A Short Tutorial on Using MuST

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What is MuST?

MuST stands for **Mu**ltiple **S**cattering **T**heory

- Multiple scattering theory is a method for solving the Kohn-Sham equation, which is an one-electron Schrödinger equation describing the electronic structure in solids
- Specifically, it calculate the Green function of the Kohn-Sham equation, and determine the electron density by taking the imaginary part of the Green function

MuST is a computational tool for *ab initio* electronic structure calculations

- So called *ab initio*, it implies that the electronic structure is determined based on fundamental physical law, which in this case is quantum mechanics, rather than on empirical models with adjustable parameters
- Other popular ab initio software packages include VASP, WIEN2K, ELK, Abinit, Quantum Espresso, etc., which are based on different methods (other than multiple scattering theory) for solving the Kohn-Sham equation.

Obtaining the package

```
$ git clone https://github.com/mstsuite/MuST
```

A directory called `MuST` is created in your local space

Take CuZn as an example

CuZn is also known as *brass*.

According to Wikipedia: Although forms of brass have been in use since prehistory, its true nature as a copper-zinc alloy was not understood until the post-medieval period.

Brass has long been a popular material for decoration for its bright gold-like appearance, e.g. for drawer pulls and doorknobs. It has also been widely used for all sorts of utensils due to many properties, such as low melting point, workability (both with hand tools and with modern turning and milling machines), durability, electrical and thermal conductivity.

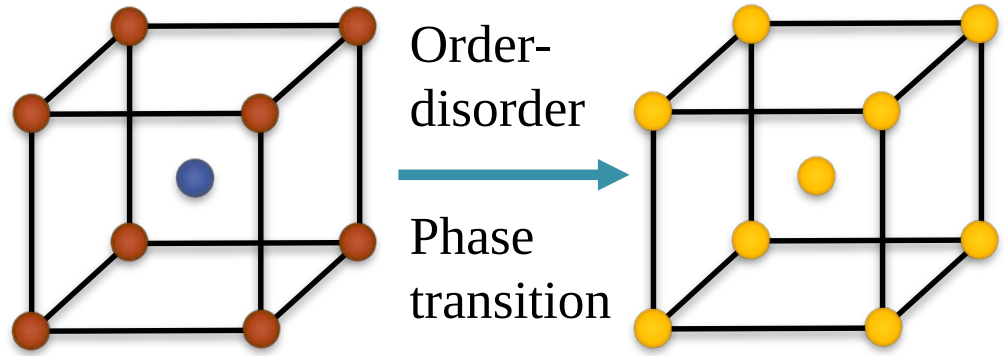
At zero temperature (T = 0 K), CuZn exists as an ordered intermetallic compound in B2 structure (β' phase). As T increases and reaches around 730 K, the materials becomes a random alloy in A2 structure (β phase).

T < 730 K

Cu:

Zn:

β' Phase (B2)



Order-disorder

Phase transition

T > 730 K

Cu/Zn:

β Phase (A2)

BCC structure

https://must-tutorial.com

Click Hub

Your username is your password

Your name	Username
	student1
	student2
	student3
	student4
	student5
	student6
	student7
	student8
	student9
	student10
	student11
	student12
	student13
	student14
	student15
	student16
	student17
	student18
	student19

A computational study of CuZn

The input data used in this tutorial can be found under "`MuST/Tutorials/CuZn`"

The computational tool is "`mst2`" can be found under "`MuST/bin`" or "`MuST/MST/bin`"

Three input files are required

- Description data: i_new.
- The system structure data: position.dat.
- Starting potential data for Cu and Zn: Cu_mt_v, Zn_mt_v

Running "`mst2`" on a number of CPU cores as follow:

```
$ mpirun -np #_CPU_cores MuST/bin/mst2 < i_new
```

replacing "`#_CPU_cores`" by a specific number

`MuST/Tutorials/CuZn/B2`

- CuZn in B2 structure (an ordered structure like CsCl) calculated with **KKR** method

`MuST/Tutorials/CuZn/BCC`

- CuZn random alloy in BCC structure (A2) calculated with **KKR-CPA** method

`MuST/Tutorials/CuZn/SuperCell`

- 16-atom super cell with 8 Cu and 8 Zn atoms placed on the underlying BCC lattice. **LSMS** method is used.

