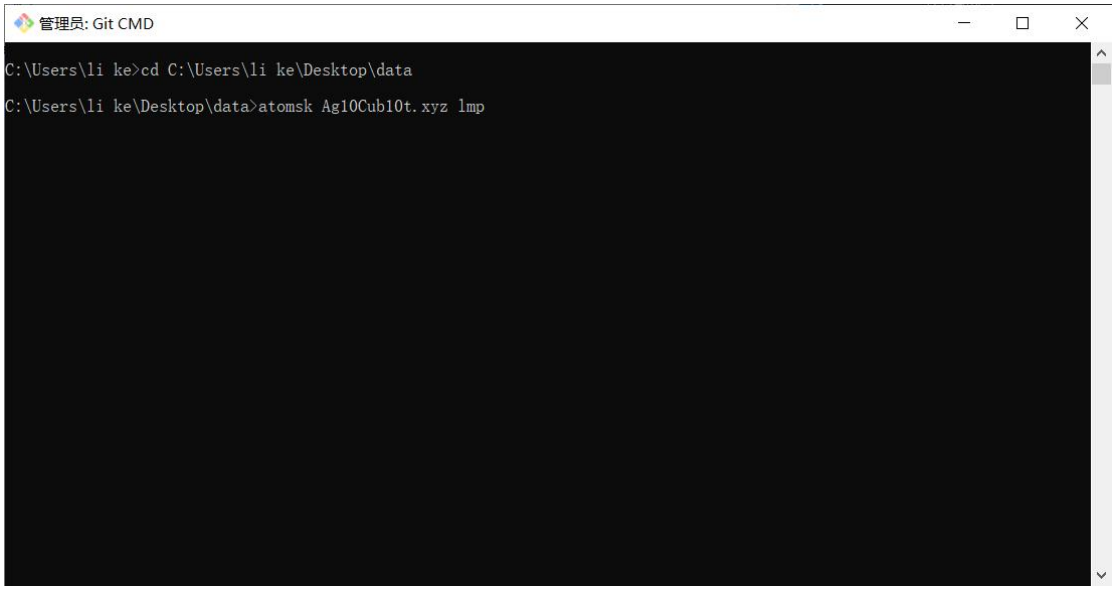
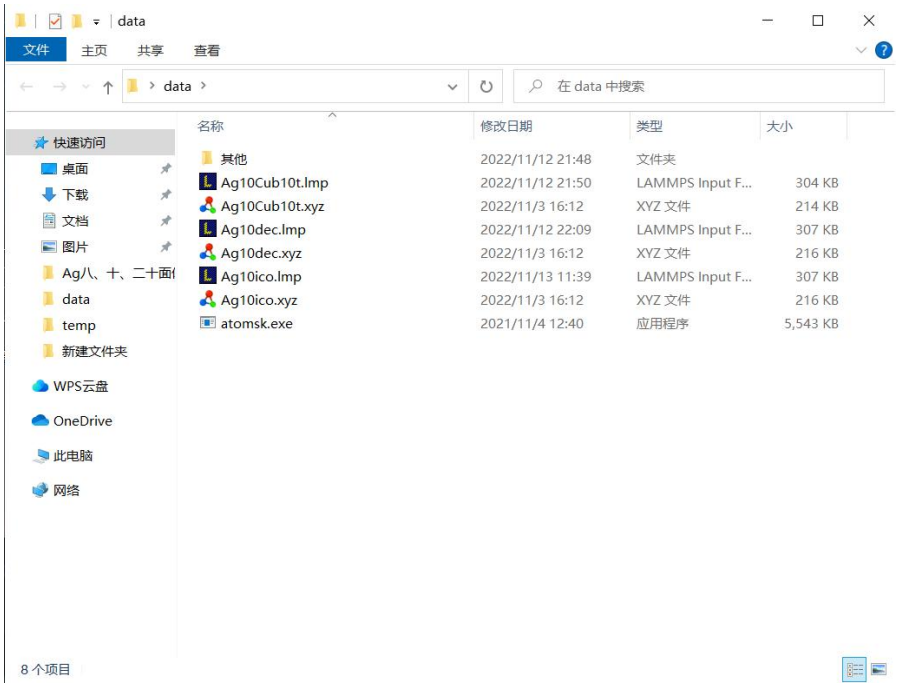
打开 atomsk.exe 所在文件夹

