

# HTEM user manual

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# 1 How to install HTEM

```
1 | tar -zvxf HTEM.tar.gz
2 | cd HTEM
3 | **You should modified the the vasp.config and HTEM_slurm_sub.sh files
   first!**
4 | pip install .
```

**vasp.config:** POTCAR path for VASP and cores for slurm script.

```
1 | path_PBE=/public1/home/xxxx/PBE
2 | cores=96
```

**HTEM\_slurm\_sub.sh:** script for sbatch vasp jobs.

```
1 | #!/bin/bash
2 | #SBATCH -N 1
3 | #SBATCH -n 96
4 |
5 | mpirun vasp_std
```

# 2 Runstyle and Script

## 2.1 Runstyle introduction

**gen:** Generate KPOINT files and INCAR files .

```
1 | 1.1 HTEM gen -k 2,2,2 -encut 400 -sigma 0.2 -T 0 -P 0,10,11 -mode cold
2 | 1.2 HTEM gen -k 2,2,2 -encut 400 -sigma 0.2 -mode QSA -in state.in
3 | 1.3 HTEM gen -k 2,2,2 -encut 400 -mode NVT -in state.in
4 | 1.4 HTEM gen -k 2,2,2 -encut 400 -T 300,1200,4 -P 0,10,3 -mode NPT
```

**create:** Generate KPOINT files and INCAR files .

```
1 | 2 HTEM create
```

**strain:** Generate KPOINT files and INCAR files .

```
1 | 3.1 HTEM strain -ms 0.02 -ns 9 -mthd Energy
2 | 3.2 HTEM strain -ms 0.02 -ns 8 -mthd Stress
```

**strain calculation prepare:** Generate KPOINT files and INCAR files .

```
1 | 4.1 HTEM relax2
2 | 4.2 HTEM static
3 | 4.3 HTEM NVT
4 | 4.4 HTEM NPT
```

**get\_results:** Generate KPOINT files and INCAR files .

```
1 | 5 HTEM get_results
```

**model:** Generate KPOINT files and INCAR files .

```
1 | 6 HTEM model -T0 0 -Tr 0,1200,121 -Pr 0,10,11 -plt png -weight 1.6 -read  
Elasticity_T.dat
```

**anisotropy:** Generate KPOINT files and INCAR files .

```
1 | 7.1 HTEM anisotropy -modulus B -plt png -read Elasticity_T.dat  
2 | 7.2 HTEM anisotropy -modulus gif
```

**update:** Generate KPOINT files and INCAR files .

```
1 | HTEM update -up CONTCAR  
2 | HTEM update -up NPT
```

## 2.2 Script tool

Some scripts are in the *script\_tools* folder.

**job\_sbatches.sh:** Automatic sub calculations for relax1, relax2, static, NVT, NPT calculation with command as follows:

```
1 | job_sbatches.sh relax1/relax2/static/NVT/NPT
```

# 3 Introduction to input and output files

## 3.1 Input file

**POSCAR:** The initial input structure for VASP, essential input for HTEM.

**state.in:** The file contain thermal states information. This file can be automatically generated for -mode cold/NPT. This file is also essential for -mode QSA/NVT. If you want to calculate isentropic elasticity, the specific heat  $C_P$  and linear thermal expansion coefficient  $\alpha_i$  are necessary.

example for lattice=C:

	T(K)	v(angstrom^3/atom)	P(GPa)	rho(g/cm^3)	Cp(J/mol/K)
1	alpha_1(/K)				
2	600.0000	20.1758	0.0000	2.2207	0.0000
	0.0000				
3	1200.0000	20.2880	0.0000	2.2084	0.0000
	0.0000				

example for lattice =H/TI/TII/RI/RII,

	T(K)	v(angstrom^3/atom)	P(GPa)	rho(g/cm^3)	Cp(J/mol/K)
1	alpha_1(/K)		alpha_2(/K)		
2	600.0000	20.1758	0.0000	2.2207	0.0000
	0.0000	0.0000			
3	1200.0000	20.2880	0.0000	2.2084	0.0000
	0.0000	0.0000			

example for lattice =O/M/N,

	T(K)	v(angstrom^3/atom)	P(GPa)	rho(g/cm^3)	Cp(J/mol/K)
1	alpha_1(/K)		alpha_2(/K)	alpha_3(/K)	
2	600.0000	20.1758	0.0000	2.2207	0.0000
	0.0000	0.0000	0.0000		
3	1200.0000	20.2880	0.0000	2.2084	0.0000
	0.0000	0.0000	0.0000		