Running MuST on Jetstream via Jupyter Hub

What is Jetstream?

- Link: https://jetstream-cloud.org/
- A cloud-based computing environment that provides pre-configured virtual machines
- Jetstream can be accessed via Jupiter Hub, a multi-user version of Jupyter Notebook that enables team work on shared resources

A short YouTube video on running the CuZn examples

- https://www.youtube.com/watch?v=ev3nHISrs5Q

Steps to run the tutorial example under "`MuST/Tutorials/CuZn/B2`"

- Go to webpage: https://must-tutorial.com
- Click Hub shown on the top banner of the webpage
- Enter your username (`student1`, `student2`, …, or `student40`) and password
- Pull down the menu under New on the upper-right corner and click Terminal
- At the prompt in the new terminal, enter the following commands to run CuZn in the B2 structure:

```
$ cp -r /srv/Tutorials ~/
$ cd Tutorials/CuZn/B2
$ mpirun –n 4 mst2 < i_new
```

In the same way, you can run examples under `Tutorials/CuZn/BCC` and `Tutorials/CuZn/SuperCell`

An example of running KKR

An example under "MuST/Tutorials/CuZn/B2"

The data are in atomic units:
Length in Bohr radii, 1 a.u. = 0.529 Å
Energy in Rydberg, 1 Ryd = 13.6 eV

Description data: i_new

```
No. Atoms in System (> 0) :: 2
Atomic Position File Name :: position.dat
Default Potential Input File Name :: Cu_mt_v, Zn_mt_v
Method of SCF Calculation :: 2
  2. KKR
Default Lmax-T matrix     :: 3
Kx, Ky, Kz Division (> 0) :: 12  12  12
Potential Type (>= 0)     ::  0
     0. Muffin-tin
```

← Lines without "::" are treated as comment and are ignored

```
$ cd Tutorials/CuZn/B2
$ mpirun –n 4 mst2 < i_new
$ tail o_n00000_CuZn
```

Configuration data: position.dat

```
5.53
# Bravais lattice
    1.00000000000    0.00000000000    0.0000000000
    0.00000000000    1.00000000000    0.0000000000
    0.00000000000    0.00000000000    1.0000000000
# Atomic position
Cu  0.00000000000    0.00000000000    0.00000000000
Zn  0.50000000000    0.50000000000    0.50000000000
```

← A factor to be multiplied to the following data

← Lines starting with "#" are treated as comment

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An example of running KKR-CPA

An example found under "MuST/Tutorials/CuZn/BCC"

Description data: i_new

```
No. Atoms in System (> 0) :: 1
Atomic Position File Name :: position.dat
Default Potential Input File Name :: Cu_mt_v, Zn_mt_v
Method of SCF Calculation :: 3
          3. KKR-CPA
Default Lmax-T matrix     :: 3
Kx, Ky, Kz Division (> 0) :: 12  12  12
Potential Type (>= 0)     ::  0
     0. Muffin-tin
```

```
$ cd Tutorials/CuZn/BCC
$ mpirun –n 4 mst2 < i_new
$ more k_n00000_CuZn
```

Configuration data: position.dat

```
5.53
# Bravais lattice
 0.50000000000    0.50000000000   -0.5000000000
 0.50000000000   -0.50000000000    0.5000000000
-0.50000000000    0.50000000000    0.5000000000
# Atomic position
CPA  0.00000000000    0.00000000000    0.00000000000  Cu  0.50   Zn  0.50
```

Output file: k_n00000_CuZn

```
Source Code Version             : : v1.4.0
System Description              : CuZn random alloy, bcc structure
Number of Atoms in Unit Cell    : 1
Number of Atomic Species        : 1
Number of Atoms in Each Type    : 1(CPA)
Unit Cell Volume (au^3)         : 0.84556189D+02
Average Atomic Volume (au^3)    : 84.55619
Energy Offset                   : -3414
```

This is the number of "atom types"

