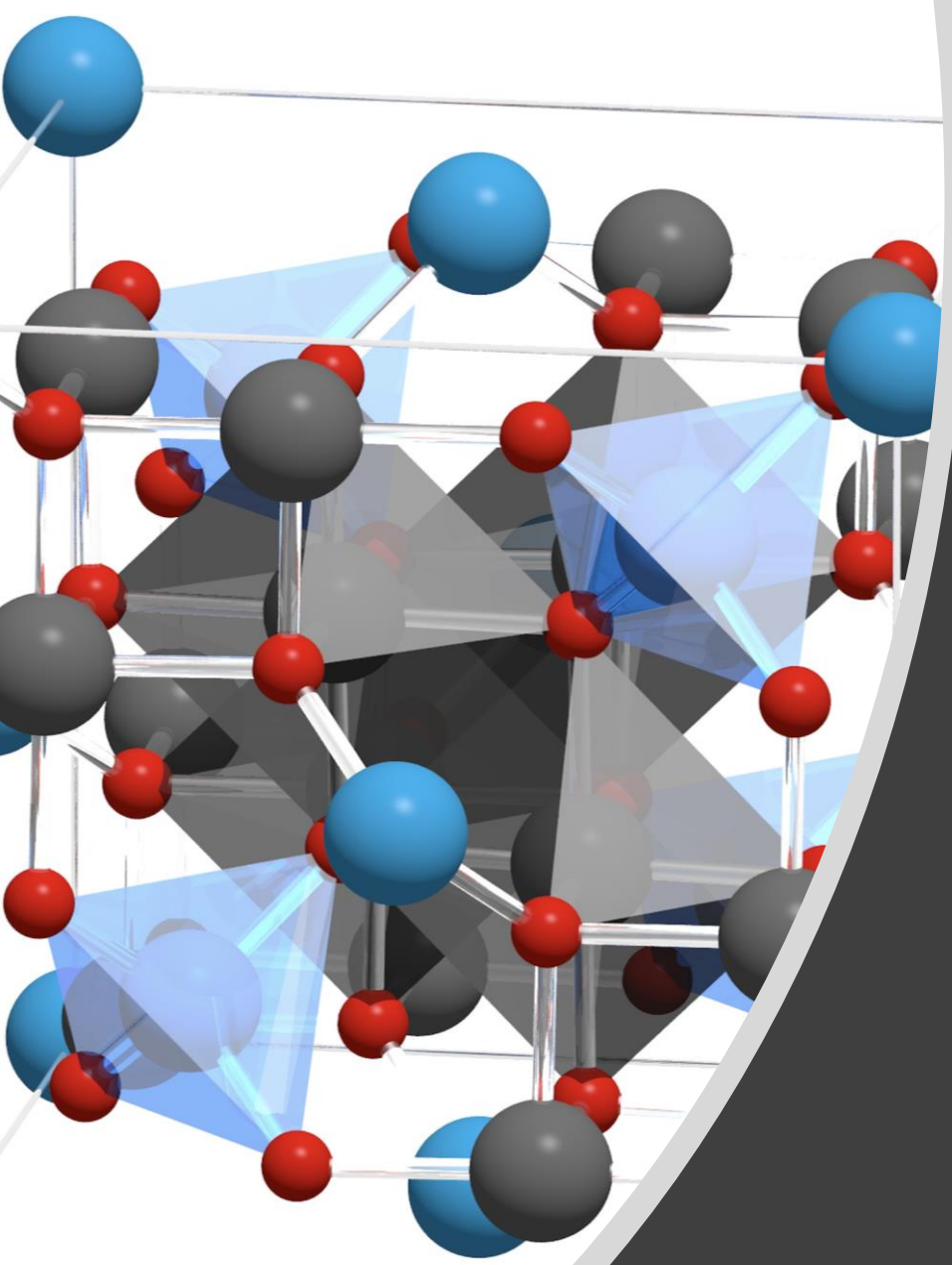


Working with Magnetite

Daniel Meilak, University of York

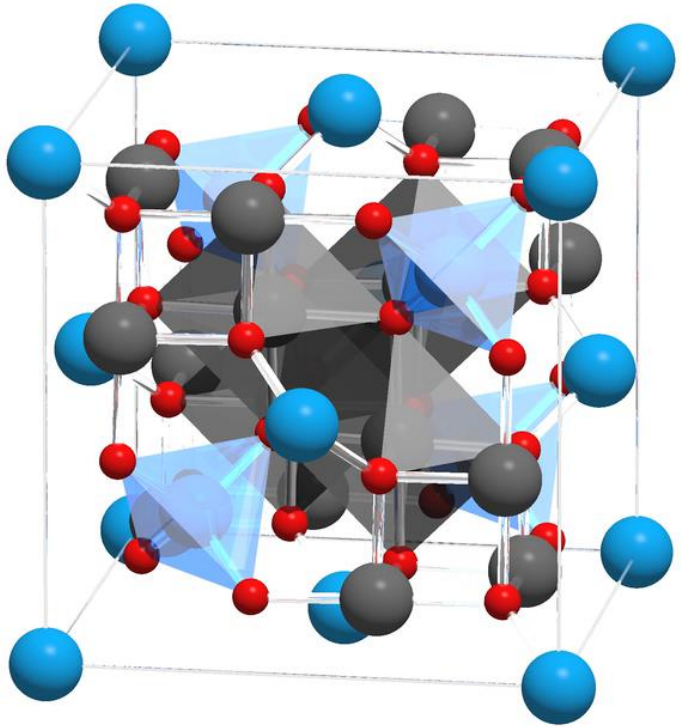
Magnetite is a ferrimagnet

Fd3m symmetry, inverse spinel

56 atoms

Two sublattices:
Tetrahedral and Octahedral

Weak cubic anisotropy



How do you construct the unit cell?

Take someone else's work (with references). Assume it's correct.

Or make it yourself!

Use a crystallographic database such as Bilbao crystallographic server.

http://www.cryst.ehu.es/

You can use the symmetry sites to find the atomic coordinates.

Magnetite is Fd-3m. 8a 16d 32e sites.

32	e	(x,x,x | 0,0,0) (x+1/4,x+1/4,-x | 0,0,0) (x,-x+1/4,-x+1/4 | 0,0,0) (-x+1/4,-x+1/4,x | 0,0,0)	(x+1/4,-x,x+1/4 | 0,0,0) (-x,x+1/4,x+1/4 | 0,0,0) (-x+1/4,x,-x+1/4 | 0,0,0) (-x,-x,-x | 0,0,0)
16	d	(1/2,1/2,1/2 | 0,0,0) (3/4,3/4,1/2 | 0,0,0)	(3/4,1/2,3/4 | 0,0,0) (1/2,3/4,3/4 | 0,0,0)
16	c	(0,0,0 | 0,0,0) (1/4,1/4,0 | 0,0,0)	(1/4,0,1/4 | 0,0,0) (0,1/4,1/4 | 0,0,0)
8	b	(3/8,3/8,3/8 | 0,0,0)	(5/8,5/8,5/8 | 0,0,0)
8	a	(1/8,1/8,1/8 | 0,0,0)	(7/8,7/8,7/8 | 0,0,0)

X refers to the oxygen atom offset.

You can find this online in papers,

experimental data etc

We're going to simulate magnetite at 0 Kelvin and visualise the system with spins.

You should be able to find a unit cell file "magnetite.ucf" in the vampire-workshop folders

However it's your job to create input and material files.

Input file checklist:

Try making a spherical nanoparticle
create:crystal-structure:sc
system dimentions
- -lattice constant
- -system size (try 2.5nm)

dimensions:particle-size=x, make it a little smaller than the system size
Material file name
material:unit-cell-file=magnetite.ucf
Temperature of 0 Kelvin
Monte Carlo solver
Time series simulation
Time step increment of 10
Total steps 100,000
output:output-rate=10000
config:atoms
config:atoms-output-rate=100000

Material File checklist:

3 materials:
Material name
Spin moments (Tet 5 !muB and Oct 4.5 !muB)
Material element
Initial spin direction is random
unit-cell-category for material 1&2
Cubic anisotropy constant: -1.77E-24
Exchange matrices:
- $-J_{TT}$ = -6.31E-22
- $-J_{TO} = J_{OT}$ = -5.07E-22
- $-J_{OO}$ = 9.76E-22

3rd material, oxygen is non-magnetic
Use non-magnetic=remove

Use the Vampire Manual to look up parameters

Once it’s working, feel free to try out different parameters to get a feel for how they change simulation time and physics.

Try increasing the size of the system and particle

Try decreasing the total number of steps

Try using faceted nanoparticles (make sure your system is a few nm larger than the particle)

```
create:faceted-particle = 1.0833333,2,1.0833333
```

Remember to visualise the particle using RASmol/Vesta/POVray

Use output options like “material-mean-magnetisation-length” to make plots of the normalised magnetisation of the sublattices.

