```
1
2#create a simulation box
3
4 dimension 3
5 units metal
6 boundary p p p
7 atom style atomic
8
9 lattice fcc 4.58
10 region myregion block 0 10 0 10 0 10
11 create_box 1 myregion
12 create_atoms 1 region myregion
13
14 mass 1 39.984
15
16 pair_style lj/cut 10
17 pair_coeff 1 1 0.01006418 3.3952
18
19 minimize 1e-20 1e-20 10000 10000
20
21 timestep 0.001
22
23 velocity all create 5 12345 dist Gaussian mom yes rot yes
24
25 compute srdf all rdf 100 1 1 cutoff 10.0
26 fix myfix all ave/time 1 10000 10000 c_srdf[1] c_srdf[2] c_srdf[3] file Arrdf_solid.txt mode vector
27 fix 1 all nve
28
29 dump dump_1 all custom 100 rdf.dump id type x y z ix iy iz vx vy vz
30 thermo_style custom step time temp pe ke etotal press vol
```

31 thermo 1000

32 run 10000

33 undump dump_1

36 unfix