

1 CONTROL

DLPOLY: LiNbO3

```
temperature 2000.000000
pressure 0.000000
steps 800000
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

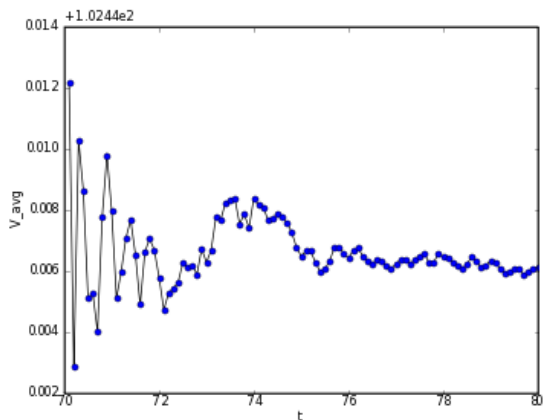


Figure 1: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=100$ K (run20080612).

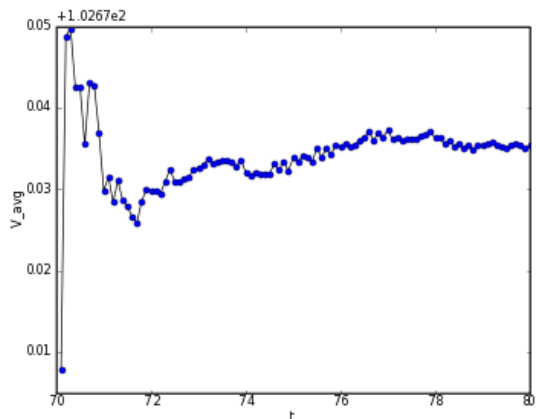


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=200$ K (run20080612).

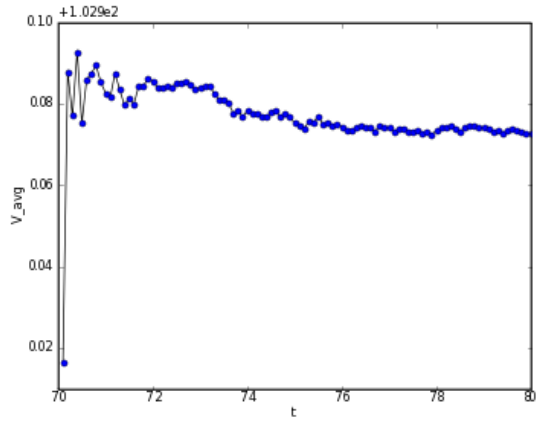


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=300$ K (run20080612).

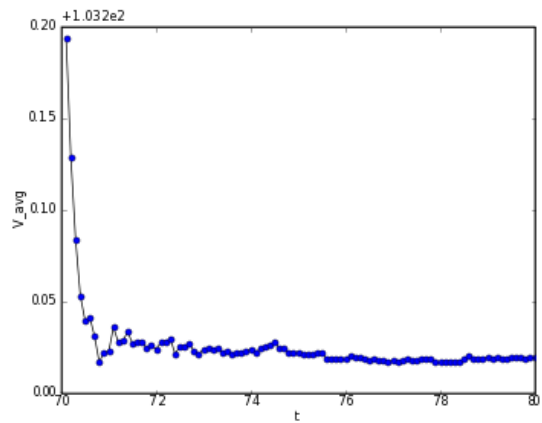


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=400$ K (run20080612).

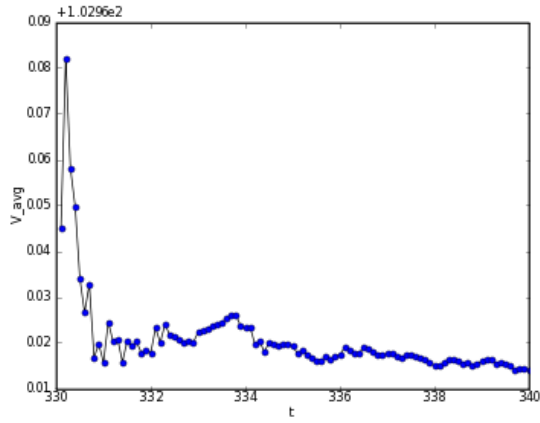


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=500$ K (run20080612).

