amcheck - tutorial

This tutorial describes the installation and usage of the `amcheck` package that allows one to check whether the given crystal structure with a given magnetic pattern is an altermanget. You will learn how to use a command-line tool to analyze a magnetic material of interest.

The underlying code is available in the Github repository and the theory behind it is described in the Ref. [1].

1 Installation

We will install the `amcheck` package inside a virtual environment: this allows the package to use the libraries it depends on with specific versions and prevents the interference with other packages. For more information on the virtual environments, read the following page. Note that this tutorial assumes you are using Linux with `python` already installed in the system: small adjustments might be necessary for other operating systems.

To create a virtual environment named `py-amcheck` run the following command:

```
python -m venv py-amcheck
```

It will create the following directory structure:

```
.
└── py-amcheck
    ├── bin
    ├── include
    ├── lib
    ├── lib64 -> lib
    └── pyvenv.cfg
```

where the package files and it's dependencies will be stored.

To use this environenment one needs to activate it via a command:

```
source py-amcheck/bin/activate
```

Upon the successful activation, the prompt of your terminal window will be prefixed with the `(py-amcheck)` tag and it will look like this: `(py-amcheck) [andriy@computer ~]$`.

One can exit the environment using the 'deactivate' command.

To install the `amcheck` packages in this virtual environment, one needs to run:

```
pip install amcheck
```

This command should be ran only once: next time you activate the environment the package will be already present there.

To check that the installation was successful and the `amcheck` package is available, run

```
amcheck --help
```

to see the description of the `amcheck` command-line tool parameters:

```
(py-amcheck) [andriy@computer ~]$ amcheck -help
usage: amcheck [-h] [--version] [-v] [-s SYMPREC] [-ms MAG_SYMPREC] [-t TOL]
               [--ahc] file [file ...]

A tool to check if a given material is an altermagnet.

positional arguments:
  file                  name of the structure file to analyze

options:
  -h, --help            show this help message and exit
  --version             show program's version number and exit
  -v, --verbose         verbosely list the information during the execution
  -s, --symprec SYMPREC
                        tolerance spglib uses during the symmetry analysis
  -ms, --mag_symprec MAG_SYMPREC
                        tolerance for magnetic moments spglib uses during
                        the magnetic symmetry analysis
  -t, --tol, --tolerance TOL
                        tolerance for internal numerical checks
  --ahc                 determine the possible form of Anomalous Hall Coefficient
```

2   Examples

In following it will be assumed that the virtual environment containing `amcheck` is activated and the active directory is the `examples` directory that contains the crystal structure files to be analyzed. For the sake of self-containment, all of the mentioned crystal structures are provided in the Appendix.

2.1 MnF_2

We will get familiar with the `amcheck` command-line interface tool by analyzing MnF_2 compound: it has rutile structure, space group #136, with two magnetic Mn ions and four non-magnetic F ions [2]. The structure file for this example is `MnF2.cif` (for more details on Crystallographic Information File (CIF) check Ref. [3]) and we want to note that although the unit cell contains 2 Mn ions and 4 F ions, the file contains only two designations:

```
   Mn          1.0     0.000000     0.000000     0.000000   Uiso  0.050000 Mn
   F           1.0     0.304910     0.304910     0.000000   Uiso  0.050000 F
```

The reason is that it is enough to specify the positions of one of each ions and the rest can be reconstructed using the information on underlying symmetries: in the `MnF2.cif` file this information is stored after the `_space_group_symop_operation_xyz` keyword.

To run the `amcheck` tool one simply invokes the following command:

```
amcheck MnF2.cif
```

and after printing the following information, the tool waits for the input from the user:

```
================================================================================
Processing: MnF2.cif
--------------------------------------------------------------------------------
Spacegroup: P4_2/mnm (136)

Writing the used structure to auxiliary file: check MnF2.cif_amcheck.vasp.
```

```
Orbit of Mn atoms at positions:
1 (1) [0.  0.  0.]
2 (2) [0.5 0.5 0.5]
Type spin (u, U, d, D, n, N, nn or NN) for each of them (space separated):
```

At first it lists what file is being processed, `MnF2.cif`, followed by the determined space group of non-magnetic crystal, `P4_2/mnm (136)`.