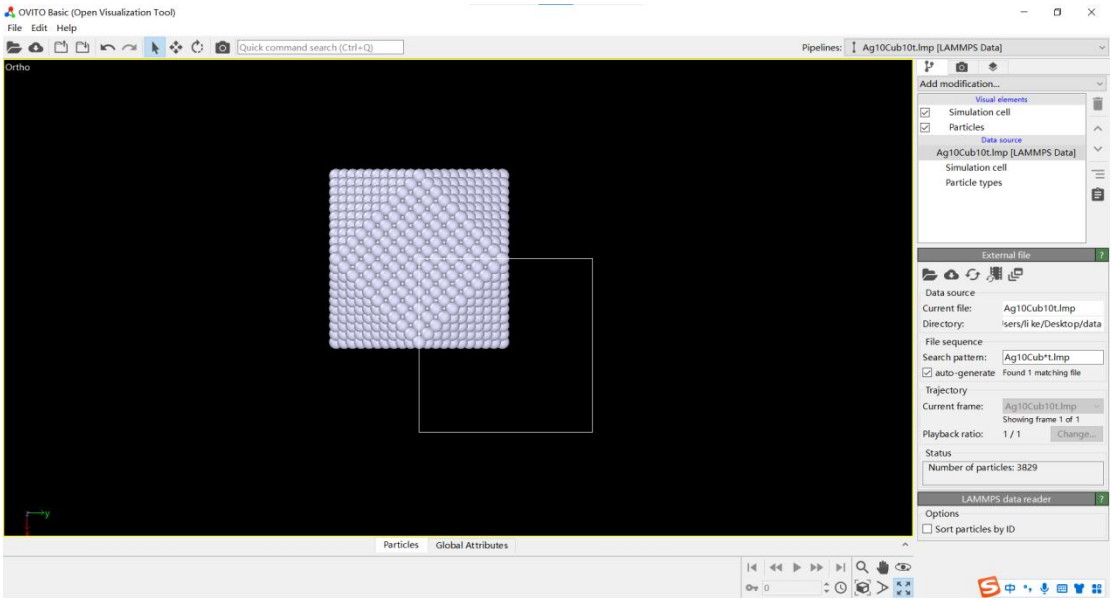
把 Ag10Cub10t.xyz 放到上述文件夹中

输入命令　把 xyz 格式转化成 lmp 格式



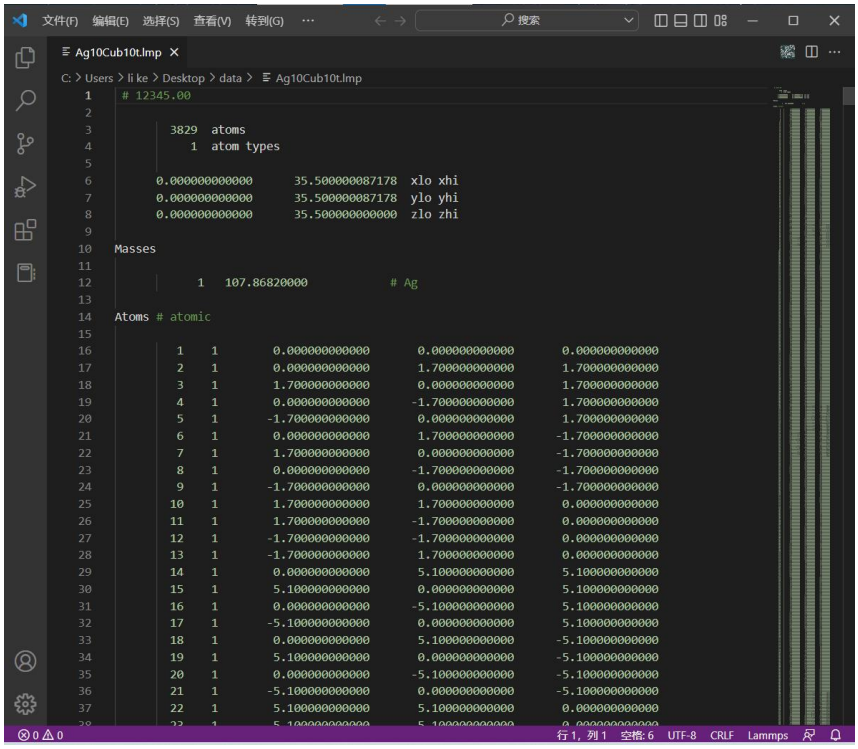


打开文件后发现模型没有位于中心位置

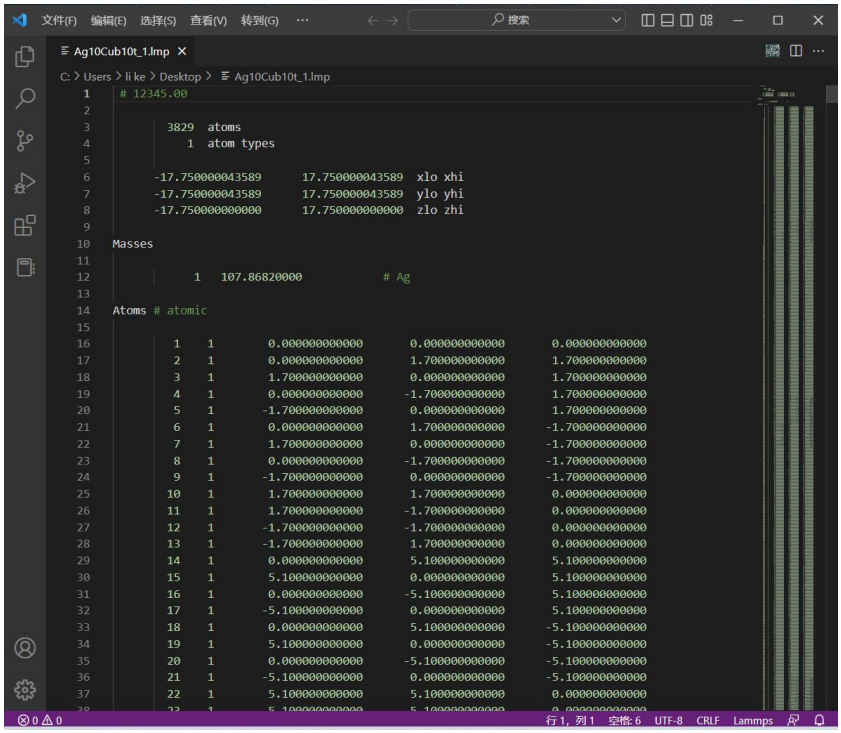


修改文件坐标

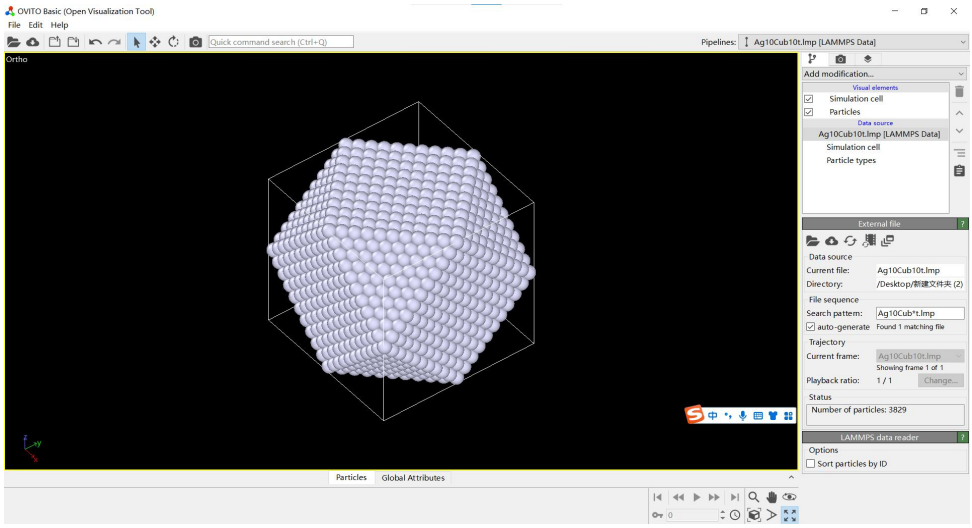
修改前的坐标如下图



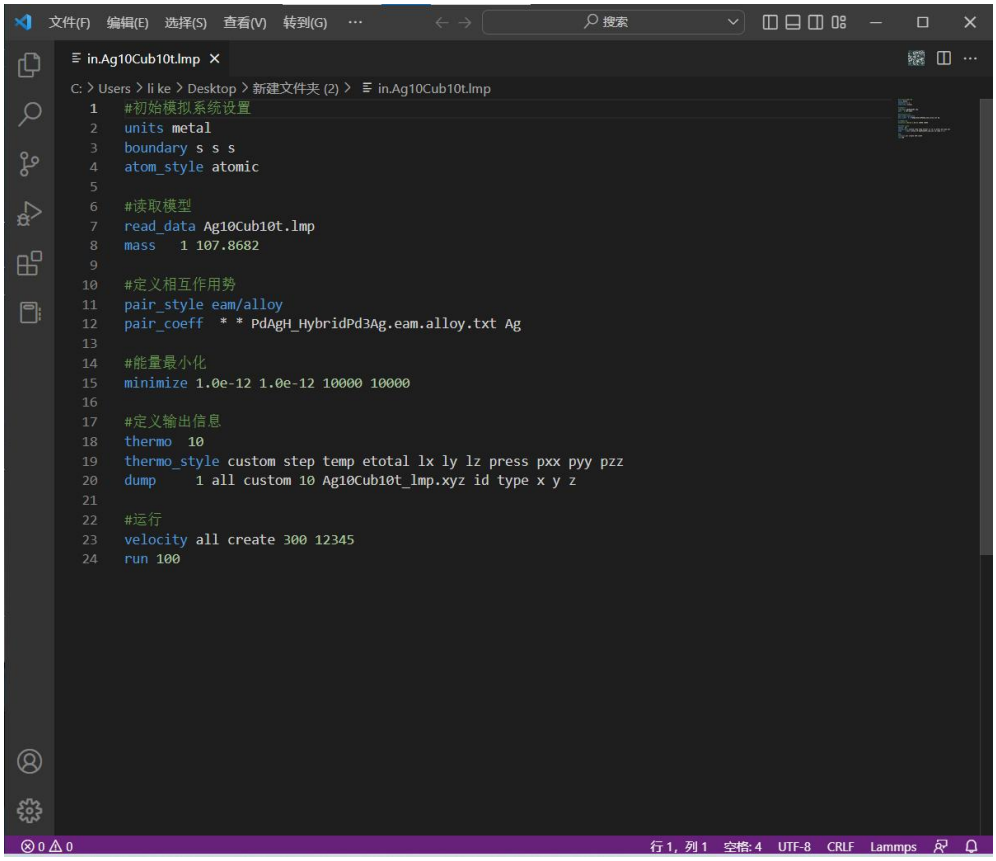
修改后的坐标如下图



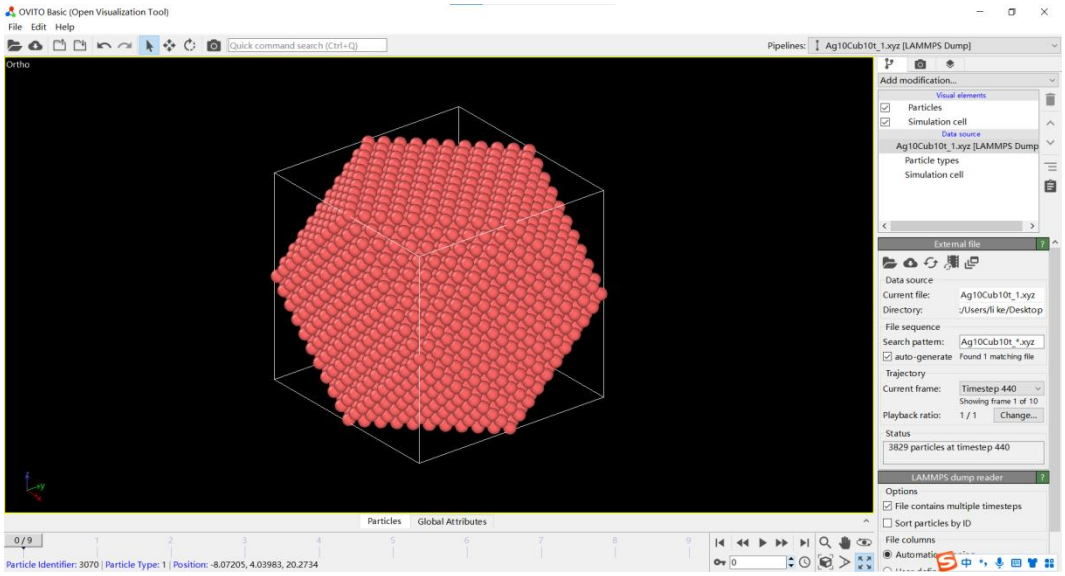
修改坐标后



in 文件


文件(F) 编辑(E) 选择(S) 查看(V) 转到(G) ···
搜索
in.Ag10Cub10t.lmp
