

1 CONTROL

DLPOLY: LiNbO3

```
temperature 100.000000
pressure 0.000000
steps 200000
equilibration 40000
print every 1000
stats every 1000
timestep 0.0002000000 ps
ensemble nst ber 0.600000 0.500000 (ps)
traj 1 1000 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

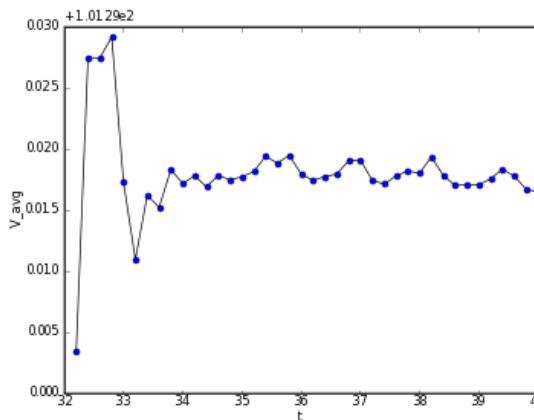


Figure 1: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=100 K (new080506).

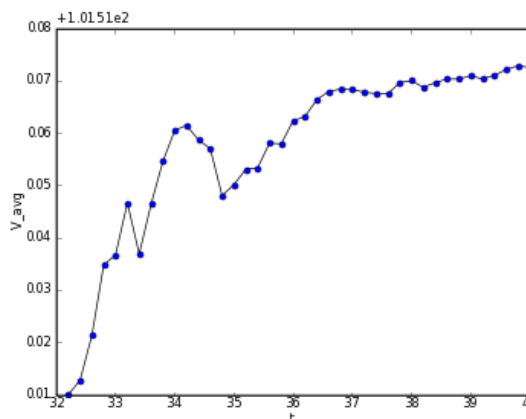


Figure 2: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=200 K (new080506).

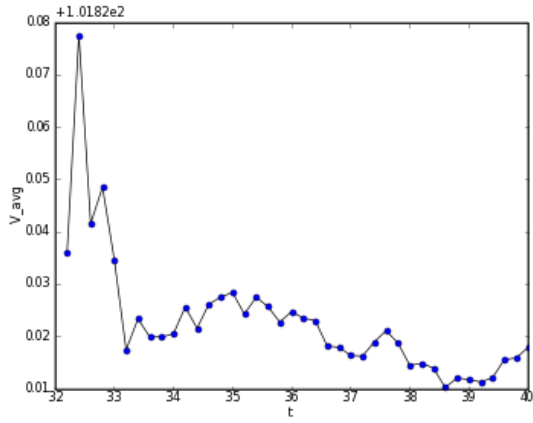


Figure 3: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=300 K (new080506).

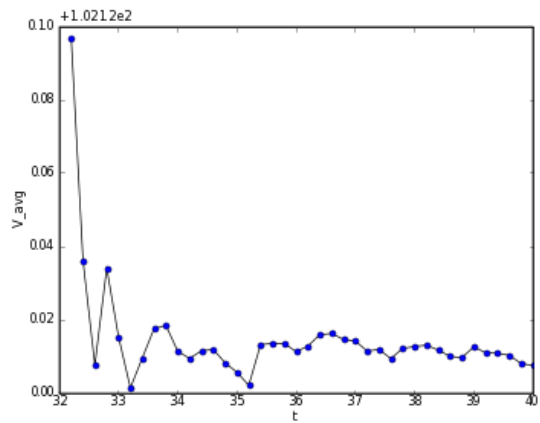


Figure 4: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=400 K (new080506).

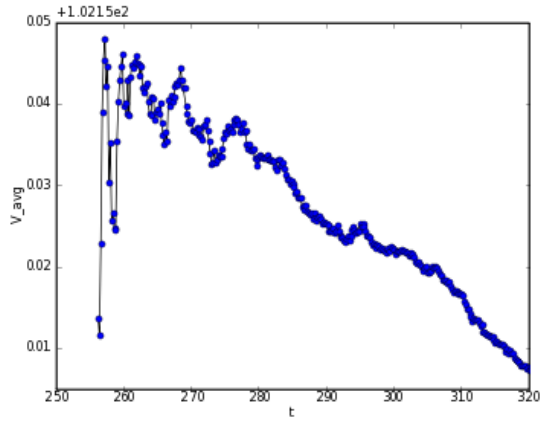


Figure 5: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=500$ K (new080506).