To have a visual aid, useful when analyzing more complicated structures, the tool creates an auxiliary file, in this case named the `MnF2.cif_amcheck.vasp` file (see Sec. 3.1), which contains the list of atoms in the `POSCAR` format [4] ordered in the same way as they appear in the output. One can open this file with a crystal visualization software, like VESTA; for the reference visualization see Fig. 1.
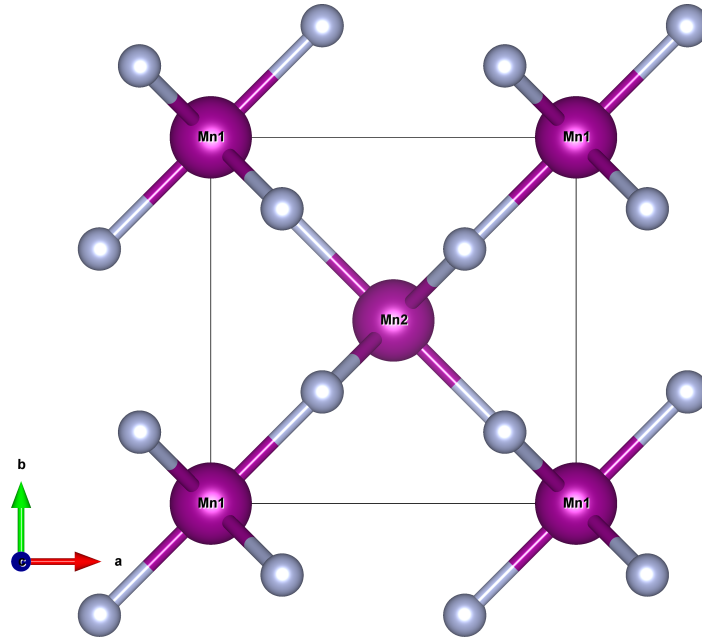

Figure 1: MnF$_2$ crystal structure with two magnetic Mn ions.

Note that the tool lists two Mn ions and their positions (here highlighted in blue). The two Mn ions are equivalent by symmetry and we will refer to them as to belonging to the same orbit. All of the atoms in the input file will be grouped into orbits and user needs to input the spin pattern for each orbit, i.e. assign a magnetic label for each atom.

It is assumed that space and spin coordinates are decoupled and that spin is a pseudoscalar quantity, i.e., merely "up" or "down" and not a pseudovector; the latter is done when magnetic space group formalism is employed. Since the exact value of the local magnetic moment is not important for the determination if the material is possibly an altermagnet based on the symmetry consideration, it is assumed that atoms within the same orbit have the same value of local magnetic moment.

To proceed with the analysis, one need to specify the spin pattern for Mn ions. One uses "u" or "U" symbols to assign spin up label and "d" or "D" for spin down. Assuming that the spin orientations on each Mn atom are anti-parallel, type in

```
u d
```

to specify that the first Mn ions has spin up and the second has spin down.

In return, the tool will print the block for the 4 F ions:

```
Orbit of F atoms at positions:
3 (1) [0.30491 0.30491 0.     ]
4 (2) [0.69509 0.69509 0.     ]
5 (3) [0.19509 0.80491 0.5    ]
6 (4) [0.80491 0.19509 0.5    ]
Type spin (u, U, d, D, n, N, nn or NN) for each of them (space separated):
```

and will wait for the user input.

F ions are non-magnetic and the corresponding label is "n" or "N". To label an entire orbit as non-magnetic, use "nn" or "NN" intsead of typing labels for each atom.

To proceed with the analysis, type:

```
n n n n
```

At the end of the output the answer is given:

```
Altermagnet? True
```

MnF_2 in this magnetic configuration is an altermagnet.

All in all, the full interaction with the tool with user input highlighted in blue is:

```
(py-amcheck) [andriy@computer examples]$ amcheck MnF2.cif
================================================================================
Processing: MnF2.cif
--------------------------------------------------------------------------------
Spacegroup: P4_2/mnm (136)

Writing the used structure to auxiliary file: check MnF2.cif_amcheck.vasp.

Orbit of Mn atoms at positions:
1 (1) [0. 0. 0.]
2 (2) [0.5 0.5 0.5]
Type spin (u, U, d, D, n, N, nn or NN) for each of them (space separated):
u d

Orbit of F atoms at positions:
3 (1) [0.30491 0.30491 0.      ]
4 (2) [0.69509 0.69509 0.      ]
5 (3) [0.19509 0.80491 0.5     ]
6 (4) [0.80491 0.19509 0.5     ]
Type spin (u, U, d, D, n, N, nn or NN) for each of them (space separated):
n n n n
Group of non-magnetic atoms (F): skipping.

Altermagnet? True
```

> **Question 1:** For Mn atom there was only one non-equivalent spin pattern: "u d". The "d u" is equivalent to it by symmetry, i.e. when you flip all of the spins you get an equivalent state; try it out using the tool. Let's imagine that the F ion is magnetic. How many non-equivalent net-moment-compensated spin configurations would there be for four ions?