C: > Users > li ke > Desktop > 新建文件夹 (2) > in.Ag10Cub10t.lmp
#初始模拟系统设置
units metal
boundary s s s
atom_style atomic
#读取模型
read_data Ag10Cub10t.lmp
mass 1 107.8682
#定义相互作用势
pair_style eam/alloy
pair_coeff * * PdAgH_HybridPd3Ag.eam.alloy.txt Ag
#能量最小化
minimize 1.0e-12 1.0e-12 10000 10000
#定义输出信息
thermo 10
thermo_style custom step temp etotal lx ly lz press pxx pyy pzz
dump 1 all custom 10 Ag10Cub10t_lmp.xyz id type x y z
#运行
velocity all create 300 12345
run 100
⊗ 0 ⚠ 0
行 1，列 1 空格: 4 UTF-8 CRLF Lammps

运行后的结果


OVITO Basic (Open Visualization Tool)
File Edit Help
Quick command search (Ctrl+Q)
Pipelines: Ag10Cub10t_1.xyz [LAMMPS Dump]
Ortho
Add modification...
Particles
Simulation cell
Ag10Cub10t_1.xyz [LAMMPS Dump]
Particle types
Simulation cell
External file
Data source
Current file: Ag10Cub10t_1.xyz
Directory: :/Users/li ke/Desktop
File sequence
Search pattern: Ag10Cub10t_*.xyz
auto-generate Found 1 matching file
Trajectory
Current frame: Timestep 440
Showing frame 1 of 10
Playback ratio: 1 / 1 Change...
Status
3829 particles at timestep 440
LAMMPS dump reader
Options
File contains multiple timesteps
Sort particles by ID
File columns
Particles Global Attributes
Particle Identifier: 3070 | Particle Type: 1 | Position: -8.07205, 4.03983, 20.2734