**软件说明书**

1. **执行程序 – 磁转变温度扫描**
2. 解析晶体结构文件模式

程序设置为可以自动读取VASP类型的晶体结构文件数据，并自动获取对应的近邻表。此处用经典的二维磁性材料CrI3作为例子，在该模式下需要两个文件即INPUT及POSCAR文件。

**POSCAR:**

CONTCAR

1.00

7.0103 0.0000 0.0000

-3.5051 6.0710 0.0000

0.0000 0.0000 19.9866

Cr I

2 6

Direct

0.6666700 0.3333300 0.5015400

0.3333300 0.6666700 0.5015400

0.6396700 0.0000000 0.4234200

0.0000000 0.6396700 0.4234200

0.3603299 0.3603299 0.4234200

0.0000000 0.3600200 0.5797899

0.3600200 0.0000000 0.5797899

0.6399800 0.6399800 0.5797899

**INPUT:**

[System]

Method = Heisenberg # Heisenberg or Ising

System = Tc # Tc or Loop

Setting = Auto # Auto or Set

[Lattice]

Sample = 5 # Default 1

Lattice = 50 # Default 10

Temperature = 10 70 1 # Default 5 500 5 K

[Magnetic]

% Cr 3

J = 0.002944

A = 0 0 0.000744 0 0 0

此时INPUT文件中的Setting参数需要设置为Auto。Lattice中的Sample表示为每次会同时运行几个环境，增加该参数可以能够有效消除微扰带来的毛刺；Lattice参数表示在有效的周期性边界上需要扩展多大的胞，越大的胞可以带来更多的多样性，结果也更加真实；Temperature参数读取是三个浮点数，表示的扫描温度的初始，结束及步长。以上的参数的增加都将带来计算的增加，故需要根据实际情况分析。

执行程序后可以在输出文件OUTCAR中查看近邻表及参数设置是否正确，例如下图中Cr的近邻环境都是正确的。

\*\* multiple model of the curie temperature -- version 0.03 \*\*

## Parallel version (MPI), running on 28 processors ##

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* ECHO INPUT PARAMETERS \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* [System] \*

\* Method = Heisenberg \*

\* System = Tc \*

\* Setting = Auto \*

\* Dimension = True True False \*

\* \*

\* [Lattice] \*

\* Sample = 5 \*

\* Lattice = 50 \*

\* Temperature[start,end,step] = 10 70 1 \*

\* H\_field = 0 0 0 \*

\* TotalSteps = 300000 \*

\* RelaxSteps = 100000 \*

\* LogicCell = False \*

\* \*

\* [Magnetic] \*

\* No.1 (Cr, 0) M = 3 A = ( 0, 0, 0.000744, \*

\* 0, 0, 0) \*

\* J1 = 0.002944 \*

\* ==> +0 -1 +0 (Cr, 1) <== \*

\* ==> +1 +0 +0 (Cr, 1) <== \*

\* ==> +0 +0 +0 (Cr, 1) <== \*

\* \*

\* No.2 (Cr, 1) M = 3 A = ( 0, 0, 0.000744, \*

\* 0, 0, 0) \*

\* J1 = 0.002944 \*

\* ==> +0 +1 +0 (Cr, 0) <== \*

\* ==> -1 +0 +0 (Cr, 0) <== \*

\* ==> +0 +0 +0 (Cr, 0) <== \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* END OF INPUT PARAMETERS \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

1. 手动设置模式

若此时晶格数据文件较难获得或需要抽象为更为简单的结构时，用户可以自行设置近邻表及相关数据。依旧采用二维磁性材料CrI3作为例子，在该模式下只需要一个文件即INPUT文件。同样的执行后可以通过查看OUTCAR查看相关设置是否正确。

[System]

Method = Heisenberg # Heisenberg or Ising

System = Tc # Tc or Loop

Setting = Set # Auto or Set

[Lattice]

Sample = 5 # Default 1

Lattice = 50 # Default 10

Temperature = 10 100 1 # Default 5 500 5 K

[Set]

