

# 1 CONTROL

```
DLPOLY: LiNbO3
temperature 800.000000
pressure 0.000000
steps 700000
equilibration 50000
print every 500
stats every 500
timestep 0.0002000000 ps
ensemble nst ber 0.500000 0.500000 (ps)
traj 1 500 0
rdf 1000
multiple step 1
cap 1000
scale 307
primary cutoff 10.000
cutoff 10.000
delr width 1.000
rvdw cutoff 10.000
ewald precision 1.0E-6
shake tolerance 1.0E-6
quaternion tolerance 1.0E-5
job time 1520000
close time 200
finish
```

# 2 result

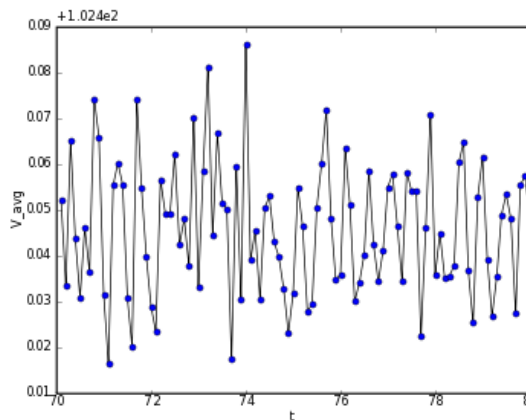


Figure 1: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=100$  K (new080514heat).

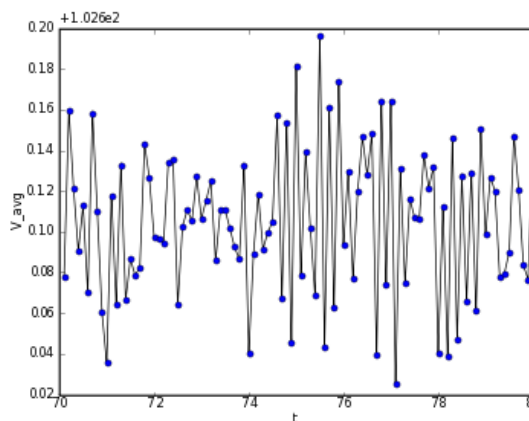


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=200$  K (new080514heat).

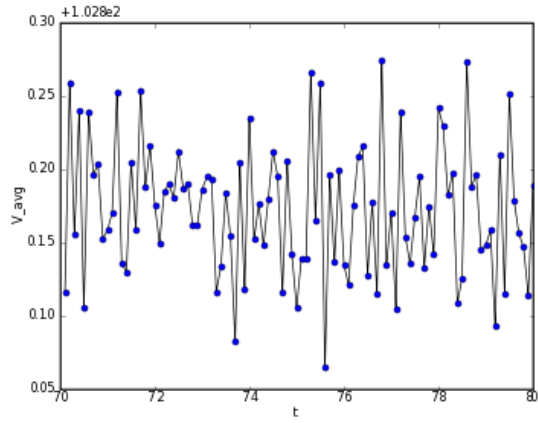


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=300$  K (new080514heat).

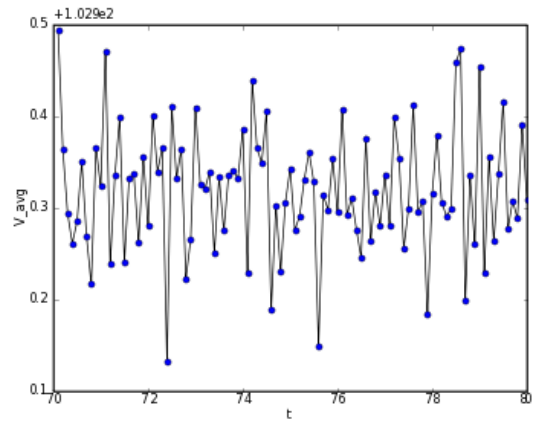


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=400$  K (new080514heat).

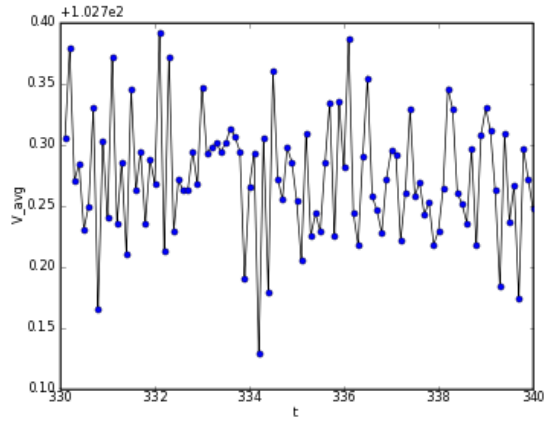


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=500$  K (new080514heat).

