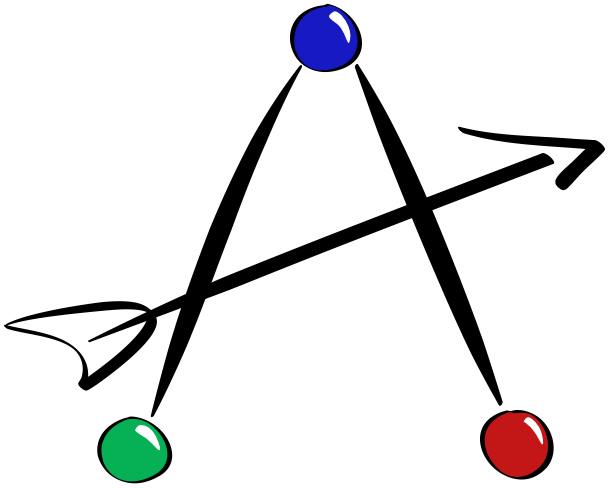

Ab initio Restructuring Tool Enabling the Modelling of Interface Structures (ARTEMIS): A User Guide

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Contents

Chapter 1

Features/Capabilites

ARTEMIS is a tool intended to help users with interface generation. Here is a list of the features it currently supports:

- Read and write geometry structure files of the formats used by VASP, CASTEP and Quantum Espresso.
- Generate slabs along user-defined Miller planes (generates all possible surface terminations in this plane)
- Determine lattice matches within defined strain tolerances for two parent structures given by the user and generate interfaces based on these.
- Determine the primitive layer of the parent structures and use these to build the parent regions of the interface structures to user-defined thicknesses.
- Identify unique surface terminations for structures along user-defined Miller planes and print slabs of these for the user to study.
- Identify unique terminations of the parent structures for Miller planes and use these to generate unique interfaces with these being the surfaces at the interface.
- Generate unique interface shifts to allow the user to explore the energetic space of interfacial alignment.

- Generate unique interface swaps (intermixing) to allow the user to explore graded interfaces.
- Take in pregenerated interface structures and determine the location of their interfaces.
- Take in pregenerated interface structures and perform shifts and swaps on them to generate further potential interfaces.

Chapter 2

Credits and Licence

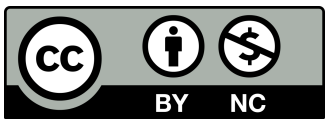
2.1 Credits

The ARTEMIS code was developed by Ned Thaddeus Taylor and Steven Paul Hepplestone. Many of the subroutines and functions used by the code were developed by Ned Thaddeus Taylor and Francis Huw Davies. During his Summer project, Isiah Edward Mikel Rudkin worked alongside Ned to develop the shifting and swapping modules of ARTEMIS, along with helping test the code.

For further information about the group behind ARTEMIS, follow the link http://www.artemis-materials.co.uk/.

For support and sending bug-reports, please contact the following email address: support@artemis-materials.co.uk

2.2 Licence



2.3 Beta testers

The following people have engaged in useful discussions that have helped to improve the quality of the program and have tested it to help find bugs in the software.

1. Conor Jason Price (University of Exeter)
2. Tsz Hin Chan (University of Exeter)
3. Joe Pitfield (University of Exeter)
4. Edward Allery David Baker (University of Exeter)
5. Shane Graham Davies (University of Exeter)

Chapter 3

Getting started

3.1 Requirements

The following utilities are required to install ARTEMIS:

- gcc version 7.2.0 (GNU Compiler Collection). Type `gcc --version` to verify this. This package can be downloaded from https://gcc.gnu.org/
- GNU make (any version). Type `make --version` to verify this. This package can be downloaded from https://gcc.gnu.org/

ARTEMIS has currently been tested to work using both the gcc fortran compiler mentioned above and the Intel fortran compiler (ifort version 17.0.4). Keep in mind, though, that ARTEMIS has been developed using the gcc fortran compiler and, as such, has been more thoroughly tested using this compiler. Whilst compilation should work with newer versions of the compilers, this has not been tested.