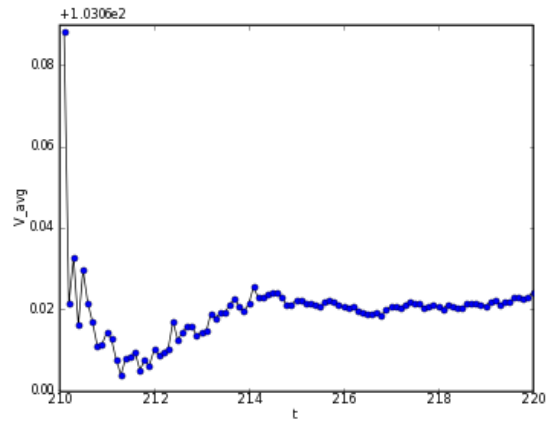


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=600$ K (run20080612).

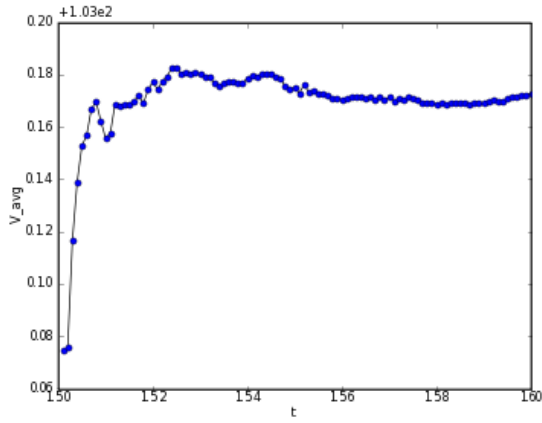


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=700$ K (run20080612).

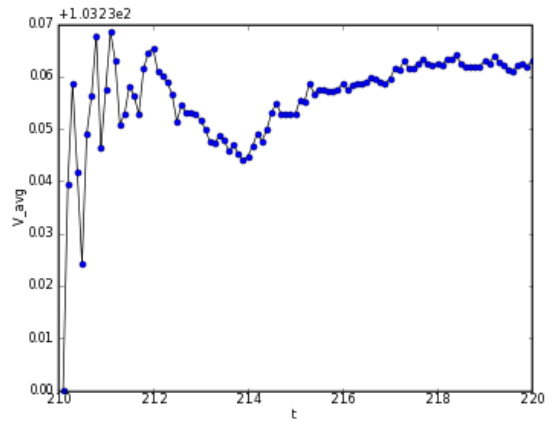


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=800$ K (run20080612).

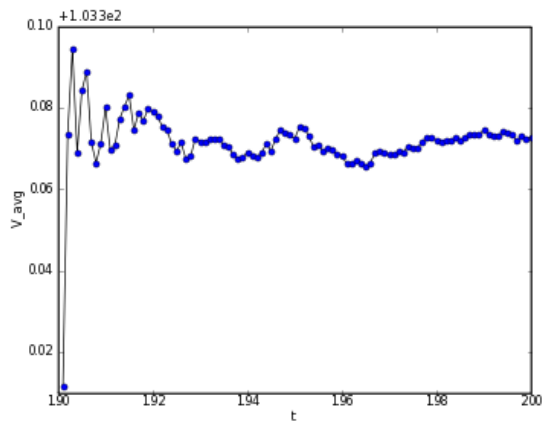


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=900$ K (run20080612).

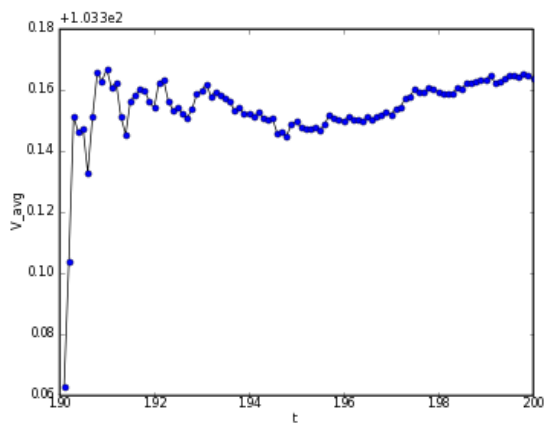


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1000$ K (run20080612).

