ANEXOS

Anexo I Código y Scripts de LAMMPS

A continuación se recogen los scripts utilizados en las simulaciones:

1. **Script generación del modelo de YSZ**

```
# YSZ_A.in----------------------------------------------------------------------
# This file was generated by Fran Gil - ITAINNOVA
# Modelling zirconium dioxide ZrO2 doped with yttrium(III) oxide Y2O3 (YSZ)
# Requires: unitcell.data and Buckingham_Coulomb_Real.ff
#-------------------------------------------------------------------------------

# Setup conditions
units real
atom_style full
boundary p p p
processors 1 1 1

# Zirconium dioxide lattice setup
read_data unitcell.data
replicate 12 12 12

# Substitution of zirconium by yttrium
group zrc type 1
group oxy type 2
set group zrc type/ratio 3 0.148 1234
group ytt type 3

# Random creation of vacancies
set group oxy type/ratio 4 0.0370 1234
group vacancy type 4
delete_atoms group vacancy

# Forcefield
```

```
variable forcefield index Buckingham_Coulomb_Real
include ${forcefield}.ff

# Time integration
timestep 4
write_data end_state.out nocoeff
```

2. Script equilibrado NVT

```
# NVT_1000K.in----------------------------------------------------
# This file was generated by Fran Gil - ITAINNOVA
# NVT equilibrium at Tª= 1000K
# Requires: YSZ_A.data and Buckingham_Coulomb.ff
#----------------------------------------------------------------

units      real
atom_style         full
boundary           p p p
processors 2 2 2
read_data          YSZ_A.data

# forcefield
variable forcefield index Buckingham_Coulomb_Real
include ${forcefield}.ff

# thermo
timestep 1
thermo_style       custom step time etotal pe ke temp press
thermo   1000
thermo_modify      norm no
atom_modify        sort 10 1000

# Initial velocity
velocity     all create 1000 10000 mom yes rot yes dist gaussian

# Initial minimization
```

```
minimize        0.0 1e-10 10000 10000
reset_timestep  0

# stress
compute temp all temp
compute pressure all pressure temp
variable st_total1 equal -c_pressure[1]
variable st_total2 equal -c_pressure[2]
variable st_total3 equal -c_pressure[3]
variable st_total4 equal -c_pressure[4]
variable st_total5 equal -c_pressure[5]
variable st_total6 equal -c_pressure[6]

# energy
variable etotal equal etotal
variable ekin equal ke
variable epot equal pe
variable eele equal ecoul+elong
variable density equal density

# dimensions
variable temp equal temp
variable density equal density
variable vol equal vol
variable cella equal cella
variable cellb equal cellb
variable cellc equal cellc
variable press equal press

# results
fix         stress all ave/time 1 1 1000 v_density v_vol v_cella v_cellb v_cellc v_press v_st_total1
v_st_total2 v_st_total3 v_st_total4 v_st_total5 v_st_total6 ave one file stress.dump
fix         energy all ave/time 1 1 1000 v_etotal v_ekin v_epot v_eele v_density v_temp ave one file
energy.dump
dump        snaps all custom 1000 snaps.dump id mol type q x y z

# time integration
```

```
fix nvt all nvt temp 1000.0 1000.0 100.0
run 400000
write_data end_state.out nocoeff
```