2.2 NiAs-structure: high-pressure FeO and MnTe

In this example we will use the NiAs structure (Sec. 3.2) as a prototype and examine how the position of magnetic atom affects the possibility of the compound to be an altermagnet. The prototype unit cell contains two Ni atoms and two As atoms as depicted in Fig. 2.

> **Question 2:** This structure contains spatial inversion: taking into account all the possible translation operations, how many inversion centers are in the unit cell?
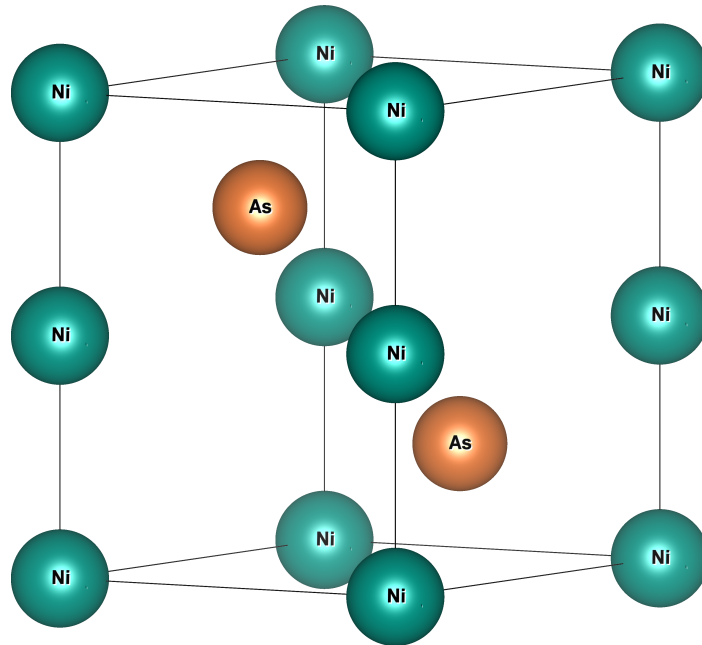
Figure 2: NiAs crystal structure: teal and orange spheres are Ni and As atoms.

Question 3: Taking into account the equivalence of atoms by translation, examine what is the action of inversion on Ni atoms and on As atoms. For material to be altermagnetic, what atoms, Ni or As, should be magnetic and have "u d" spin pattern?

In the first example we will substitute As atoms with Fe and Ni atoms with O. This corresponds to the FeO structure at high pressure (hp-FeO), see the `FeO.vasp` file (Sec. 3.3). Use the following command:

```
amcheck FeO.vasp
```

and specify "u d" spin pattern for Fe and specify that O is non-magnetic, "n n".
The result is that hp-FeO is an antiferromagnet, since Fe atoms are exchanged by the inversion.
Next, we will have a look at MnTe, where As atoms are substituted with Te and Ni atoms with Mn, see the `MnTe.vasp` file (Sec. 3.4).
Use the following command:

```
amcheck MnTe.vasp
```

and specify "u d" spin pattern for Mn and specify that Te is non-magnetic, "n n". Confirm that MnTe is an altermagnet.

Answers

1. There will be three non-equivalent spin configurations: "u u d d", "u d d u", and "u d u d".

2. There will be 8 inversion centers in the unit cell at positions: $(0, 0, 0)$, $(0.5, 0, 0)$, $(0.5, 0.5, 0)$, $(0, 0.5, 0)$, $(0, 0, 0.5)$, $(0.5, 0, 0.5)$, $(0.5, 0.5, 0.5)$, and $(0, 0.5, 0.5)$.

3. The spatial inversion exchanges As atoms but leaves Ni atoms unchanged, because it brings one Ni atom to the one which is equivalent to it by a translation, i.e. connected by an integer multiple of a lattice vector. Thus, to have an altermagnet, a magnetic atom should be at the position of Ni atom.