You can also use this unitcell file to look at materials related to magnetite, such as cobalt ferrite, by doping the system with Cobalt. The anisotropy and exchange constants will also have to be changed to produce reasonable physics however.

Doping with Cobalt Ferrite:

material[1] is Tet, material[2] is Oct, material[3] is Oxygen

Set material[2]:alloy-host. We know that Cobalt forms part of the octahedral sites

material[4] is Cobalt. However we do not want it to be places in the system automatically.

material[4]:minimum-height=0.0

material[4]:maximum-height=0.0

Material[2]:alloy-fraction[4]=0.5

Cobalt Ferrite also has a different easy axis of [100] and much stronger anisotropy around 10* higher.

Extra Slides

```
# Unit cell size:
8.397   8.397   8.397
# Unit cell vectors:
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
# Atoms num, id cx cy cz mat lc hc
56
0       0.125   0.125   0.125   0       0       0
1       0.875   0.375   0.375   0       1       0
2       0.125   0.625   0.625   0       2       0
3       0.875   0.875   0.875   0       3       0
4       0.625   0.125   0.625   0       4       0
5       0.375   0.375   0.875   0       5       0
6       0.625   0.625   0.125   0       6       0
7       0.375   0.875   0.375   0       7       0
8       0.5     0.5     0.5     1       8       1
9       0.249999        0.749999        0       1       9       1
10      0.749999        0       0.249999        1       10      1
11      0       0.249999        0.749999        1       11      1
12      0.5     0       0       1       12      1
13      0.249999        0.249999        0.5     1       13      1
14      0.749999        0.5     0.749999        1       14      1
15      0       0.749999        0.249999        1       15      1
16      0       0.5     0       1       16      1
17      0.749999        0.749999        0.5     1       17      1
18      0.249999        0       0.749999        1       18      1
19      0.5     0.249999        0.249999        1       19      1
20      0       0       0.5     1       20      1
21      0.749999        0.249999        0       1       21      1
22      0.249999        0.5     0.249999        1       22      1
23      0.5     0.749999        0.749999        1       23      1
24      0.2549  0.2549  0.2549  2       24      2
25      0.4951  0.9951  0.7549  2       25      2
```

Lattice parameters. Overwrite value in input file

Unit Cell vectors. Must be cubic

Atomic positions.
Columns are:
Atom number
Fractional x-coord
Fractional y-coord
Fractional z-coord
Material number

```
47      0.7451  0.0049  0.0049  2       47      2
48      0.7549  0.7549  0.2549  2       48      2
49      0.9951  0.4951  0.7549  2       49      2
50      0.4951  0.2549  0.4951  2       50      2
51      0.2549  0.9951  0.9951  2       51      2
52      0.5049  0.0049  0.2451  2       52      2
53      0.2451  0.2451  0.7451  2       53      2
54      0.0049  0.7451  0.0049  2       54      2
55      0.7451  0.5049  0.5049  2       55      2
#Interactions n exctype, id i j dx dy   dz        Jij
768     normalised-isotropic
0       0       3       -1      -1      -1      1
1       0       41      -1      -1      0       1
2       3       41      0       0       1       1
3       41      0       1       1       0       1
4       41      3       0       0       -1      1
5       0       1       -1      0       0       1
6       1       41      0       -1      0       1
7       41      1       0       1       0       1
8       0       10      -1      0       0       1
9       10      41      0       -1      0       1
10      41      10      0       1       0       1
11      0       7       0       -1      0       1
12      7       41      -1      0       0       1
13      41      7       1       0       0       1
14      0       15      0       -1      0       1
15      15      41      -1      0       0       1
16      41      15      1       0       0       1
17      0       20      0       0       0       1
18      20      41      -1      -1      0       1
19      41      20      1       1       0       1
20      0       34      -1      0       -1      1
21      3       34      0       1       0       1
```

■
■
■

```
765     23      5       0       0       0       1
766     23      9       0       0       1       1
767     23      8       0       0       0       1
```

Using the exchange constants J_{ij}, we need to work out the exchange values between each atom i and j in the system.

```
material[1]:exchange-matrix[1] = -6.30863E-22
material[1]:exchange-matrix[2] = -5.06981E-21
material[1]:exchange-matrix[3] = 0
```

Columns are:
Interaction id
i atom number
j atom number (don't include i=j)
unit cell id x-coord
unit cell id y-coord
unit cell id z-coord
Interaction number (always 1 in this version of vampire)