3. Script equilibrado NPT

```
# NPT_1bar_A.in-----------------------------------------------------
# This file was generated by Fran Gil - ITAINNOVA
# NPT equilibrium at P= 1 bar
# Requires: YSZ_NVT_A.data and Buckingham_Coulomb.ff
#-------------------------------------------------------------------

units      real
atom_style         full
boundary           p p p
processors 2 2 2
read_data          YSZ_NVT_A.data

# Forcefield
variable forcefield index Buckingham_Coulomb_Real
include ${forcefield}.ff

# thermo
timestep 1
thermo_style       custom step time etotal pe ke temp press
thermo   1000
thermo_modify      norm no
atom_modify        sort 10 1000

# initial minimization
minimize           0.0 1e-10 10000 10000
reset_timestep     0

# stress
compute temp all temp
compute pressure all pressure temp
```

```
variable st_total1 equal -c_pressure[1]
variable st_total2 equal -c_pressure[2]
variable st_total3 equal -c_pressure[3]
variable st_total4 equal -c_pressure[4]
variable st_total5 equal -c_pressure[5]
variable st_total6 equal -c_pressure[6]

# energy
variable etotal equal etotal
variable ekin equal ke
variable epot equal pe
variable eele equal ecoul+elong
variable density equal density

# dimensions
variable temp equal temp
variable density equal density
variable vol equal vol
variable cella equal cella
variable cellb equal cellb
variable cellc equal cellc
variable press equal press

# results
fix         stress all ave/time 1 1 1000 v_density v_vol v_cella v_cellb v_cellc v_press v_st_total1 v_st_total2 v_st_total3 v_st_total4 v_st_total5 v_st_total6 ave one file stress.dump
fix         energy all ave/time 1 1 1000 v_etotal v_ekin v_epot v_eele v_density v_temp ave one file energy.dump
dump     snaps all custom 5000 snaps.dump id mol type q x y z

# time integration
fix         npt all npt temp 1000.0 1000.0 100 iso 1.0 1.0 100
run 100000
unfix npt
fix npt2 all npt temp 1000.0 1000.0 100 aniso 1.0 1.0 100
run 900000
write_data end_state.out nocoeff
```

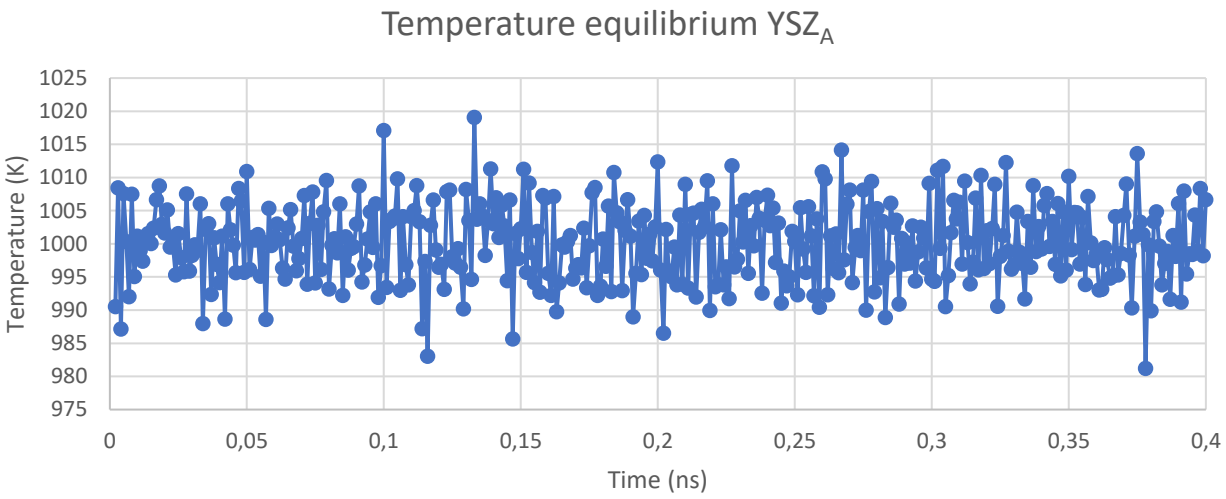
4. Script cálculo de conductivida térmica