**config:** The file contain config information. Can automatically save essential command information. You can also use this file to replace optional inputs for command.

```
1 lattice = C
2 sgn = 227
3 M = 28.085000000000022
4 mode = cold
5 encut = 400
6 sigma = 0.2
7 MLFF = False
8 ksetting = [2, 2, 2]
9 pressure = [0.0, 10.0, 11]
10 temperature = 0.0
11 natom = 64
12 nstrain = 8
13 maxstrain = 0.02
14 method = stress
```

```
15 | inputfile = state_new.in  
16 | nstate = 11  
17 | upmode = CONTCAR  
18 | forder = 2
```

The following files can automatically be generated using **HTEM gen**, you can also modified them after **HTEM gen!!!**

**POTCAR:** POTCAR file for VASP input.

**INCAR.relax1:** INCAR file for **command 2** to relax the initial structures at different states. ISIF = 4 for relax lattices and atomic positions at constant volume. ISIF = 3 for relax lattices and atomic positions at constant pressure.

**INCAR.relax2:** INCAR file for **command 4.1** to relax the strained structures.

**INCAR.static:** INCAR file for **command 4.2** to perform SCF for the strained structures.

**INCAR.NVT:** INCAR file for **command 4.3** to perform NVT simulations for the strained structures.

**INCAR.NPT:** INCAR file for **command 4.4** to perform NPT simulations at specific states.

## 3.2 Output file

**Elasticity\_T.dat:** The isothermal elasticity files.

**Elasticity\_S.dat:** The isentropic elasticity files.

**figures/model/Elasticity\_T\_model.dat:** The modeled isothermal elasticity.

**figures/model/Elasticity\_S\_model.dat:** The modeled isentropic elasticity.

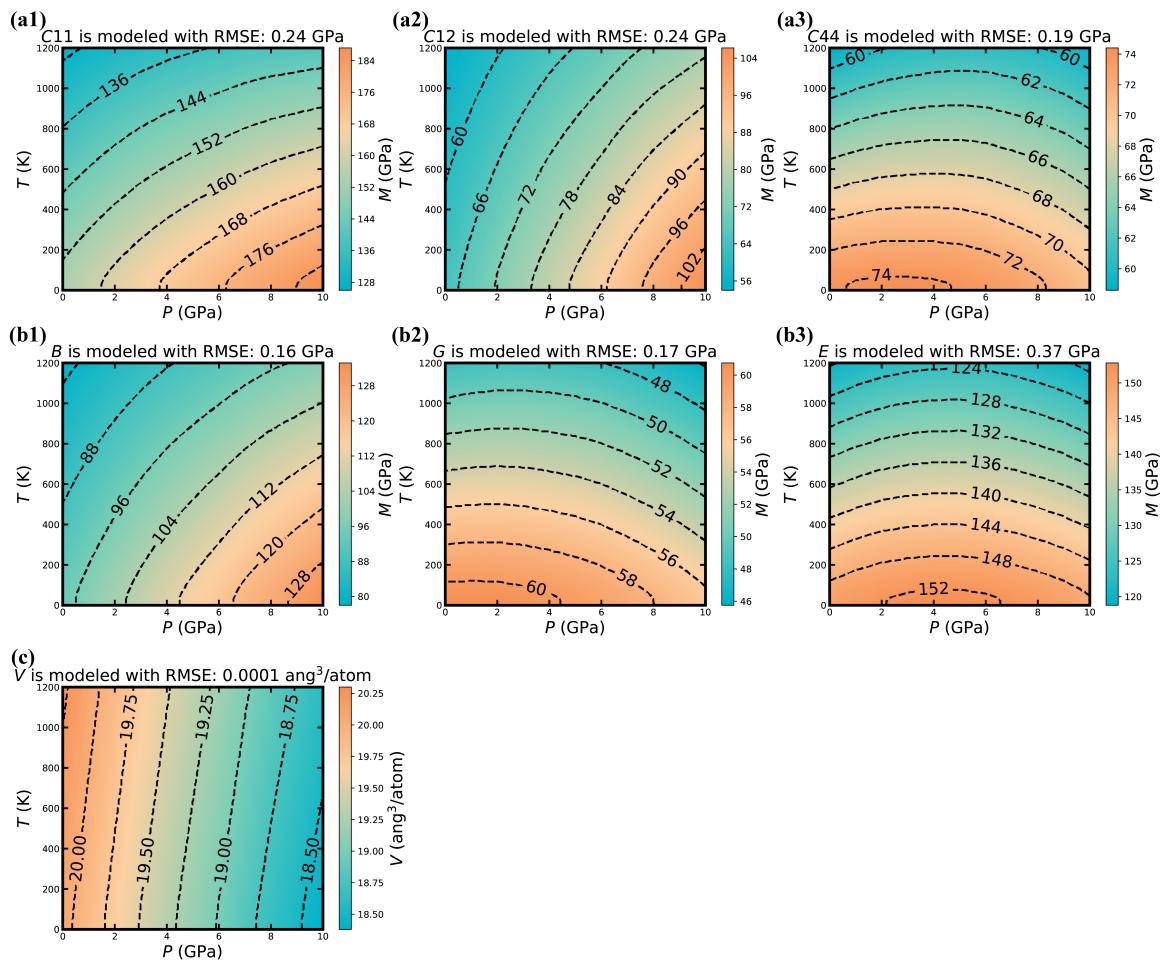
**figures/model/Elasticity\_model.dat:** The modeled elasticity using external input.