3 Appendix

3.1 MnF$_2$ crystal structure

The following `MnF2.cif` file contains the crystal structure of MnF$_2$ compound [2]:

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'MnF2'
_cell_length_a                         4.873600
_cell_length_b                         4.873600
_cell_length_c                         3.310200
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           78.623794
_space_group_name_H-M_alt             'P 42/m n m'
_space_group_IT_number                 136

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x, -y, z'
   'x, y, -z'
   '-y+1/2, x+1/2, z+1/2'
   'y+1/2, -x+1/2, -z+1/2'
   'y+1/2, -x+1/2, z+1/2'
   '-y+1/2, x+1/2, -z+1/2'
   '-x+1/2, y+1/2, -z+1/2'
   'x+1/2, -y+1/2, z+1/2'
   'x+1/2, -y+1/2, -z+1/2'
   '-x+1/2, y+1/2, z+1/2'
   'y, x, -z'
   '-y, -x, z'
   '-y, -x, -z'
   'y, x, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Mn         1.0      0.000000     0.000000     0.000000    Uiso  0.050000 Mn
   F          1.0      0.304910     0.304910     0.000000    Uiso  0.050000 F
```

3.2 NiAs

The following `NiAs.cif` file contains the crystal structure of NiAs compound [5]:

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'NiAs'
_cell_length_a                         3.620000
_cell_length_b                         3.620000
_cell_length_c                         5.040000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           57.197662
_space_group_name_H-M_alt             'P 63/m m c'
_space_group_IT_number                 194

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   '-y, x-y, z'
   'y, -x+y, -z'
   '-x+y, -x, z'
   'x-y, x, -z'
   '-x, -y, z+1/2'
   'x, y, -z+1/2'
   'y, -x+y, z+1/2'
   '-y, x-y, -z+1/2'
   'x-y, x, z+1/2'
   '-x+y, -x, -z+1/2'
   'y, x, -z'
   '-y, -x, z'
   'x-y, -y, -z'
   '-x+y, y, z'
   '-x, -x+y, -z'
   'x, x-y, z'
   '-y, -x, -z+1/2'
   'y, x, z+1/2'
   '-x+y, y, -z+1/2'
   'x-y, -y, z+1/2'
   'x, x-y, -z+1/2'
   '-x, -x+y, z+1/2'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
```

```
_atom_site_U_iso_or_equiv
_atom_site_type_symbol
Ni       1.0     0.000000     0.000000     0.000000   Uiso  0.050000 Ni
As       1.0     0.333333     0.666667     0.250000   Uiso  0.050000 As
```

3.3   FeO

The following `FeO.vasp` file contains the crystal structure of FeO compound at high pressure [6]:

```
hp-FeO. Unit cell parameters from: 10.1126/science.266.5191.1678
1.0
        2.5739998817        0.0000000000        0.0000000000
       -1.2869999409        2.2291492869        0.0000000000
        0.0000000000        0.0000000000        5.1719999313
Fe    O
 2    2
Direct
     0.333333343        0.666666687        0.250000000
     0.666666627        0.333333313        0.750000000
     0.000000000        0.000000000        0.000000000
     0.000000000        0.000000000        0.500000000
```

3.4   MnTe

The following `MnTe.vasp` file contains the crystal structure of MnTe compound [7]:

```
MnTe. Unit cell parameters from sd_0379437 of Springer Materials
1.0
        4.1260000000        0.0000000000        0.0000000000
       -2.0630000000        3.5732200000        0.0000000000
        0.0000000000        0.0000000000        6.7240000000
Mn    Te
 2    2
Direct
     0.000000000        0.000000000        0.000000000
     0.000000000        0.000000000        0.500000000
     0.333333343        0.666666687        0.250000000
     0.666666627        0.333333313        0.750000000
```

References

[1] A. Smolyanyuk, L. Šmejkal, and I. I. Mazin, "A tool to check whether a symmetry-compensated collinear magnetic material is antiferro- or altermagnetic," *SciPost Phys. Codebases*, p. 30, 2024.

[2] W. Jauch, G. J. McIntyre, and A. J. Schultz, "Single-crystal neutron diffraction studies of MnF_2 as a function of temperature: the effect of magnetostriction," *Acta Crystallographica Section B*, vol. 46, pp. 739–742, Dec 1990.

[3] I. D. Brown and B. McMahon, "CIF: the computer language of crystallography," *Acta Crystallographica Section B*, vol. 58, pp. 317–324, Jun 2002.

[4] https://www.vasp.at/wiki/index.php/POSCAR.

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[6] Y. Fei and H. kwang Mao, "In Situ Determination of the NiAs Phase of FeO at High Pressure and Temperature," *Science*, vol. 266, no. 5191, pp. 1678–1680, 1994.

[7] G. I. Makovetskii, A. I. Galyas, G. M. Severin, and K. I. Yanushkevich, "ChemInform Abstract: Synthesis of Solid Solutions of Cr1-xMnxTe ($0 \leq x \leq 1$).," *ChemInform*, vol. 28, no. 4, 1997.