=ON, which runs RELAX\_STATIC=2 for each strained structure.

- 8) Since multiple calculations are performed for each independent direction, there is a certain amount of redundancy. In the event of failure of some of these calculations, and therefore options have been implemented within AEL to allow for the possibility of one or more failed runs in each independent direction. Failed runs can be detected automatically (by the absence of a LOCK or OUTCAR file in the directory), and the option of whether or not to skip these runs can be set by including the following line in the aflow.in file:

```
[AFLOW_AEL]AUTOSKIPFAILEDARUNS=option
```

The default is "OFF" so that no runs are skipped automatically; instead detection of a failed run will cause an error unless this particular run was explicitly listed to be skipped.

Specific runs can be listed for skipping by including the following line in the aflow.in file:

```
[AFLOW_AEL]SKIPFAILEDARUNS=directory_name_list
```

where "directory\_name\_list" is a string with the list of directory names containing the failed runs to be skipped. A fitting algorithm is used to determine the best fit. If there is more than one failed run, the individual directory names should be listed on a single line separated by commas.

AEL only permits a certain number of runs for any given independent strain direction to be skipped. The maximum number of runs permitted to be skipped in any strain direction can be set by including the following line in the aflow.in file:

```
[AFLOW_AEL]SKIPARUNSMAX=number
```

The default value is 1, so that only one run can be skipped per independent direction. Note that there is always at least one run in the number of runs in a given direction which can be skipped which is equal to half of the initial number of runs in that direction.

- 9) The main output file for the AEL method is aflow.ael.out. It contains the AEL results for the Poisson ratio, bulk modulus (Voigt, Reuss, and Voigt-Reuss-Hill (VRH)), shear modulus (Voigt, Reuss, and Voigt-Reuss-Hill (VRH)), speed of sound, AEL Debye temperature, and elastic anisotropy. It also contains the elastic constants in the form of the stiffness tensor and the compliance tensor.
- 10) The AFLOW AEL method allows the user to choose whether or not to automatically write the directional elastic moduli (Young's moduli, etc.) to a file. The writing of this file can be controlled by including the following entry in the aflow.in file:

```
[AFLOW_AEL]WRITEFULLRESULTS=option
```

The default is "OFF", so that these tensors are not written.

Finally, the values of the Poisson ratio, bulk modulus, shear modulus and elastic anisotropy are written in a script-parsable format in the file aellib.dat. The format used is the same as that used for the file aflowlib.dat. The elastic constants (in the form of the stiffness and compliance tensor) are also written to files independently of the value of the WRITEFULLRESULTS setting.