**figures/model/Elasticity\_T\_model\_cal.dat:** The elasticity calculated by using isothermal modeled elasticity.

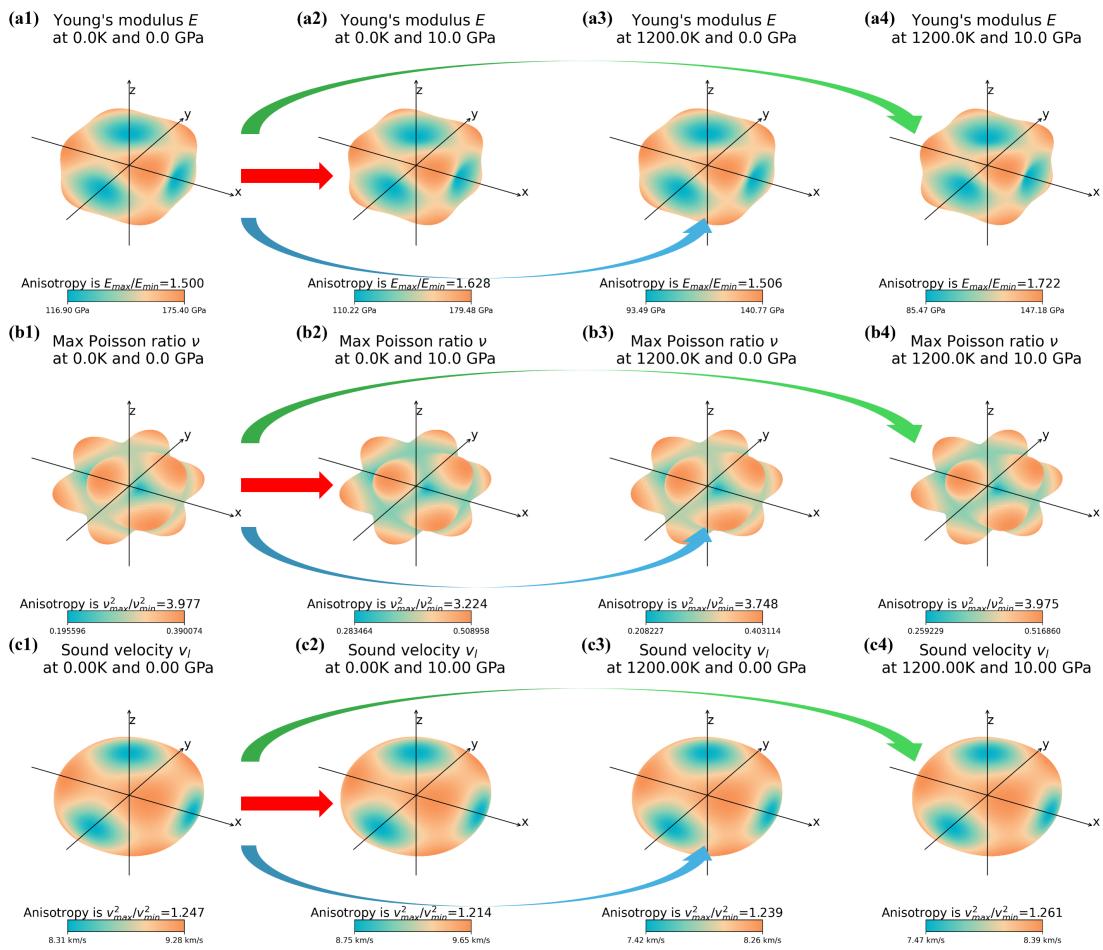
**figures/model/Elasticity\_S\_model\_cal.dat:** The elasticity calculated by using isentropic modeled elasticity.