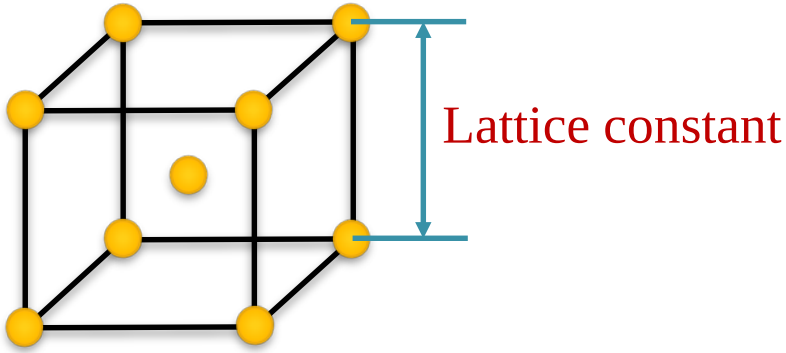
In the units of Rydberg

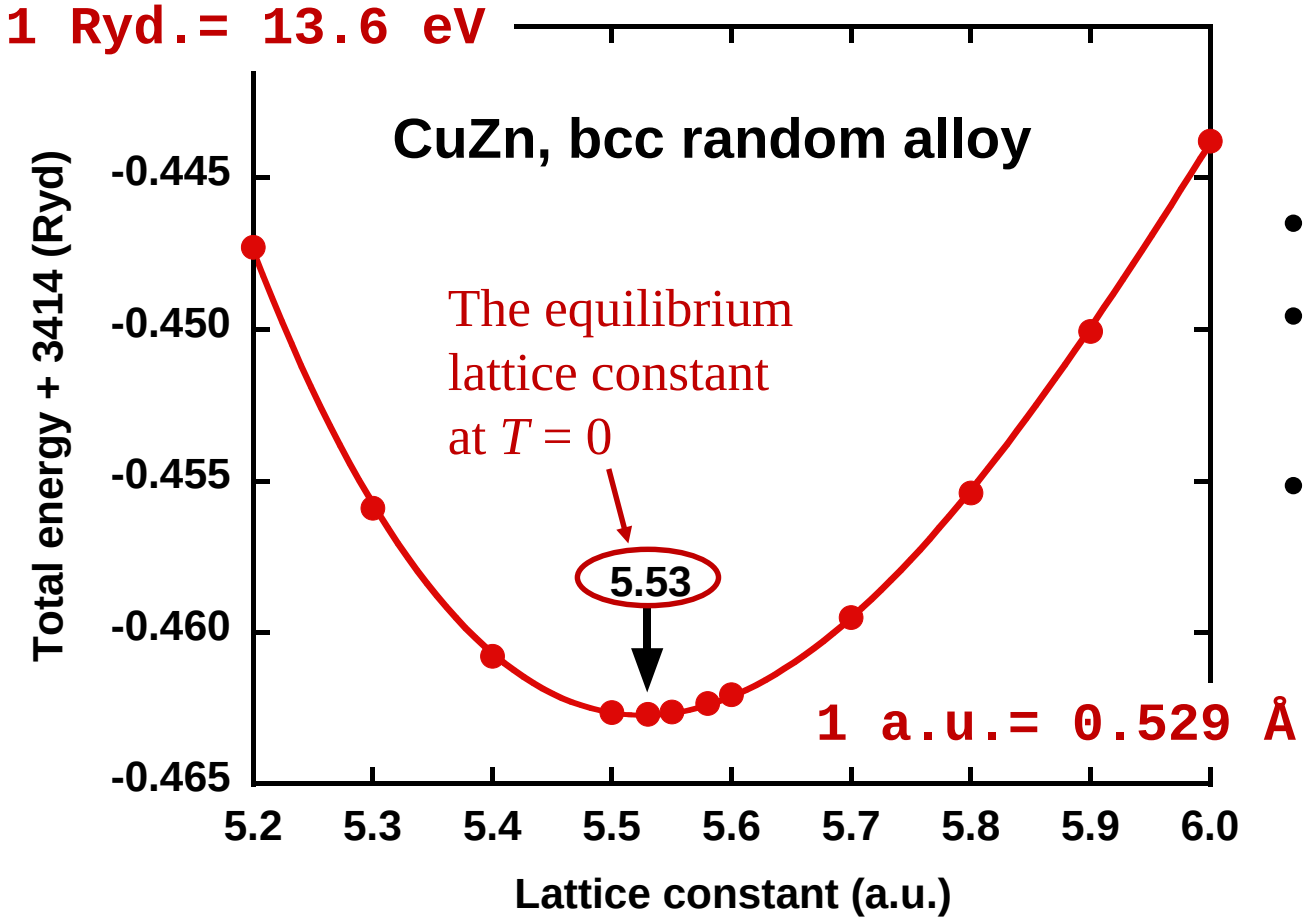
	Iter	Energy	3PV	Efermi	Rms_rho	Rms_pot	Mix	Alg	Alpha
**	1	-0.456493	0.11459	0.63849	0.163E-03	0.308E-01	pot	B	0.1000
	2	-0.460514	-0.17648	0.64229	0.244E-03	0.187E-01	pot	B	0.1000
	3	-0.461988	-0.26012	0.64443	0.133E-03	0.688E-02	pot	B	0.1000
	4	-0.462651	0.09343	0.64221	0.214E-03	0.168E-02	pot	B	0.1000
	5	-0.462625	-0.13011	0.64353	0.722E-04	0.127E-02	pot	B	0.1000
	6	-0.462672	-0.11879	0.64305	0.399E-04	0.508E-03	pot	B	0.1000
	7	-0.462692	-0.07019	0.64268	0.249E-04	0.169E-03	pot	B	0.1000
	8	-0.462693	-0.05639	0.64258	0.524E-05	0.780E-04	pot	B	0.1000
	9	-0.462691	-0.05746	0.64264	0.408E-05	0.807E-05	pot	B	0.1000
	10	-0.462691	-0.05643	0.64264	0.344E-06	0.261E-05	pot	B	0.1000
	11	-0.462692	-0.05659	0.64263	0.296E-06	0.193E-05	pot	B	0.1000
	12	-0.462692	-0.05660	0.64263	0.520E-08	0.180E-05	pot	B	0.1000
	13	-0.462692	-0.05676	0.64263	0.664E-07	0.419E-06	pot	B	0.1000
	14	-0.462692	-0.05663	0.64263	0.471E-07	0.141E-05	pot	B	0.1000
	15	-0.462692	-0.05687	0.64263	0.859E-07	0.460E-06	pot	B	
	16	-0.462692	-0.05682	0.64263	0.177E-07	0.840E-07	pot	B	
	17	-0.462692	-0.05681	0.64263	0.190E-08	0.306E-07	pot	B	