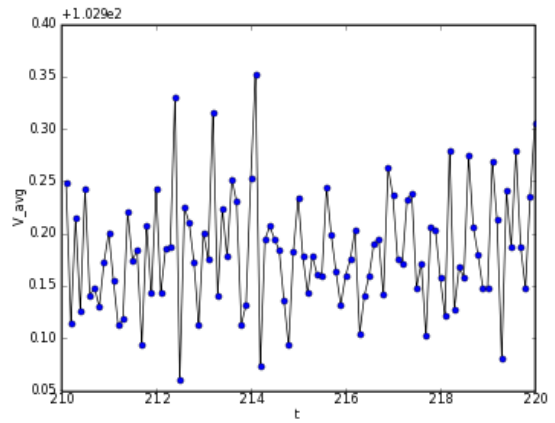


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=600$  K (new080514heat).

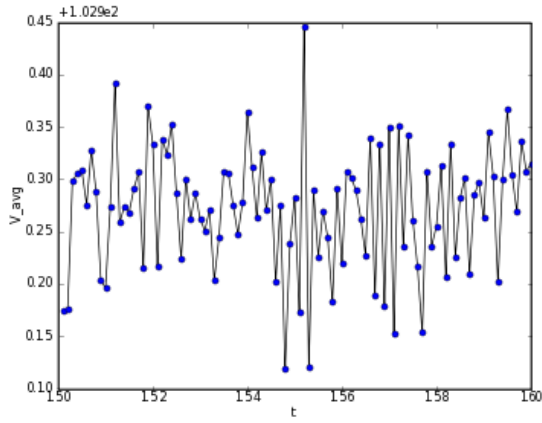


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=700$  K (new080514heat).

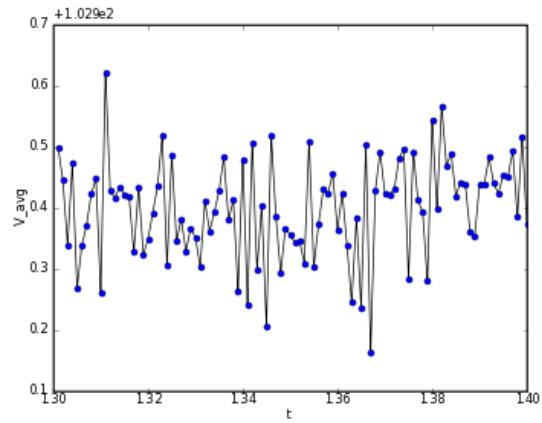


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=800$  K (new080514heat).

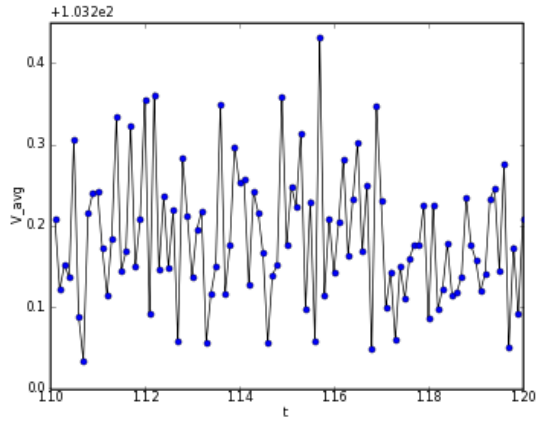


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=900$  K (new080514heat).

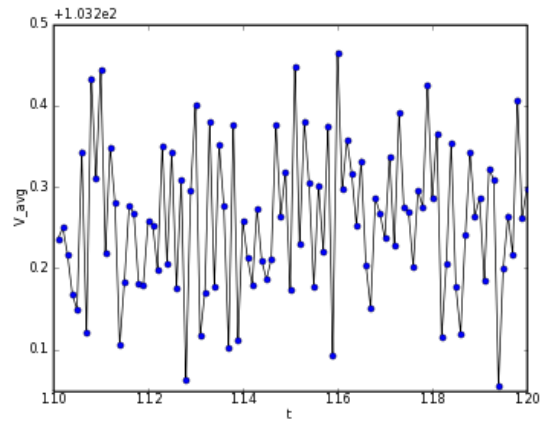


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1000$  K (new080514heat).