**figures/model/Elasticity\_model\_cal.dat:** The elasticity calculated by using modeled elasticity.

**figures/anisotropy/{Cij/B/G/E/V}\_{\_T/\_S/ }.{eps/png}:** The file of modeled elasticity **Cij/ B/ G/ E/ V** for **\_T(isothermal) / \_S(isentropic)/ (external input)** with type **{png/eps}**.



**figures/anisotropy/{B/E/G\_min/G\_max/G\_average/v\_min/v\_max/v\_average/v\_l/v\_s1/v\_2}**  
 $\{\text{T/S}\}_{\{\text{num}\}}.\{\text{png/eps/dat}\}$ : The anisotropy file of **B / E / G\_min / G\_max / G\_average / v\_min / v\_max / v\_average / v\_l / v\_s1 / v\_2** for **\_T(isothermal) / \_S(isentropic) / (external input)** at state **{num}** with type **{png/eps/dat}**.



**figures/anisotropy/{B/E/G\_min/G\_max/G\_average/v\_min/v\_max/v\_average/v\_l/v\_s1/v\_2}\_{T/S}.gif:** The anisotropy process file of **B / E / G\_min / G\_max / G\_average / v\_min / v\_max / v\_average / v\_l / v\_s1 / v\_2** for **\_T(isothermal) / \_S(isentropic)/ (external input).**