- 11) EXAMPLE: CaO FCC with default AEL settings (note that this will give the same results if all of the "[AFLOW\_AEL]" lines except "[AFLOW\_AEL]CALC" are removed or commented out):

```

[AFLOW] *****
[AFLOW] Test file for AEL calculation of CaO (fcc)
[AFLOW] *****
[AFLOW] input file for aflow
[AFLOW_MODE=VASP]
[AFLOW] *****
[AFLOW_MODE_ZIP=bzip2]
[AFLOW_MODE_BINARY=vasp46s]
[AFLOW] *****
[AFLOW_MODE_MPI]
[AFLOW_MODE_MPI_MODE] NCPUS=MAX
[AFLOW_MODE_MPI_MODE] COMMAND ="mpirun -np"
[AFLOW_MODE_MPI_MODE] AUTOTUNE
[AFLOW_MODE_MPI_MODE] BINARY="mpivasp46s"
[AFLOW] *****
[AFLOW_SYMMETRY] CALC
#[AFLOW_SYMMETRY] SGROUP_WRITE
#[AFLOW_SYMMETRY] SGROUP_RADIUS=7.77
[AFLOW] *****
#[AFLOW_NEIGHBOURS] CALC
[AFLOW_NEIGHBOURS] RADIUS=7.7
[AFLOW_NEIGHBOURS] DRADIUS=0.1
[AFLOW] *****
#[AFLOW_APL] CALC // README_AFLOW_APL.TXT
[AFLOW_APL] ENGINE=DM // README_AFLOW_APL.TXT
[AFLOW_APL] DISMAG=0.015 // README_AFLOW_APL.TXT
[AFLOW_APL] MINATOMS=100 // README_AFLOW_APL.TXT
#[AFLOW_APL] SUPERCELL=3x3x3 // README_AFLOW_APL.TXT
[AFLOW_APL] DC=y // README_AFLOW_APL.TXT
[AFLOW_APL] DPM=y // README_AFLOW_APL.TXT
[AFLOW_APL] ZEROSTATE=y // README_AFLOW_APL.TXT
[AFLOW_APL] DOS=y // README_AFLOW_APL.TXT
[AFLOW_APL] TP=y // README_AFLOW_APL.TXT
[AFLOW_APL] TPT=0:2000:10 // README_AFLOW_APL.TXT
[AFLOW] *****
#[AFLOW_QHA] CALC // README_AFLOW_APL.TXT
[AFLOW_QHA] GP_VOL_DISTORTION_PERCENTAGE=0.03 // README_AFLOW_APL.TXT
[AFLOW_QHA] DISPLACEMENTS=y // README_AFLOW_APL.TXT
[AFLOW_QHA] PROJECTION_DIR=1:1:1 // README_AFLOW_APL.TXT
[AFLOW_QHA] EOS=n // README_AFLOW_APL.TXT
[AFLOW_QHA] EOS_VOLRANGE_DIST=-2:4:0.5 // README_AFLOW_APL.TXT
[AFLOW_QHA] EOS_KPOINTS_MODE=32768:10000:20:100000 // README_AFLOW_APL.TXT
[AFLOW] *****
#[AFLOW_AAPL] CALC // README_AFLOW_APL.TXT
[AFLOW_AAPL] TDMAG=0.015 // README_AFLOW_APL.TXT
[AFLOW_AAPL] CUT_SHELL=4 // README_AFLOW_APL.TXT
[AFLOW_AAPL] CUT_RAD=4.5 // README_AFLOW_APL.TXT
[AFLOW_AAPL] SUMRULE=1E-5 // README_AFLOW_APL.TXT
[AFLOW_AAPL] BTE=FULL // README_AFLOW_APL.TXT
[AFLOW_AAPL] THERMALGRID=21x21x21 // README_AFLOW_APL.TXT
[AFLOW_AAPL] ISOTOPE=y // README_AFLOW_APL.TXT
[AFLOW_AAPL] CUMULATIVEK=y // README_AFLOW_APL.TXT
[AFLOW_AAPL] BOUNDARY=n // README_AFLOW_APL.TXT
[AFLOW_AAPL] NANO_SIZE=100 // README_AFLOW_APL.TXT
[AFLOW_AAPL] TCT=200:700:20 // README_AFLOW_APL.TXT
[AFLOW] *****
#[VASP_RUN] RELAX_STATIC_BANDS=2 // GENERATE | STATIC | RELAX=N | RELAX_STATIC=N | STATIC
#[VASP_FORCE_OPTION] NEGLECT_NOMIX
[VASP_FORCE_OPTION] CHGCAR=OFF // ON | OFF (default ON)
#[VASP_FORCE_OPTION] KPOINTS=keyword[,keyword] // EVEN | ODD | KSHIFT_GAMMA_EVEN | KSHIFT_GAMMA_ODD | KS
[VASP_FORCE_OPTION] SYM=ON // ON | OFF (default ON)
[VASP_FORCE_OPTION] AUTO_PSEUDOPOTENTIALS=potpaw_PBE // pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_P

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[VASP_FORCE_OPTION]NBANDS // Estimate Bands (better than VASP)
#[VASP_FORCE_OPTION]SPIN=ON,REMOVE_RELAX_1 // (ON | OFF (default ON)), REMOVE_RELAX_1 | _2
#[VASP_FORCE_OPTION]AUTO_MAGMOM=ON // ON | OFF (default OFF)
[VASP_FORCE_OPTION]RELAX_MODE=ENERGY // ENERGY | FORCES | ENERGY_FORCES | FORCES_ENERGY (default OFF)
[VASP_FORCE_OPTION]PREC=HIGH // (LOW | MEDIUM | NORMAL | HIGH | ACCURATE), PRESERVED (default OFF)
[VASP_FORCE_OPTION]ALGO=FAST // (NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED (default OFF)
#[VASP_FORCE_OPTION]NOTUNE
[VASP_FORCE_OPTION]TYPE=DEFAULT // METAL | INSULATOR | SEMICONDUCTOR | DEFAULT (default OFF)
[VASP_FORCE_OPTION]CONVERT_UNIT_CELL=SPRIM // SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART,
#[VASP_FORCE_OPTION]VOLUME+=10.0
#[VASP_FORCE_OPTION]VOLUME*=1.05
[AFLOW] *****
[AFLOW] *****
[VASP_INCAR_MODE_EXPLICIT]START
SYSTEM=Ca101_ICSD_26959
NELM = 120
NELMIN=2
LPLANE=.TRUE.
LREAL=.FALSE.
LSCALU=.FALSE.
#NBANDS=XX # for hand modification
#IALGO=48 # for hand modification
[VASP_INCAR_MODE_EXPLICIT]STOP
[AFLOW] *****
[VASP_KPOINTS_MODE_IMPLICIT]
[VASP_KPOINTS_FILE]KSCHEME=M
[VASP_KPOINTS_FILE]KPPRA=8000
[VASP_KPOINTS_FILE]STATIC_KSCHEME=M
[VASP_KPOINTS_FILE]STATIC_KPPRA=10000
[VASP_KPOINTS_FILE]BANDS_LATTICE=FCC
[VASP_KPOINTS_FILE]BANDS_GRID=20
[AFLOW] *****
[AFLOW_AEL]CALC
[AFLOW_AEL]NNORMALSTRAINS=4
[AFLOW_AEL]NSHEARSTRAINS=4
[AFLOW_AEL]NORMALSTRAINSTEP=0.005
[AFLOW_AEL]SHEARSTRAINSTEP=0.005
[AFLOW_AEL]NEGSTRAINS=ON
[AFLOW_AEL]NINDSTRAINS=3
[AFLOW_AEL]STRAINSYMMETRY=OFF
[AFLOW_AEL]CHECKELASTICSYMMETRY=OFF
[AFLOW_AEL]SYMTOLFRAC=0.05
[AFLOW_AEL]WRITEFULLRESULTS=OFF
[AFLOW_AEL]CALCSTRAINORIGIN=OFF
[AFLOW_AEL]FITRELAXEDSTRUCT=OFF
[AFLOW_AEL]FITSTRAINORIGIN=OFF
[AFLOW_AEL]VASPRUNXMLSTRESS=OFF
[AFLOW_AEL]PRECACALGONORM=ON
[AFLOW] *****
[VASP_POSCAR_MODE_EXPLICIT]START
Ca101 #225 - (Ca101_ICSD_26959) - Ca101 [Ca101] cF8 Fm-3m CaO 225 Ca101_ICSD_26959 ICSD_26959 (icsd library) (
1.224745
0.0000000000000000 1.95061033183634 1.95061033183634
1.95061033183634 0.0000000000000000 1.95061033183634
1.95061033183634 1.95061033183634 0.0000000000000000
1 1
Direct(2) [A1B1]
0.0000000000000000 0.0000000000000000 0.0000000000000000 Ca
0.5000000000000000 0.5000000000000000 0.5000000000000000 0
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *****
[VASP_POTCAR_MODE_IMPLICIT]
[VASP_POTCAR_FILE]Ca
[VASP_POTCAR_FILE]0
[AFLOW] potpaw_PBE: Ca_sv 0

