When converting the P1 cif file for the FeAl-crystal to a code specific input file via cif2cell, you may run into this error message:

***Warning: Space group operation check failed for Hall symbol Unknown (H-M symbol P21/m21/m2/n(originchoice2)).

The reason for this error is that cif2cell cannot correctly read/interpret the information for the _symmetry_space_group_name_H-M keyword in the cif file, for space groups for which there is freedom in the origin choice.

We'll describe 3 workarounds :

Solution 1

This error appears only if you have added symmetry information to the cif file via FINDSYM (it is this step that introduces the _symmetry_space_group_name_H-M keyword in the cif file. If you use a DFT code that does not heavily use symmetry (like Quantum Espresso), it is harmless to use cif2cell directly on the P1 cif. This will result in a correct input file. Note, however, that in this way you may not detect situations where the P1 cif file has more atoms than strictly needed – you may end up spending too much calculations time with your DFT code.

Solution 2

This is the critical part of the cif file (produced by FINDSYM) that is related to the error message:

```
_symmetry_space_group_name_H-M "P 21/m 21/m 2/n (origin choice 2)"
_symmetry_Int_Tables_number 59
_space_group.reference_setting '059:-P 2ab 2a'
_space_group.transform_Pp_abc a,b,c;0,0,0
```

This tells us we have space group nr. 59, in a setting described by the H-M symbol (first line). The notation of the latter is not correctly understood by cif2cell. If you replace this long notation by its short version, cif2cell will read it correctly. You can find the short notation at https://en.wikipedia.org/wiki/List_of_space_groups :

59			Pmmn	P 2_1/m 2_1/m 2/n

The proper format for cif2cell is "P m m n :2" : spaces, and a :2 to indicate the origin choice. Your cif file should read as follows:

```
_symmetry_space_group_name_H-M "P m m n :2"
_symmetry_Int_Tables_number 59
_space_group.reference_setting '059:-P 2ab 2a'
_space_group.transform_Pp_abc a,b,c;0,0,0
```

The table on Wikipedia is not complete for all possible settings, however. Therefore, this solution includes some guesswork. The next solution is more fool-proof.

Solution 3

The H-M symbol does not entirely define the setting for all space groups, for some groups – and nr. 59 is an example of this -- there are ambiguities left. That is taken care of by the _space_group.reference_setting symbol. We could therefore remove the H-M symbol and take a different notation instead that has all information included. The Hall symbol does that job, and _space_group.reference_setting basically includes the Hall symbol already. You can check it in this exhaustive list of Hall symbols :

http://cci.lbl.gov/sginfo/hall_symbols.html

This is the relevant section :

```
59:1      P m m n:1      P 2 2ab -1ab
59:2      P m m n:2     -P 2ab 2a
59:1cab   P n m m:1      P 2bc 2 -1bc
59:2cab   P n m m:2     -P 2c 2bc
59:1bca   P m n m:1      P 2ac 2ac -1ac
59:2bca   P m n m:2     -P 2c 2a
```

The middle column is the H-M symbol in a notation that cif2cell understands. The right column is the Hall symbol.

What is now the procedure:

_space_group.reference_setting tells you “059: -P 2ab 2a”. What follows after the “:” is the Hall symbol. Look for the line with “-P 2ab 2a” in the table. You then read at that line the correct short H-M symbol for solution 2, if you want. But you can also remove the line with _symmetry_space_group_name_H-M keyword, alter _space_group.reference_setting into _space_group_name_Hall, and give it as value ‘-P 2ab 2a’. The cif file looks now like this:

```
_symmetry_Int_Tables_number 59
_space_group_name_Hall '-P 2ab 2a'
_space_group.transform_Pp_abc a,b,c;0,0,0
```

And this will work too.