## 4. Command option

```
1 usage: HTEM [-h] [-mode cold/QSA/NVT/NPT] [-k 0.1/4,4,4] [-T 300/300,500,3]
2 [-P 0/0,10,3] [-lt C/H/TI/TII/RI/RII/O/M/N] [-in state.in] [-e 500] [-s
3 0.20] [-M M] [-na NATOM] [-sgn SGN] [-MLFF True/False] [-mthd Energy/Stress]
4 [-ns 9] [-forder 3/2] [-ms 0.02] [-nstate NSTATE] [-plt False/png/eps] [-
5 read file] [-modulus B/G/E/v/sound/gif] [-T0 0] [-Tr 0,2000,101] [-Pr
6 0,10,101] [-weight 2] [-up CONTCAR/NPT] runstyle
7
8 HTEM: High-throughput Toolkits for Elasticity Modeling
9
10 optional arguments:
11   -h, --help            show this help message and exit
12
13 Basic Parameters:
14   runstyle              one of arguments in ['create', 'strain', 'relax2',
15   'static', 'NPT', 'NVT', 'get_results', 'anisotropy', 'gen', 'model',
16   'update'] should be input
17   -mode cold/QSA/NVT/NPT
18                   Choose the calculation mode: cold, QSA, NVT, NPT
19
20 Parameters for automatically generate input files for HTEM:
21   -k 0.1/4,4,4 , --ksetting 0.1/4,4,4
22                   KSPACING or KMESH, eg. 0.1 for KSPACING or 4,4,4 for
23 KMESH
24   -T 300/300,500,3 , --temperature 300/300,500,3
25                   Temperature of the system, unit K, eg. 300 for 300K
26 or 300,500,3 for 300-500K with 3 points and 100K step size
27   -P 0/0,10,3 , --pressure 0/0,10,3
28                   Pressure of the system, unit GPa, eg. 0 for 0GPa or
29 0,10,3 for 0-10GPa with 3 points and 5GPa step size
30   -lt C/H/TI/TII/RI/RII/O/M/N, --lattice C/H/TI/TII/RI/RII/O/M/N
31                   Choose the lattice type: C, H, TI, TII, RI, RII, O,
32 M, N, can be read from POSCAR
33   -in state.in, --inputfile state.in
34                   Name of input file
35   -e 500, --encut 500 ENCUT of INCAR file
36   -s 0.20, --sigma 0.20
37                   SIGMA of INCAR file, 0.05~0.30
38   -M M, --M M          Averaged atomic mass, can be read from POSCAR
39   -na NATOM, --natom NATOM
40                   The number of atoms of POSCAR, can be read from
41 POSCAR
42   -sgn SGN             Space Group Number in 1~229, can be read from POSCAR
43   -MLFF True/False, --MLFF True/False
44                   Choose the MLFF mode for INCAR file: True, False
45
46 Parameters related to the calculation method:
47   -mthd Energy/Stress, --method Energy/Stress
48                   Choose the calculation method: Energy, Stress.
49 Energy is only supported by mode cold and QSA
50   -ns 9, --nstrain 9    Number of strained structures for each strain.
51   -forder 3/2           Fitting order of solution: default 3 for Strain-
52 Energy and 2 for Strain-Stress
53   -ms 0.02, --maxstrain 0.02
54                   Max strain, eg. 0.01~0.05
```

```
41 -nstate NSTATE, --nstate NSTATE
42                                     The number of calculated states, can be read from
43 inputFile
44
45 Plot Parameters:
46 -plt False/png/eps     Choose the plot mode: False, png, eps
47 -read file, --read_file file
48                                     Read the elasticity data from the file
49
50 Anisotropy Parameters:
51 -modulus B/G/E/v/sound/gif, --modulus B/G/E/v/sound/gif
52                                     Choose the modulus to calculate the anisotropy: B,
53 G, E, v, sound. This parameter is for mode plot
54
55 Model Parameters:
56 -T0 0, --T_ref 0      The reference temperature for SAM
57 -Tr 0,2000,101 , --T_range 0,2000,101
58                                     Temperature range for SAM elasticity modeling, eg.
59 0,2000,101 for 0-2000K with 101 points and 20K step size
60 -Pr 0,10,101 , --P_range 0,10,101
61                                     Pressure range for SAM elasticity modeling, eg.
62 0,10,101 for 0-10GPa with 101 points and 0.1GPa step size
63 -weight 2              The weight coefficient of SAM, please set it between
64 1 and 2
65
66 Update state files parameters:
67 -up CONTCAR/NPT, --upmode CONTCAR/NPT
68                                     Update the inputFile's volume and density for each
69 state, eg. for state.in', two mode: CONTCAR, NPT
```

## 5. Templates

One can using **command run's run steps** as a script to automatically calculation or using **run with config's run steps** as a script with the **config** file. If you want to read information from POSCAR, you should delete **lattice**, **sgn**, **M** from **config** file.

### 5.1 cold calculation at 0 GPa

#### 5.1.1 command run

**run steps:**

```
1 HTEM gen -k 0.1 -e 400 -s 0.2 -T 0 -P 0 -mode cold
2 HTEM create
3 job_sbash.sh relax1
4 HTEM strain -ms 0.02 -ns 8 -mthd Stress
5 HTEM relax2
6 job_sbash.sh relax2
7 HTEM static
8 job_sbash.sh static
9 HTEM update -up CONTCAR
10 HTEM get_results
```

#### 5.1.2 run with config

**config file:**

```
1 lattice = C
2 sgn = 227
3 M = 28.0850000000000022
4 mode = cold
5 encut = 400
6 sigma = 0.2
7 ksetting = 0.1
8 pressure = 0
9 temperature = 0.0
10 nstrain = 9
11 maxstrain = 0.02
12 method = Energy
13 inputfile = state.in
14 nstate = 1
15 upmode = CONTCAR
16 forder = 2
```