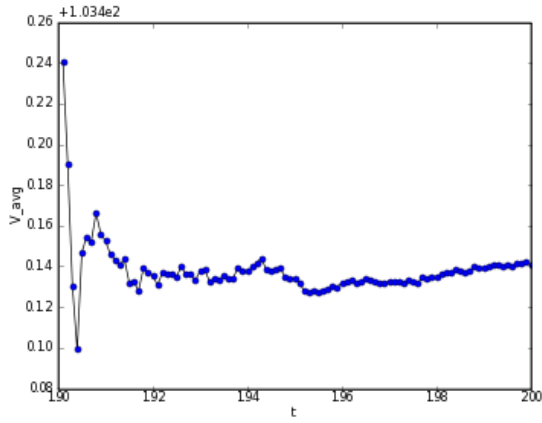


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1100$ K (run20080612).

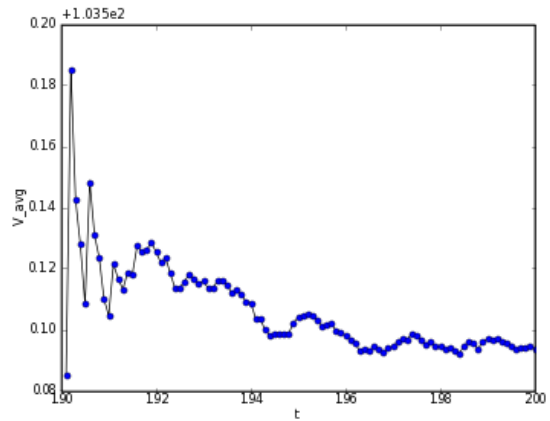


Figure 12: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1200$ K (run20080612).

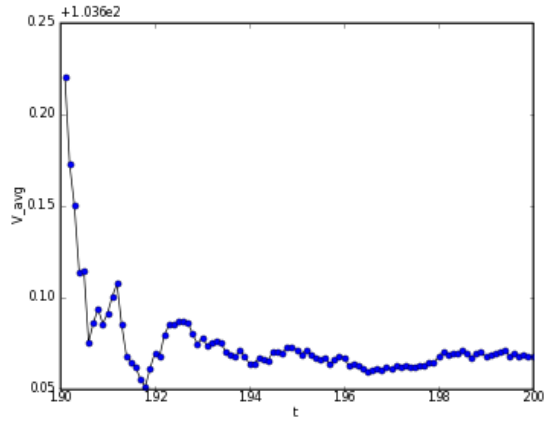


Figure 13: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1300$ K (run20080612).

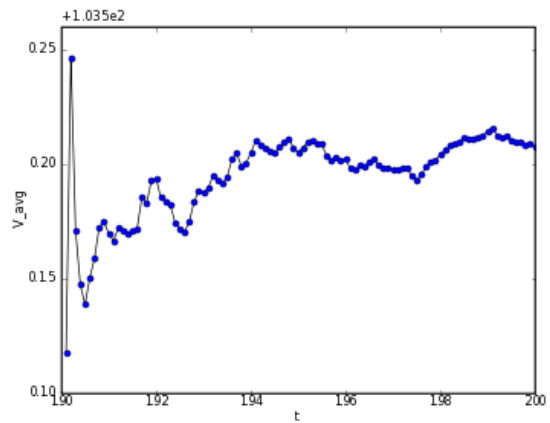


Figure 14: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1400$ K (run20080612).

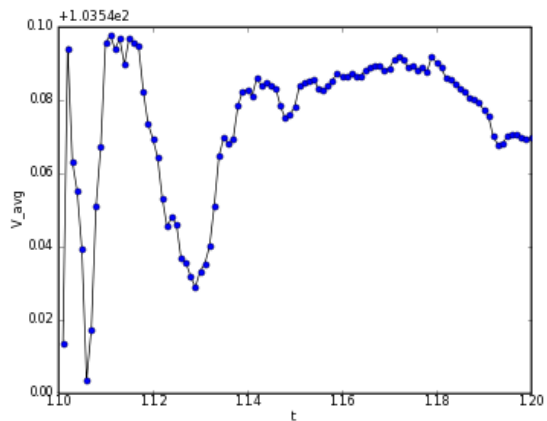


Figure 15: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1500$ K (run20080612).