% Cr 3

J = 0.002944

A = 0 0 0.000744 0 0 0

J1 0 0 0 2

J1 +1 0 0 2

J1 0 +1 0 2

% Cr 3

J = 0.002944

A = 0 0 0.000744 0 0 0

J1 0 0 0 1

J1 -1 0 0 1

J1 0 -1 0 1

1. 分析数据

执行中会生出两个文件OUTCAR及Data.dat，OUTCAR存储了相关的参数及模拟分析执行程度。Data.dat中存储磁性相关的数据，分别为内能，热容，磁矩和磁化率用于后续的数据分析。

**OUTCAR:**

\*\* multiple model of the curie temperature -- version 0.03 \*\*

## Parallel version (MPI), running on 28 processors ##

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* ECHO INPUT PARAMETERS \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* [System] \*

\* Method = Heisenberg \*

\* System = Tc \*

\* Setting = Auto \*

\* Dimension = True True False \*

\* \*

\* [Lattice] \*

\* Sample = 5 \*

\* Lattice = 50 \*

\* Temperature[start,end,step] = 10 70 1 \*

\* H\_field = 0 0 0 \*

\* TotalSteps = 300000 \*

\* RelaxSteps = 100000 \*

\* LogicCell = False \*

\* \*

\* [Magnetic] \*

\* No.1 (Cr, 0) M = 3 A = ( 0, 0, 0.000744, \*

\* 0, 0, 0) \*

\* J1 = 0.002944 \*

\* ==> +0 -1 +0 (Cr, 1) <== \*

\* ==> +1 +0 +0 (Cr, 1) <== \*

\* ==> +0 +0 +0 (Cr, 1) <== \*

\* \*

\* No.2 (Cr, 1) M = 3 A = ( 0, 0, 0.000744, \*

\* 0, 0, 0) \*

\* J1 = 0.002944 \*

\* ==> +0 +1 +0 (Cr, 0) <== \*

\* ==> -1 +0 +0 (Cr, 0) <== \*

\* ==> +0 +0 +0 (Cr, 0) <== \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* END OF INPUT PARAMETERS \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

T = 10| delta = 0.0400 [###################################] Rate = 51.50%

T = 11| delta = 0.0400 [###################################] Rate = 53.53%

T = 12| delta = 0.0500 [###################################] Rate = 50.98%

T = 13| delta = 0.0500 [###################################] Rate = 52.74%

T = 14| delta = 0.0600 [###################################] Rate = 50.74%

T = 15| delta = 0.0600 [###################################] Rate = 52.29%

T = 16| delta = 0.0700 [###################################] Rate = 50.66%

T = 17| delta = 0.0700 [###################################] Rate = 52.05%

T = 18| delta = 0.0800 [###################################] Rate = 50.69%

T = 19| delta = 0.0800 [###################################] Rate = 51.97%

**Data.dat:**

Temperature Energy Capacity Magnetic Susceptibility

10 -0.0107240 1.821527E-08 2.8256272 1.243809E-02

11 -0.0106322 1.840921E-08 2.8067080 1.421968E-02

12 -0.0105400 1.865170E-08 2.7875326 1.596653E-02

13 -0.0104470 1.867857E-08 2.7680349 1.774003E-02

14 -0.0103532 1.876691E-08 2.7481668 1.951585E-02

……

56 -0.0049336 1.567349E-08 0.1074436 4.878433E-01

57 -0.0048570 1.500697E-08 0.1035059 4.327720E-01

58 -0.0047839 1.443587E-08 0.1007834 3.992886E-01

59 -0.0047134 1.378165E-08 0.0981459 3.667351E-01

60 -0.0046455 1.333115E-08 0.0957825 3.425392E-01

分析Data.dat文件中的数据即可。



1. **执行程序 – 磁滞回线**
2. 参数设置

以下将以自动模式为例介绍磁滞回线模拟仿真时的设置，同样的在该模式下需要两个文件即INPUT及POSCAR文件。

[System]

Method = Heisenberg # Heisenberg or Ising

System = Loop # Tc or Loop

Setting = Auto # Auto or Set

[Lattice]

Sample = 5 # Default 1

Lattice = 20 # Default 10

Temperature = 10 70 1 # Default 5 500 5 K

[Magnetic]

% Cr 3

J = 0.002944

A = 0 0 0.000744 0 0 0

[Loop]