**run steps:**

```
1 HTEM gen
2 HTEM create
3 job_sbatch.sh relax1
4 HTEM strain
5 HTEM relax2
6 job_sbatch.sh relax2
7 HTEM static
8 job_sbatch.sh static
9 HTEM update
10 HTEM get_results
```

## 5.2 cold calculation

**input file:** Supercell **POSCAR** for Si with 64 atoms.

### 5.2.1 command run

**run steps:**

```
1 HTEM gen -k 2,2,2 -e 400 -s 0.2 -T 0 -P 0,10,11 -mode cold
2 HTEM create
3 job_sbatch.sh relax1
4 HTEM strain -ms 0.02 -ns 8 -mthd stress
5 HTEM relax2
6 job_sbatch.sh relax2
7 HTEM update -up CONTCAR
8 HTEM get_results
```

### 5.2.2 run with config

**config file:**

```
1 lattice = C
2 sgn = 227
3 M = 28.0850000000000022
4 mode = cold
5 encut = 400
6 sigma = 0.2
7 ksetting = [2, 2, 2]
8 pressure = [0.0, 10.0, 11]
9 temperature = 0.0
10 natom = 64
11 nstrain = 8
12 maxstrain = 0.02
13 method = Stress
14 inputfile = state.in
15 nstate = 11
16 upmode = CONTCAR
17 forder = 2
```

**run steps:**

```
1 HTEM gen
2 HTEM create
3 job_sbatch.sh relax1
4 HTEM strain
5 HTEM relax2
6 job_sbatch.sh relax2
7 HTEM update
8 HTEM get_results
```

## 5.3 NPT calculation

**input file:** Supercell **POSCAR** for Si with 64 atoms.

### 5.3.1 command run

**run steps:**

```
1 HTEM gen -k 2,2,2 -e 400 -T 300,1200,4 -P 0,10,3 -mode NPT
2 HTEM create
3 HTEM strain -ms 0.03 -mthd Stress
4 HTEM NPT
5 job_sbatch.sh NPT
6 HTEM update -up NPT
7 HTEM get_results
```

### 5.3.2 run with config

**config file:**

```
1 lattice = C
2 sgn = 227
3 M = 28.085000000000022
4 mode = NPT
5 encut = 400
6 sigma = 0.2
7 MLFF = False
8 ksetting = [2, 2, 2]
9 pressure = [0.0, 10.0, 3]
10 temperature = [300.0, 1200.0, 4]
11 natom = 64
12 method = Stress
13 inputfile = state.in
14 nstate = 12
15 maxstrain = 0.03
16 upmode = NPT
17 forder = 2
```

**run steps:**

```
1 HTEM gen
2 HTEM create
3 HTEM strain
4 HTEM NPT
5 job_sbatch.sh NPT
6 HTEM update
7 HTEM get_results
```

## 5.4 QSA calculation

**input file:** Supercell **POSCAR** for Si with 64 atoms. States in **state.in** file will be calculated.

### 5.4.1 command run

**run steps:**

```
1 HTEM gen -k 2,2,2 -e 400 -s 0.2 -mode QSA -in state.in
2 HTEM create
3 job_sbatch.sh relax1
4 HTEM strain -ms 0.02 -ns 8 -mthd stress
5 HTEM relax2
6 job_sbatch.sh relax2
7 HTEM get_results
```

### 5.4.2 run with config

**config file:**

```
1 lattice = C
2 sgn = 227
3 M = 28.085000000000022
4 mode = QSA
5 encut = 400
6 sigma = 0.2
7 ksetting = [2, 2, 2]
8 natom = 64
9 nstrain = 8
10 maxstrain = 0.02
11 method = Stress
12 inputfile = state.in
13 forder = 2
```

**run steps:**

```
1 HTEM gen
2 HTEM create
3 job_sbatch.sh relax1
4 HTEM strain
5 HTEM relax2
6 job_sbatch.sh relax2
7 HTEM get_results
```