```

```

[AFLOW] COMPOSITION_PP=|Ca_sv1|01|
[AFLOW] COMPOSITION=|Ca1|01|
[AFLOW] VOLUME(A^3)=|0|0|
[AFLOW] MASS(amu)=|40.08|15.9994|
[AFLOW] *****
[AFLOW] AfLOW automatically generated (afLOW_avasp.cpp)
[AFLOW] *****
[AFLOW] afLOW/aconvasp/ae/apennsy v(30793) in ICSD/FCC/Ca101_ICSD_26959
[AFLOW] *****
[AFLOW] SELF-MODIFICATION
[AFLOW] Recycling CONTCAR of relax1
[AFLOW] *****
[VASP_POSCAR_MODE_EXPLICIT]START
Ca101 #225 - (Ca101_ICSD_26959) - Ca101
1.224745
  0.000000000000000  1.97560216103176  1.97560216103176
  1.97560216103176  0.000000000000000  1.97560216103176
  1.97560216103176  1.97560216103176  -0.000000000000000
1 1
Direct(2) [A1B1]
  0.000000000000000  -0.000000000000000  -0.000000000000000
  0.500000000000000  0.500000000000000  0.500000000000000
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *****
[VASP_FORCE_OPTION]SPIN=OFF // Self Correction
[AFLOW] SELF-MODIFICATION
[AFLOW] Recycling CONTCAR of relax2
[AFLOW] *****
[VASP_POSCAR_MODE_EXPLICIT]START
Ca101 #225 - (Ca101_ICSD_26959) - Ca101
1.224745
  0.000000000000000  1.97560216103176  1.97560216103176
  1.97560216103176  0.000000000000000  1.97560216103176
  1.97560216103176  1.97560216103176  0.000000000000000
1 1
Direct(2) [A1B1]
  0.000000000000000  0.000000000000000  0.000000000000000
  0.500000000000000  0.500000000000000  0.500000000000000
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *****

```