ARTEMIS is known to not compile with gcc version 4.8.0. This is due to that version not supporting the `allocate(MATRIX,source=SOURCE)` and the `movealloc()` Fortran built-in subroutines.

You may also want a first-principles electronic structure calculation code in order to make use of the output structures to determine the energetics of them.

3.2 Installation

Type `tar -xvzf ARTEMIS_X.X.X.tar.gz`

where `X.X.X` is the current version number. This command creates a directory called `DARTEMIS` in the current directory which contains the whole software package. From now on, I will refer to the access path to this directory as `DARTEMIS`.

Type `cd DARTEMIS`

By default, when making ARTEMIS, it will output the executable into a `bin` directory in `DARTEMIS`. The user can change where the executable is compiled by editing the Makefile line `BIN_DIR := ./bin` in `Makefile` to point to the location where the execultable is wanted. Type

```
make
```

This should compile the code into an executable called `artemis` in the designated bin directory. We highly recommend that the user copies this executable into their `$(HOME)/bin` directory and the manual assumes from now on that the user has done so (if not done, then whenever `artemis` is seen in the manual, replace this with the filepath to the `artemis` executable).

3.3 Test ARTEMIS with a simple example

In the `artemis` directory, three examples highlighting the use of ARTEMIS can be found in the `examples` subdirectory. The three presented examples are for generating new interfaces (`generate_interface` directory) and manipulating pregenerated interfaces (`pregenerated_interface` directory) and exploring all unique surface terminations of slabs (`identify_terminations`).

3.3.1 Generate interface example

Change to the `generate_interface` directory and type

```
artemis -f param.in
```

ARTEMIS will then read the `param.in` file and set the parameters as defined in there for the run. A directory named `DINTERFACES` will then be generated and populated with directories and structure files. As defined by the parameter file, `POSCAR_Si` and `POSCAR_Ge` are used for the two parent structure files.

This example is set up to show how ARTEMIS can find matched between two materials and perform shifts and swaps based on these generated interface structures.

3.3.2 Pregenerated interface example

Change to the `pregenerated_interface` directory and type

```
artemis -f param.in
```

ARTEMIS will then read the `param.in` file and set the parameters as defined in there for the run. A directory named `DINTERFACES` will then be generated and populated with directories and structure files.

This example is set up to show how ARTEMIS can determine the location of interfaces within a structure and can use that information to perform additional shifts and swaps to allow the user to further explore the energetic space of the interface.

3.3.3 Identify terminations example

Change to the `identify_terminations` directory and type

```
artemis -f param.in
```

ARTEMIS will then read the `param.in` file and set the parameters as defined in there for the run. A directory named `DTERMINATIONS` will be made with a `DLW_TERMS` directory (and `DUP_TERMS`, if `STRUC2_FILE` and `UP_MILLER` are defined) inside. This directory will contain the unique surface termination slab structures.

This example is set up to show how ARTEMIS can generate slabs cleaved along user-

defined Miller planes. In such a case, it will determine all unique surface terminations in that plane and print them to files termed as `POSCAR_term{1..n}`, where `n` is the number of unique surface terminations identified by ARTEMIS.

