S1: Workflows for Computing Physical Properties: Radial Distribution Functions

Qiang Zhu, Yuming Gu, Xinzhu Wang, Limu Hu

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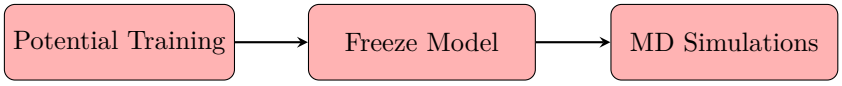
Contents

In this report, the workflow was designed and developed under airflow. The workflow is utilized here to calculate the radial distribution function of atom Cu under different simulation time.

1 Tree of the workflow



2 Potential Training & Model Freezing

For simplification, we use the datasets provided in the A1 problem. The potential was trained by deepmd-kit,[1] and was latter frozen to a model for latter molecular dyanmics simulations.

3 Molecular Dynamics Simulations

3.1 Configuration of lammps

Below are the input file we applied for molecular dynamics simulations.

```
# bulk Cu fcc

units           metal
boundary        p p p
atom_style      atomic

neighbor        2.0 bin
neigh_modify    every 10 delay 0 check no

read_data   Cu_3x3x3.lmp
mass        1 64

# here is replaced with the potential trained with deepmd-kit
pair_style  deepmd ../deepmd-train/frozen_model.pb
pair_coeff

velocity        all create 298.15 23456789

fix             1 all nvt temp 298.15 298.15 0.5
timestep        0.0005
thermo_style    custom step pe ke etotal temp press vol
thermo          100
dump        1 all custom 100 water.dump id type x y z

# section for rdf
compute gofr all rdf 100
fix rdf all ave/time 100 10 100000 c_gofr[*] file fcc-rdf.dat mode vector

run             100000
```

3.2 Preparation of the initial structure

We build a 3x3x3 supercell of Cu fcc crystal with Material Studio, and export the structure to a ***cif*** file, then Ovito[2] was utilized to convert the ***cif*** to ***lmp*** or ***data*** file which could be read by lammps.[3] The structure is shown in Figure 1

Steps for building Cu(fcc) with Material Studio:
(1). File -> Import... -> (choose dir: share/Structures/metal/pure-metals);
(2). Build -> Symmetry -> Supercell -> fill (A:3/B:3/C:3);
(3). File -> Export... -> (Choose File Type (*.cif/*.cmf))
Steps for converting ***cif*** to ***lmp*** with Ovito:
(1). File -> Load File -> (Choose the ***cif*** file we generated above);
(2). File -> Export File ->(Choose LAMMPS Data File)

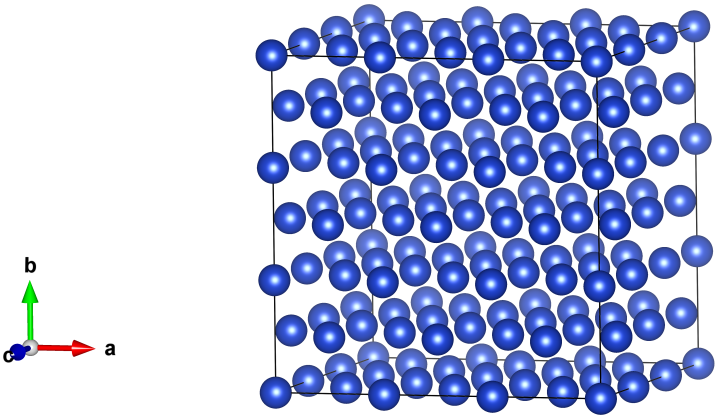


Figure 1: Illustration of the initial coordiante of Cu(fcc) with a 3x3x3 supercell

4 Plot the Data

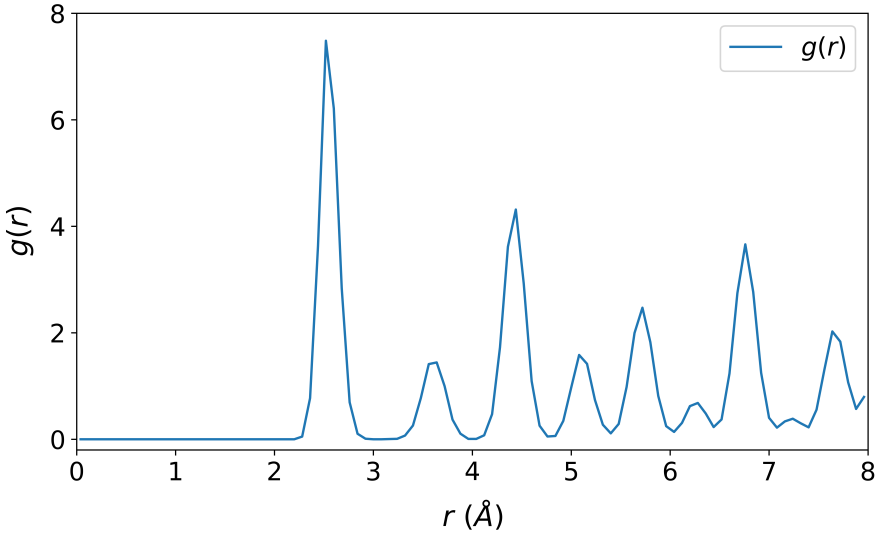


Figure 2: Radial distribution function of Cu as a function of distance r

References

[1] Han Wang, Linfeng Zhang, Jiequn Han, and Weinan E. DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. *Comput. Phys. Commun.*, 228:178–184, jul 2018.

[2] Alexander Stukowski. Visualization and analysis of atomistic simulation data with ovito–the open visualization tool. *Modelling and Simulation in Materials Science and Engineering*, 18(1):015012, 2009.

[3] Steve Plimpton. Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 117(1):1–19, 1995.