LoopTemp = 10

LoopVector = 0 0 1

LoopRange = 3E-3 1E-4

Loop模块下的参数，LoopTemp表示磁滞回线模拟所需要的温度，在开启Loop模式后将无视Lattice模块中的Temperature参数的设置，转而读取LoopTemp的温度设置；LoopVector表示外磁场的方向，分别是三个浮点数。程序会自动将该矢量标准化，因此设置好方向指向即可；LoopRange表示外磁场扫描的范围及步长，该模式对于Loop扫描为串行，因此请慎重选择步长大小。

1. 数据分析

正常运行后获得数据如下。

**Loop.dat:**

No. Temp X Y Z H-field Magnetism Energy Susceptibility Capacity

0 10 0 0 0 0 0.16649 -0.01072 3.117504E+01 2.603204E-07

1 10 0 0 0.0001 0.0001 0.16459 -0.01073 7.859074E-02 1.142373E-07

2 10 0 0 0.0002 0.0002 0.16775 -0.01074 7.907739E-02 1.141225E-07

3 10 0 0 0.0003 0.0003 0.17093 -0.01075 8.017039E-02 1.142871E-07

4 10 0 0 0.0004 0.0004 0.17418 -0.01076 8.167262E-02 1.141594E-07

……

45 10 0 0 0.0016 0.0016 2.86101 -0.01313 4.048800E-02 1.122974E-07

46 10 0 0 0.0015 0.0015 2.85938 -0.01298 4.179811E-02 1.123189E-07

47 10 0 0 0.0014 0.0014 2.85767 -0.01283 4.314872E-02 1.122799E-07

48 10 0 0 0.0013 0.0013 2.85592 -0.01268 4.461061E-02 1.124222E-07

49 10 0 0 0.0012 0.0012 2.85409 -0.01253 4.617068E-02 1.124746E-07

50 10 0 0 0.0011 0.0011 2.85221 -0.01238 4.787202E-02 1.125814E-07

将数据可视化后可得，



1. **微观结构分析**

如果分析中出现基态磁结构与预期差异较大，此时可以在System模块中开启LogicTraj参数输出各个温度下的最终磁结构。结构文件会以xsf文件格式存储，将磁矩信息保存在XCrySDen原本受力分析的部分，可以用多种手段进行局部分析。获得磁结构在不同温度下的演变情况，为后续更多有趣的分析提供基础信息。

**structure\_20\_2.xsf:**

# [mtc] model = heisenberg model, temperature = 20.

CRYSTAL

PRIMVEC

350.51500798 0.00000000 0.00000000

-175.25802945 303.55459793 0.00000000

0.00000000 0.00000000 19.98660088

PRIMCOORD

20000 1

Cr 3.50518178 2.02367711 10.02407990 0.39413764 0.67030231 1.28271210

Cr -0.00004211 4.04741502 10.02407990 0.57297770 0.63862512 1.23038794

I 4.48427880 0.00000000 8.46272678 0.00000000 0.00000000 0.00000000

I -2.24214612 3.88349548 8.46272678 0.00000000 0.00000000 0.00000000

I 1.26300689 2.18759648 8.46272678 0.00000000 0.00000000 0.00000000

I -1.26192796 2.18571460 11.58803124 0.00000000 0.00000000 0.00000000

I 2.52384835 0.00000000 11.58803124 0.00000000 0.00000000 0.00000000

I 2.24321929 3.88537754 11.58803124 0.00000000 0.00000000 0.00000000

Cr 0.00002119 8.09476907 10.02407990 0.89226531 0.90881809 0.79240916

Cr -3.50520270 10.11850698 10.02407990 0.48380701 0.86074094 1.12918368

I 0.97911821 6.07109196 8.46272678 0.00000000 0.00000000 0.00000000

I -5.74730671 9.95458744 8.46272678 0.00000000 0.00000000 0.00000000

I -2.24215370 8.25868844 8.46272678 0.00000000 0.00000000 0.00000000

I -4.76708855 8.25680656 11.58803124 0.00000000 0.00000000 0.00000000

I -0.98131224 6.07109196 11.58803124 0.00000000 0.00000000 0.00000000

I -1.26194130 9.95646950 11.58803124 0.00000000 0.00000000 0.00000000

Cr -3.50513940 14.16586103 10.02407990 0.94410331 0.07278066 1.16334512

Cr -7.01036329 16.18959894 10.02407990 0.63502174 0.72526008 1.14923679

……