Chapter 4

Version History

Format is based on [Keep a Changelog] (https://keepachangelog.com/en/1.0.0/), and this project adheres to [Semantic Versioning](https://semver.org/spec/v2.0.0.html).

```
## [Alpha 1.0.0] - 2019-05-31
### Added
- Changelog introduced
- IMATCH 0, 1 and 2
- ISHIFT 0, 1 and 2
- Symmetry checks performed over matches

### Changed
- Source code moved to src/ and Makefile compiles from ./
- Updated default infile that is generated to include new opptions


## [Beta 1.0.0] - 2019-11-28
### Added
- IMATCH 3 and 4
- ISHIFT 3 and 4
- Help and search function

### Changed
```

```
- LREDUCE default changed from TRUE to FALSE


## [Beta 1.1.0] - 2019-12-18
### Added
- LW_SURFACE, UP_SURFACE
-- user-defined surface terminations
- LW_LAYERED, UP_LAYERED
-- user defines whether material is layered


## [Public release 1.0.0] - 2020-02-26
### Added
- TOL_SYM
-- user-defined symmetry precision/tolerance
- ISWAP method 2
-- method weights swapping based on distance from interface
- Restart job prints out interface location for use by user
- Optional user defined interface location - for restart
- SWAP_DENSITY allows for consistency of swapping concentration over
  structures
- User manual (doc/manual.pdf)
- LMIRROR added for swapping
-- says whether to maintain symmetry of interfaces or to perform
   swaps on one
-- only listened to if interfaces are not symmetric
- Added support email address to README and manual
- Added date of compilation to code
- Added date of execution of code to the output
- Added make install to build ARTEMIS executable
  in $(HOME)/bin directory
- Added make uninstall to remove ARTEMIS executable
  from $(HOME)/bin directory
- Added help for OUTPUT_FILE tag in CELL_EDITS card
```

```
- Added help for LSURF_GEN tag ino CELL_EDITS card
- ISHIFT=4 method updated
-- DON for upper parent crystal is now scaled appropriately the same
   as the lattice is
-- reduces issue of DONs finding more bonds at the surface than in
   the bulk
-- Update appears in interfaces.f90 gen_interfaces subroutine
- Added LAYER_SEP flag to CELL_EDITS card
-- need to figure out solution for shared cards
- Added help for LORTHO tag in CELL_EDITS and INTERFACES cards
-- defines whether surface axis is orthogonal when using LSURF_GEN
- Added example runs input/output files and input structures
-- example for detecting pregenerated interfaces
-- example for generating new interfaces
-- example for surface generation

### Changed
- Makefile now defaults to compiling executable into user's home bin
- LREDUCE default now FALSE
- Changed io.f90 to io.F90 to allow for preprossing of file
-- now includes date of compilation
- Settings output file now contains more of the important tags
- Changed make clean to remove bin/ and obj/ directories
  in the ARTEMIS directory
- f_scale and g_scale are now global variables
  in mod_shifting.f90 for ISHIFT=4
- Changed OUTFILE tag to OUTPUT_FILE
- Changed LSURF_GEN tag help description
- STRUC2_FILE no longer a mandatory tag for all cases
-- no longer required for LSURF_GEN = TRUE
-- no longer required for TASK = 0

### Removed
- LSWAP replaced with ISWAP
```

```
-- LSWAP = F is now ISWAP = 0
-- LSWAP = T is now ISWAP = 1
- NSWAP replaced with SWAP_DENSITY
- NSWAP_OUT replaced with NSWAP
- LSURF_INFO replaced with LSURF_GEN in INTERFACES card

### Fixed
- Unique termination identifier
-- inversion symmetry matches
-- reset symmetry list after each save
- Layer identification
- basis_map subroutine in mod_sym
- Correctly print and define vector mismatch to be maximum mismatch
  of any one vector
- Correctly convert symmetries to new lattice space for use in
  mod_plane_matching.f90 and mod_lat_compare.f90
- Fixed area mismatch value printing
- Works again with Intel fortran compiler ifort 17.0.4
- Fixed denominator of ISHIFT g function
-- now normalises to bond size
- Corrected help function for LREDUCE default to FALSE
- Fixed termination idenitifier again
-- works correctly for slabs without mirror symmetry now with ladders
- Fixed error in mod_plane_matching.f90
-- did not correctly save the smallest area lattice match with the
   same symmetry
- No longer makes DINTERFACES directory when not necessary
-- e.g. does not make it when generating surfaces


## [Public release 1.0.1] - 2020-05-04

### Added
- added gen_group function into mod_misc_linalg.f90 to generate entire
```

```
  group from a subset of elements
-- used in the updated version of the setup_ladder subroutine.

### Fixed
- setup_ladder subroutine
-- now correctly identifies the separation between identical layers for
   systems with both mirrored and translation symmetries transforming
   between layers
```