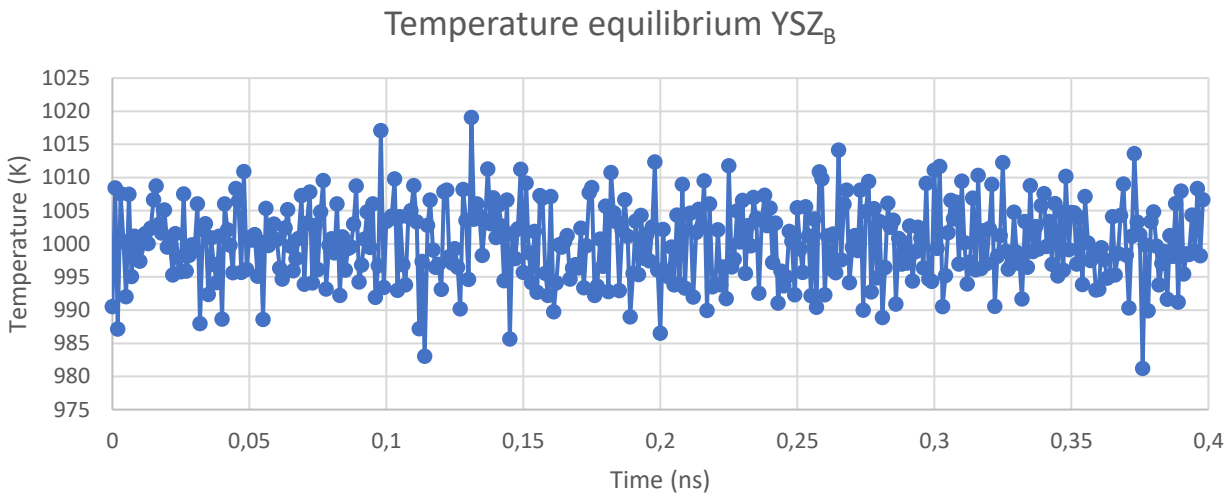
```
# Sample LAMMPS input script for thermal conductivity of YSZ_A
# Calculates the thermal conductivity using the Green-Kubo algorithm
# This file was generated by Fran Gil - ITAINNOVA
# Units: real; Temperature: 1000K; TimeStep: 1 fs; atoms: 20000
# Requires: NPT_A.data and Buckingham_Coulomb.ff
#----------------------------------------------------------------

processors 2 2 2
units real
variable T equal 1000
variable V equal vol
variable dt equal 1
variable p equal 200 # correlation length
variable s equal 20 # sample interval
variable d equal $p*$s # dump interval

# Convert from LAMMPS real units to SI
variable kB equal 1.3806504e-23 # [J/K] Boltzmann
variable KcaltoJoules equal 6.95e-21# conversion from kcal/mol to Joules (including Avogadro)
variable A2m equal 1.0e-10
variable fs2s equal 1.0e-15
variable convert equal ${KcaltoJoules}*${KcaltoJoules}/${fs2s}/${A2m}

# Setup
atom_style full
boundary p p p
read_data NPT_A.data

# Forcefield---------------------------------------------------------------------------------
variable forcefield index Buckingham_Coulomb_Real
include ${forcefield}.ff
# thermo
timestep ${dt}
```