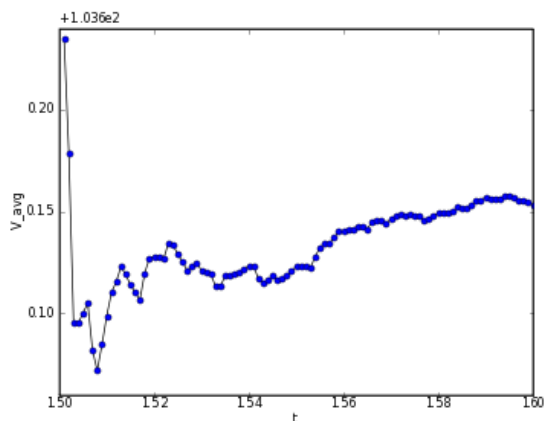


Figure 16: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1600$ K (run20080612).

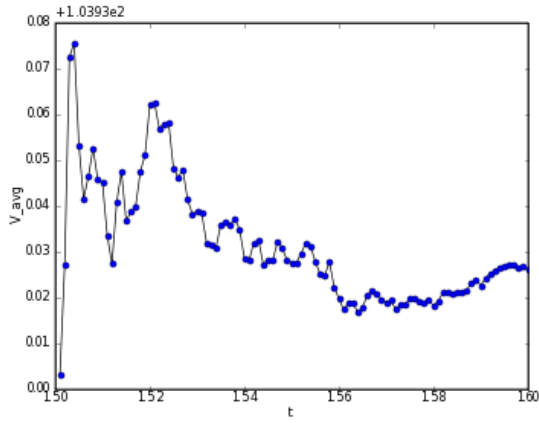


Figure 17: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1700$ K (run20080612).

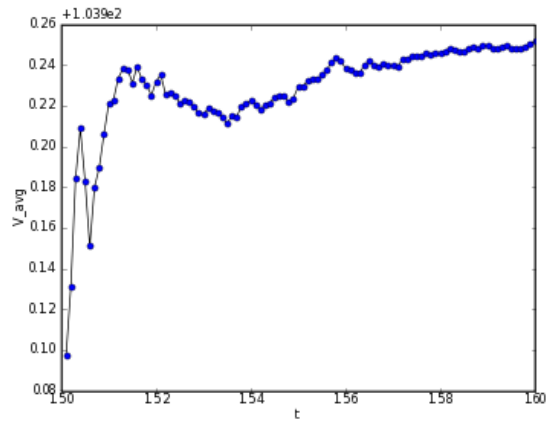


Figure 18: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1800$ K (run20080612).

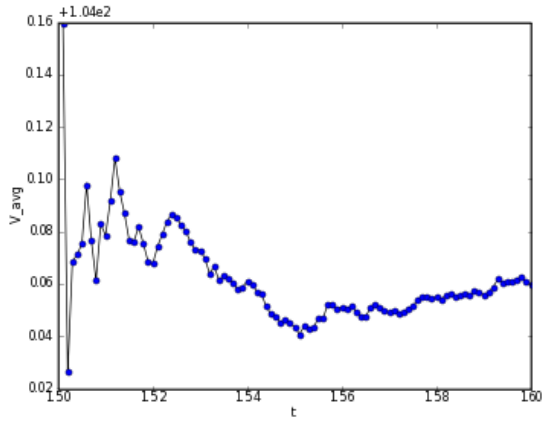


Figure 19: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1900$ K (run20080612).

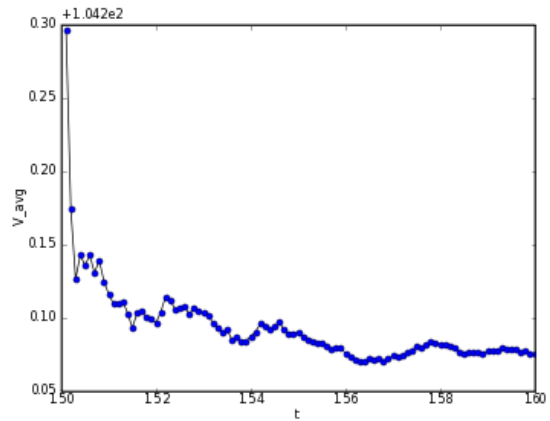


Figure 20: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=2000$ K (run20080612).