Chapter 5

User guide

5.1 Input files

The ARTEMIS code needs either two or three input files: one that provides the parameters to guide the interface generation and either one or two files that specify the geometries of the parent structure/structures. If the user intends to use a pre-generated interface and manipulate this structure, then only one geometry parent file is required. If one wants to generate a set of interfaces from the combination of two parent structures, then two geometry parent files are required (one for each of the parent structures). The geometry file formats currently supported include: VASP, CASTEP, Quantum Espresso. For an example of the parameters file, running the following command will generate such a file:

```
artemis -d param.in
```

This will generate an input file with some of the tags/parameters present. The input file is structured in the following way:

```
SETTINGS        (beginning of settings card)
  TAG =
END SETTINGS    (end of card)

INTERFACES      (beginning of interface card)
  TAG =
END INTERFACES  (end of interface card)
```

where the cards separate blocks of the parameters that are distinct in their actions. Cards are started by a `CARDNAME` and ended when met with `END[ ]CARDNAME`. Tags/-parameters are found within these tags and are used to alter the settings of the run. For an brief description of each of the tags available within each card, type

```
artemis -help all
```

This displays a list of all tags currently available within ARTEMIS, with a brief description of their use. To get a more indepth description of each one, type

```
artemis -help <TAGNAME>
```

where `<TAGNAME>` is the name of the tag that the user wants to know more about. If the user wants to find all tags relating to a certain word, then type

```
artemis -search <WORD>
```

All tags that include this word will be printed to the terminal.

The one/two parent geometry files are specified using the following tags in the `SETTINGS` card:

```
SETTINGS
  STRUC1_FILE = <PARENT_FILE_1>
  STRUC2_FILE = [PARENT_FILE_2]
END SETTINGS
```

5.2 Running the code

Once the input files have been gathered, ARTEMIS can be run by entering the command

```
artemis -f [INPUT_FILENAME]
```

where the flag `-f` takes [INPUT_FILENAME] as the input file and runs the code using the parameters specified in that file.

Once this has been run, a directory tree will be generated, depending on the options ran with. When generating interfaces, the `DINTERFACES/` directory will be made. When surface terminations are requested (`LSURF_INFO`, default = False), then `DTERMINATIONS/` will be made. Inside these directories, a directory tree containing the output structure files will be generated.

5.3 Outputs of ARTEMIS

Here is an example output directory tree generated by ARTEMIS. In this example, `NSHIFT` = 2 and `NSWAP` = 2, and the output file format of VASP has been used. For each unique interface match and termination, a directory in `DINTERFACES/` will be generated, with the form `D01/`, `D02/`, `D03/`, etc. Inside each of these, shifts of the generated interface match will be made and placed inside `DSHIFTS`. And inside each of those, any requested swaps will populate the `DSWAPS` directory.

```
|- DINTERFACES/
|  |- D01/
|  |  |- DSHIFTS/
|  |  |  |- D01/
|  |  |  |  |- POSCAR
|  |  |  |  |- DSWAPS/
|  |  |  |  |  |- D01/
|  |  |  |  |  |  |- POSCAR
|  |  |  |  |  |- D02/
|  |  |  |  |  |  |- POSCAR
|  |  |  |- D02/
|  |  |  |  |- POSCAR
|  |  |  |  |- DSWAPS/
|  |  |  |  |  |- D01/
|  |  |  |  |  |  |- POSCAR
|  |  |  |  |  |- D02/
|  |  |  |  |  |  |- POSCAR
|  |- D02
...
```

5.4 Conclusion

The ARTEMIS code is intended to help the user more easily and quickly explore the possibility space of interfaces between two materials. With its ability to determine lattice matches, perform shifts and swaps, this should help reduce potential bias that can be associated with such a problem by making it easier to create these interfaces. This should enable users to focus more heavily on the idea of interfacial aligment and give them the ability to explore the problem of interfaces with more ease.