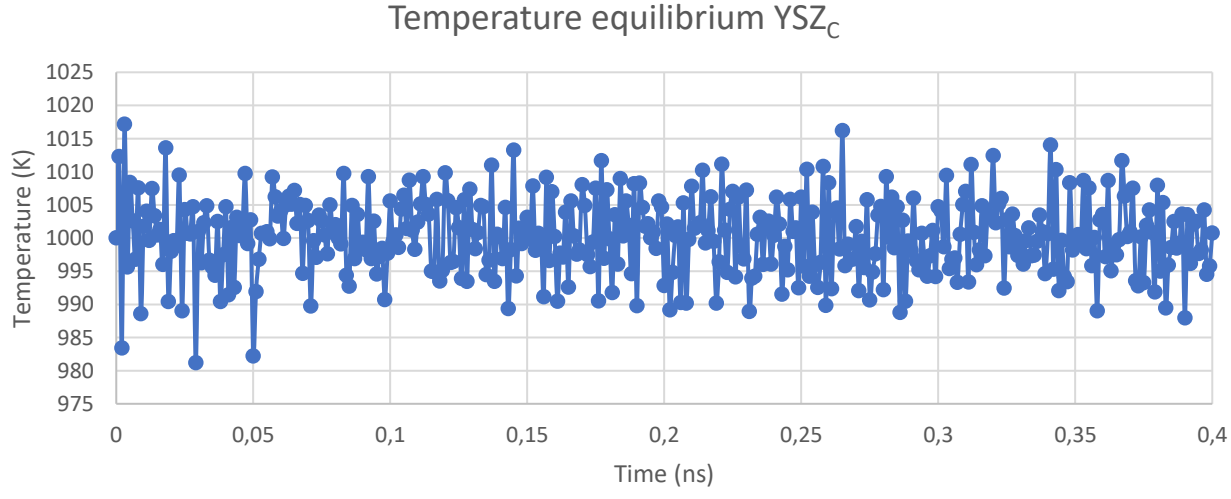
```
thermo   $d
thermo_modify    norm no
atom_modify       sort 10 1000

# Equilibration and thermalization
fix NVT all nvt temp $T $T 100

# Thermal conductivity calculation
compute myKE all ke/atom
compute myPE all pe/atom
compute myStress all stress/atom NULL virial
compute flux all heat/flux myKE myPE myStress

variable Jx equal c_flux[1]/vol
variable Jy equal c_flux[2]/vol
variable Jz equal c_flux[3]/vol

fix JJ all ave/correlate $s $p $d &
c_flux[1] c_flux[2] c_flux[3] type auto file J0Jt.dat ave running

variable scale equal ${convert}/${kB}/$T/$T/$V*$s*${dt}
variable k11 equal trap(f_JJ[3])*${scale}
variable k22 equal trap(f_JJ[4])*${scale}
variable k33 equal trap(f_JJ[5])*${scale}

dump     snaps all custom 5000 snaps.dump id mol type q x y z
thermo_style custom step temp press v_Jx v_Jy v_Jz v_k11 v_k22 v_k33 v_scale
run 1200000
variable k equal (v_k11+v_k22+v_k33)/3.0
variable ndens equal count(all)/vol
print "average conductivity: $k[W/mK] @ $T K, ${ndens} /A\^3"
write_data end_state.out nocoeff
```

Anexo II Gráficos de equilibrado

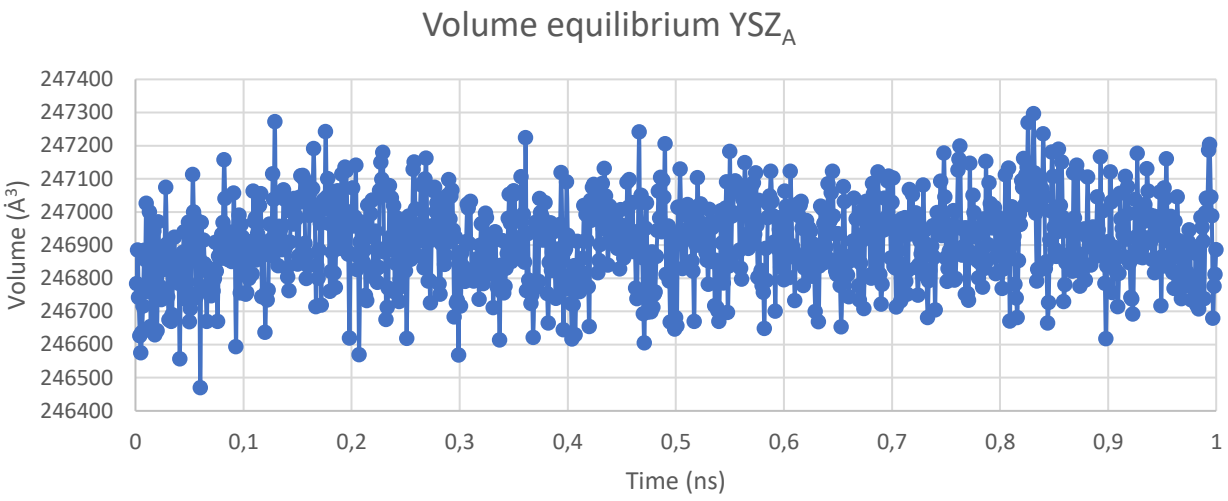
1. **Equilibrado de la temperatura a 1000K en condiciones de ensamblado NVT.**

