

Simulation details and notes

1/ AMORPHISE

The timestep on the initial run should be set low because the accelerations will be very high. We used 0.001ps.
62ps at 3400K, velocity scalling every step, ewald precision 1d-3
Ensemble nve, pressure = 0.

2/ RECRYSTALLISE

Timestep increased to 0.005ps
3000ps at 3400K, velocity scalling every step, ewald precision 1d-3
Ensemble npt, pressure = 20 GPa

3/ REDUCE PRESSURE

Timestep = 0.005ps
2500ps at 3400K, velocity scalling every step, ewald precision 1d-3
Ensemble npt hoover 1.0 1.0, pressure = 0 GPa

4/ COOL

Timestep = 0.005ps
375ps at 3000K, 60ps at 2500K, 50ps at 2000K, 50ps at 1500K, 995ps at 1000K, 50ps at 500K and 320ps at 0K.
velocity scalling every step, ewald precision 1d-3
Ensemble npt hoover 1.0 1.0, pressure = 0 GPa

5 CONDUCTIVITY CALCULATIONS USING MODEL

Timestep = 0.005ps
250ps, equilibration, ewald precision 1d-6
500ps production run - Ensemble npt hoover 1.0 1.0, Pressure = 0GPa
Performed for 2500K, 2000K, 1700K, 1500K, 1335K, 1175K, 1000K

CONTROL file

```
Ce2O3Y-R33
temperature          3400.0
pressure             0.0
steps                1000000
equilibration steps 9000000
scale every          1 steps
timestep             0.001 ps
multiple timestep    1 steps
cutoff               10.0 angstrom
delr                 2.5 angstrom

print every          10 steps
rdf sampling every  10 steps
print rdf

job time             10000000 seconds
close time           1000 seconds

ewald precision 1d-3

ensemble nve
stats every          100 steps
stack                100 deep

trajectory nstraj=0001 istraj= 100 keytrj=0

finish
```

FIELD file

```
EO2YSZ31%COMP
UNITS eV
MOLECULES 6
O CORE
NUMMOL 11904
atoms 1
O 16.0000 -2.000
finish
ZR CORE
NUMMOL 5376
atoms 1
ZR 91.2200 4.000
finish
Y CORE
NUMMOL 768
atoms 1
Y 88.9059 3.000
finish
O1 CORE
NUMMOL 12096
atoms 1
O 16.0000 -2.000
finish
CE CORE
NUMMOL 5760
atoms 1
CE 140.1200 4.000
finish
C3 CORE
NUMMOL 383
atoms 1
C3 140.1200 3.000
finish
vdw 5
CE O buck 1986.8300 0.3511 20.4000
C3 O buck 1731.6181 0.3637 14.4326
O O buck 22764.3000 0.1490 27.8900
ZR O buck 985.8700 0.3760 0.0000
Y O buck 1345.1000 0.3491 0.0000
CLOSE
```