## 5.5 NVT calculation

**input file:** Supercell **POSCAR** for Si with 64 atoms. States in **state.in** file will be calculated.

### 5.5.1 command run

**run steps:**

```
1 HTEM gen -k 2,2,2 -e 400 -mode NVT -in state.in
2 HTEM create
3 HTEM strain -ms 0.02 -ns 4 -mthd Stress
4 HTEM NVT
5 job_sbatch.sh NVT
6 HTEM get_results
```

### 5.5.2 run with config

**config file:**

```
1 lattice = C
2 sgn = 227
3 M = 28.0850000000000022
4 mode = cold
5 encut = 400
6 sigma = 0.2
7 MLFF = False
8 ksetting = [2, 2, 2]
9 natom = 64
10 nstrain = 4
11 maxstrain = 0.02
12 method = Stress
13 inputfile = state.in
14 forder = 2
```

**run steps:**

```
1 HTEM gen
2 HTEM create
3 HTEM strain
4 HTEM NVT
5 job_sbatch.sh NVT
6 HTEM get_results
```

## 5.6 model results

**input file:** Supercell **POSCAR** for Si with 64 atoms. Elasticity file such as **Elasticity\_T.dat**. One can combine **cold's** results with **other modes'** results in one elasticity file than model results.

### 5.6.1 command run

**run steps:**

```
1 | HTEM model -T0 0 -Tr 0,1200,121 -Pr 0,10,11 -plt png -weight 2 -read  
Elasticity_T.dat
```

### 5.6.2 run with config

**config:**

```
1 | sgn = 227  
2 | natom = 64  
3 | M = 28.085000000000022  
4 | weight = 2  
5 | T_ref = 0.0  
6 | read_file = Elasticity_T.dat  
7 | plt = png
```

**run steps:**

```
1 | HTEM model
```

If the average atomic mass of **POSCAR** is not proper your system, you can also modified the **M** of **config!!!** Especially for using external input elasticity to perform this step!!!

## 5.7 model results

**input file:** Supercell **POSCAR** for Si with 64 atoms. Elasticity file such as **Elasticity\_T.dat**. One can also use model's results **figures/model/Elasticity\_model\_cal.dat** as input or **select** some states' elasticity to combine a new file as input.

### 5.7.1 command run

**run steps:**

```
1 HTEM anisotropy -modulus B -plt png -read Elasticity_T.dat
2 HTEM anisotropy -modulus E -plt png -read Elasticity_T.dat
3 HTEM anisotropy -modulus G -plt png -read Elasticity_T.dat
4 HTEM anisotropy -modulus v -plt png -read Elasticity_T.dat
5 HTEM anisotropy -modulus sound -plt png -read Elasticity_T.dat
6 HTEM anisotropy -modulus gif
```

### 5.7.2 run with config

**config:**

```
1 sgn = 227
2 natom = 64
3 M = 28.085000000000022
4 read_file = Elasticity_T.dat
5 plt = png
```

**run steps:**

```
1 HTEM anisotropy -modulus B
2 HTEM anisotropy -modulus E
3 HTEM anisotropy -modulus G
4 HTEM anisotropy -modulus v
5 HTEM anisotropy -modulus sound
6 HTEM anisotropy -modulus gif
```

If the average atomic mass of **POSCAR** is not proper your system, you can also modified the **M** of **config!!!** Especially for using external input elasticity to perform this step!!!

Especially for using external input elasticity to perform this step!!!==

## **6. Examples**

---

The follows are examples in directory **example**, all these examples can run with the script **HTEM\_run.sh**. The input and output files can be seen from the previous introduction for details.

### **6.1 Cubic\_Diamond**

Cold calculation for cubic diamond.

### **6.2 model**

Si's elasticity modeling at 0-10 GPa and 0-1200 K.

### **6.3 anistropy**

Si's anisotropy analysis for isobar, isothermal and 0K0GPa\_1200K10GPa.

### **6.4 NVT**

Si's elasticity calculations with NVT modes at 0 GPa and 600K and 1200K.

### **6.5 NPT**

Si's elasticity calculations with NPT modes at 8 GPa and 600K and 1200K.