It took 17 iterations to converge

Total energy per atom
= -3414.462692 Rydberg

A plot of the total energy versus the lattice constant





What we can learn from the total energy results

- Equilibrium crystal structure at $T = 0$
- Equilibrium lattice constant of the crystal structure at $T = 0$
- Mechanical properties of the alloy
  - Faster (slower) increase in energy when the lattice is stretched or compressed from its equilibrium state is an indication of harder (softer) material

An example of running LSMS

An supercell example found under "MuST/Tutorials/CuZn/SuperCell"

Description data: i_new

```
No. Atoms in System (> 0) :: 16
Method of SCF Calculation :: 1
    1. LSMS
Default LIZ Cutoff Radius :: 12.1
```

Given only 4 cores available to run the job, change this number from 12.1 to 8.0, so to reduce the computing time

This will result a LIZ cluster with 89 atoms

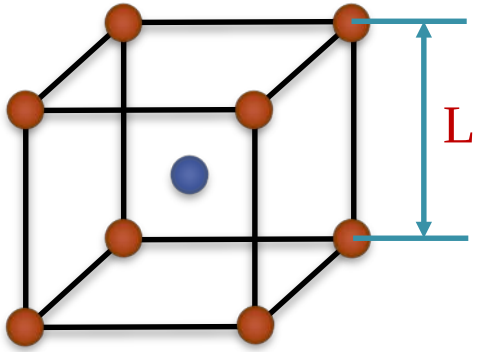
16 atoms in total:
8 Cu atoms + 8 Zn atoms

```
$ cd Tutorials/CuZn/SuperCell
$ mpirun –n 4 mst2 < i_new
```