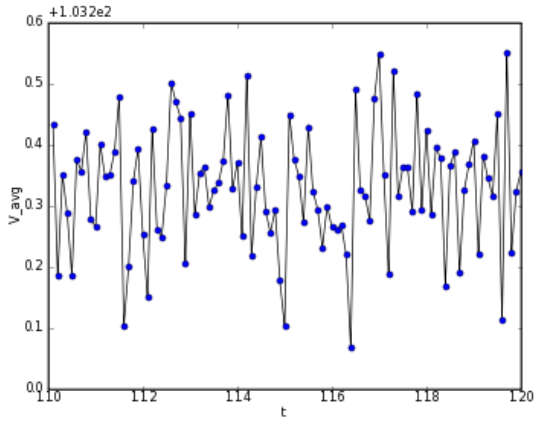


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1100$  K (new080514heat).

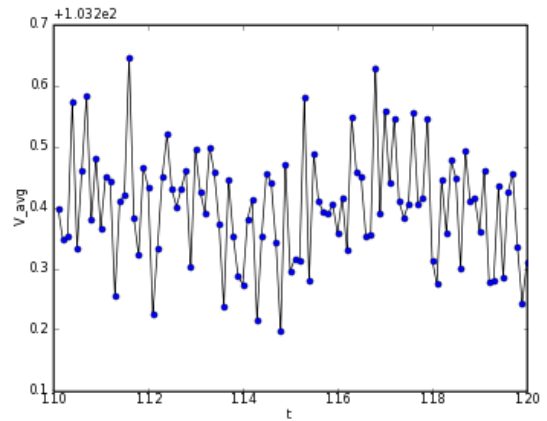


Figure 12: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1200$  K (new080514heat).

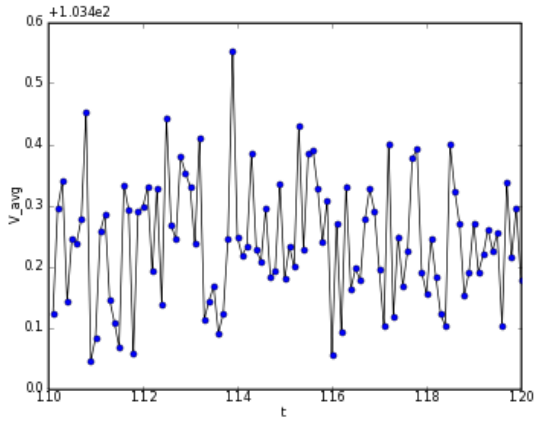


Figure 13: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1300$  K (new080514heat).

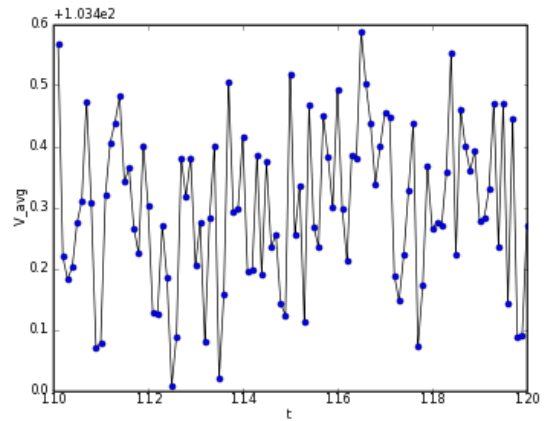


Figure 14: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1400$  K (new080514heat).

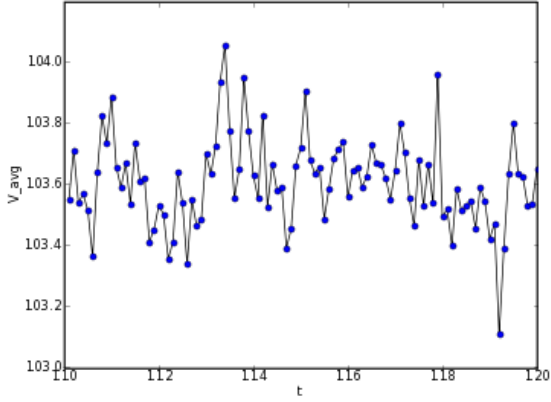


Figure 15: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1500$  K (new080514heat).