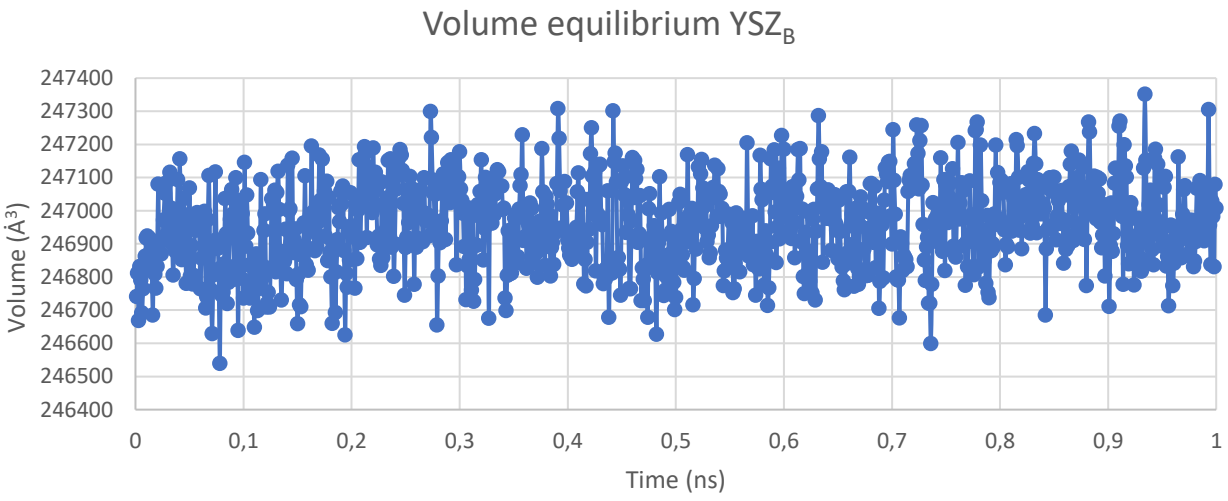


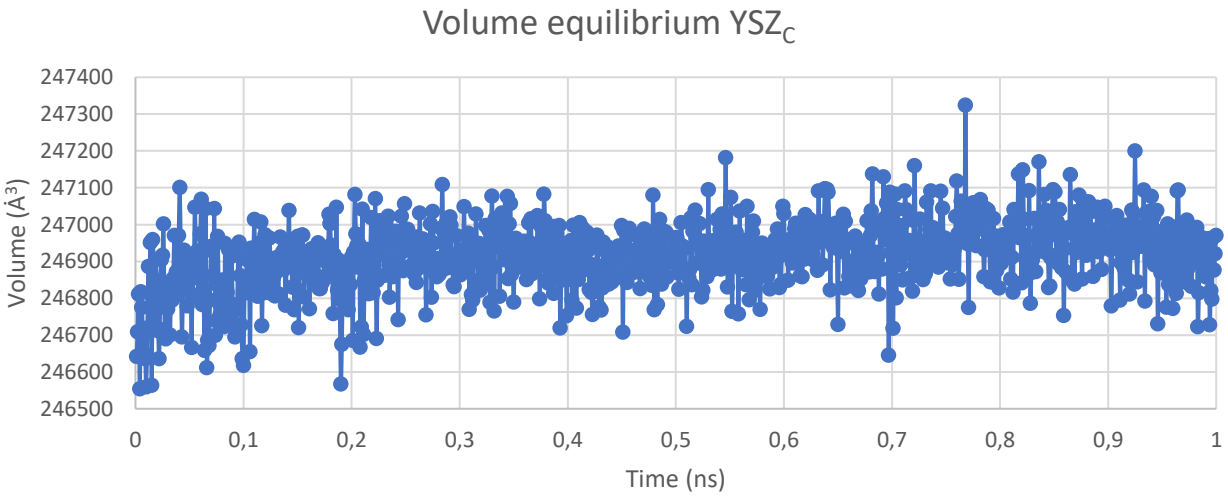




2. Equilibrados del volumen en condiciones de ensamblado NPT.







3. Control de la presión durante ensamblado NPT