Configuration data: position.dat

```
5.53
 2.00000000000      0.00000000000      0.00000000000
 0.00000000000      2.00000000000      0.00000000000
 0.00000000000      0.00000000000      2.00000000000
# Atomic position
   Cu         0.00000000000      1.00000000000      1.00000000000
   Cu         0.00000000000      1.00000000000      0.00000000000
   Cu         1.50000000000      0.50000000000      0.50000000000
   Cu         0.50000000000      1.50000000000      1.50000000000
   Cu         1.50000000000      0.50000000000      1.50000000000
   Cu         1.00000000000      0.00000000000      1.00000000000
   Cu         0.00000000000      0.00000000000      0.00000000000
   Cu         0.00000000000      0.00000000000      1.00000000000
   Zn         1.00000000000      1.00000000000      0.00000000000
   Zn         0.50000000000      1.50000000000      0.50000000000
   Zn         1.00000000000      0.00000000000      0.00000000000
   Zn         0.50000000000      0.50000000000      1.50000000000
   Zn         1.50000000000      1.50000000000      1.50000000000
   Zn         1.00000000000      1.00000000000      1.00000000000
   Zn         1.50000000000      1.50000000000      0.50000000000
   Zn         0.50000000000      0.50000000000      0.50000000000
```

The total energy of three different CuZn alloy structures



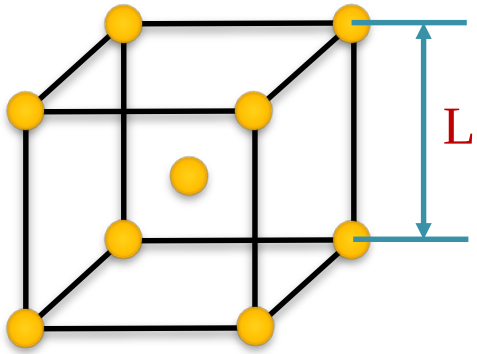
Lattice constant = 5.53 a.u.

Cu:

Zn:

Total energy per atom = -3414.468452 Ryd.

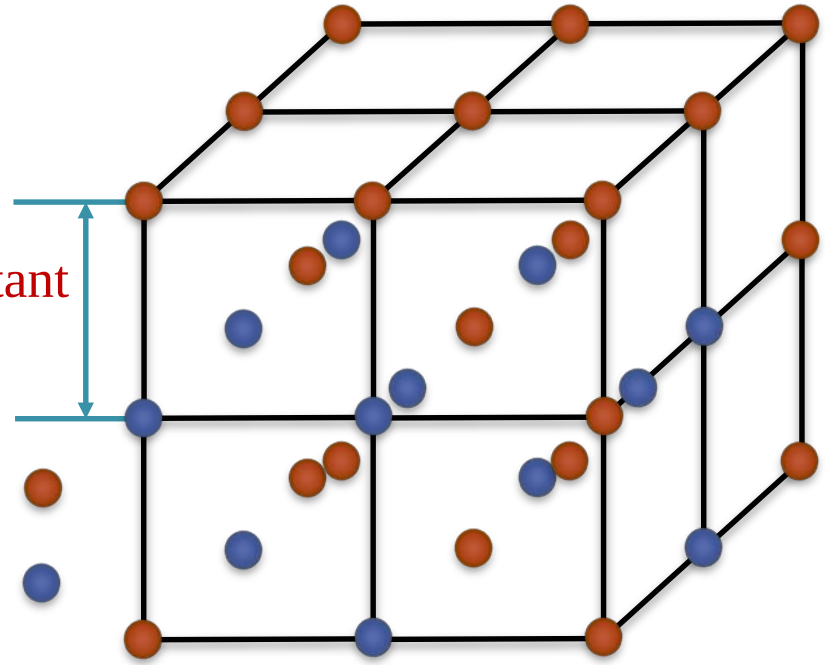
Using this energy difference (ΔE = 0.0058 Ryd = 0.0789 eV), we may estimate the transition temperature in a naive way as follows:
$T_C = \Delta E / k_B \approx \Delta E \cdot 300\ \text{K}/(0.025\ \text{eV}) = 946.6\ \text{K}$



Lattice constant = 5.53 a.u.

Cu/Zn:

Total energy per atom = -3414.462692 Ryd.



Lattice constant
= 5.53 a.u.

8 Cu:

8 Zn:

Total energy per atom = -3414.463548 Ryd.

At T = 0, CuZn prefers an ordered structure

- The ordered B2 compound has the lowest energy
- The completely random structure (A2) has the highest energy among the 3 given structures