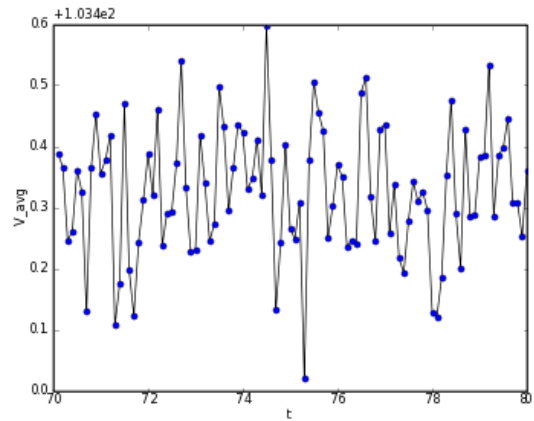


Figure 16: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1600$  K (new080514heat).



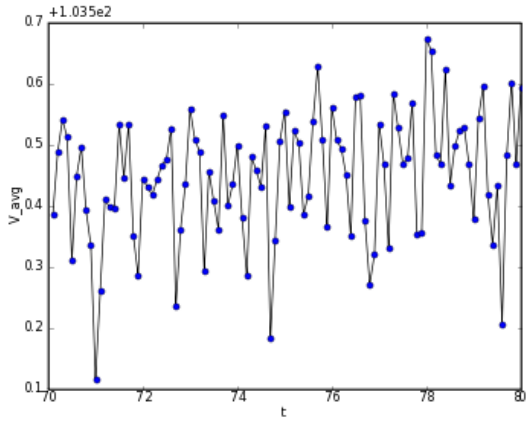


Figure 17: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1700$  K (new080514heat).

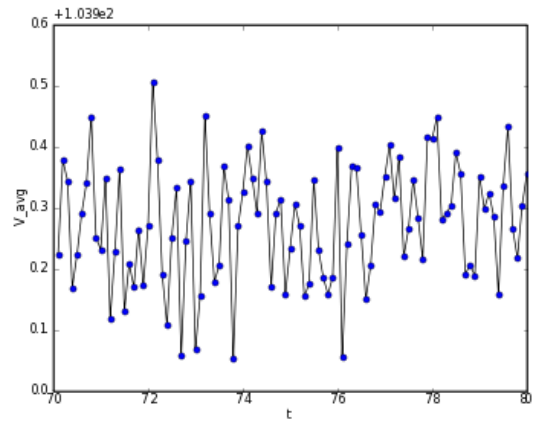


Figure 18: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1800$  K (new080514heat).

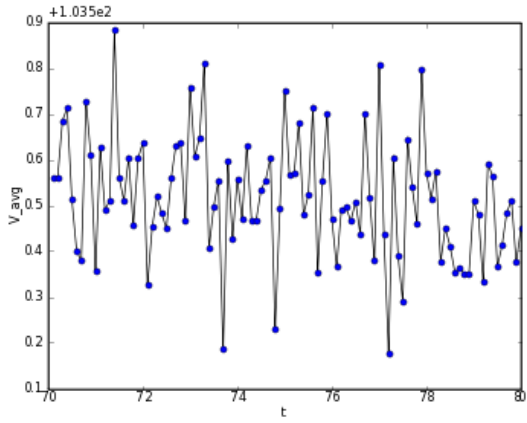


Figure 19: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=1900$  K (new080514heat).

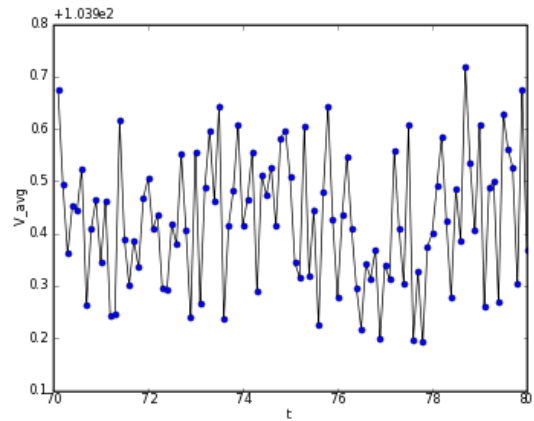


Figure 20: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature  $T=2000$  K (new080514heat).