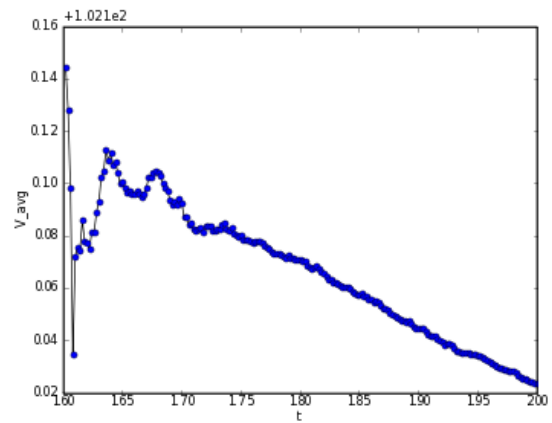


Figure 6: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=600$ K (new080506).

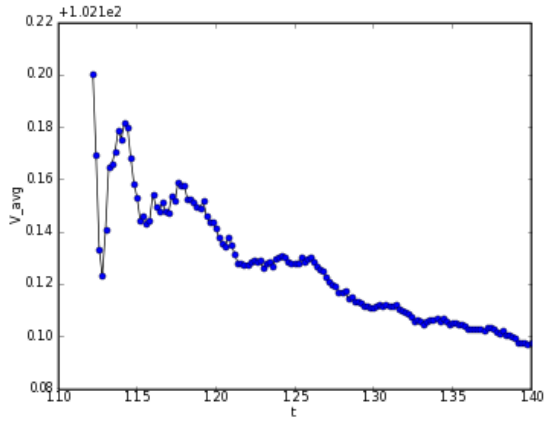


Figure 7: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=700$ K (new080506).

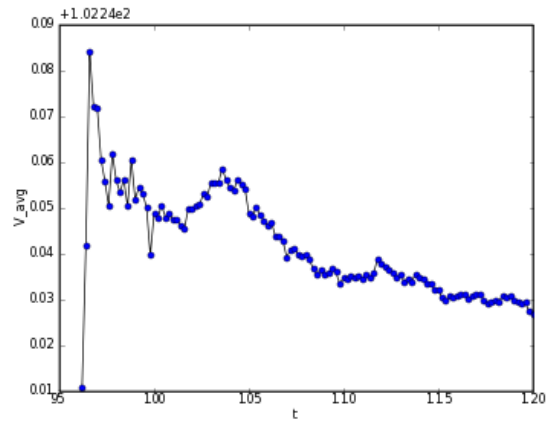


Figure 8: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=800$ K (new080506).

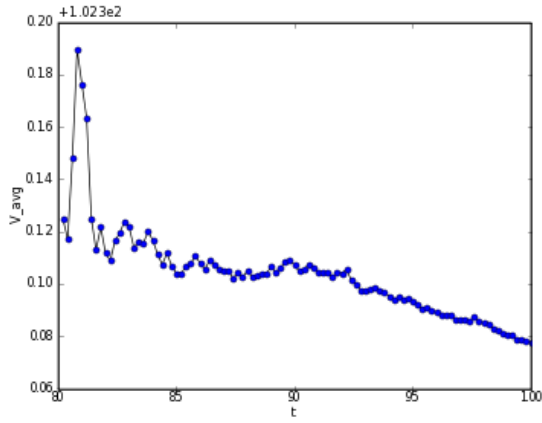


Figure 9: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=900 K (new080506).

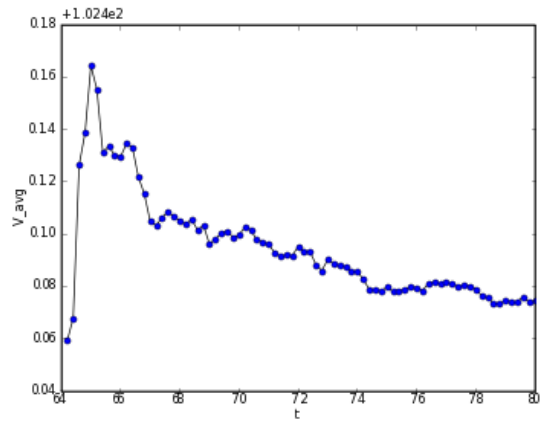


Figure 10: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=1000 K (new080506).

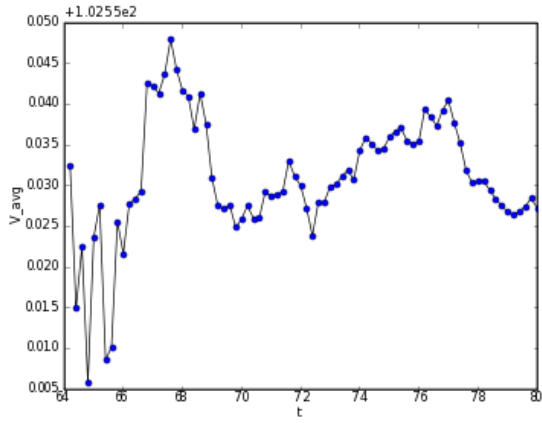


Figure 11: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1100$ K (new080506).

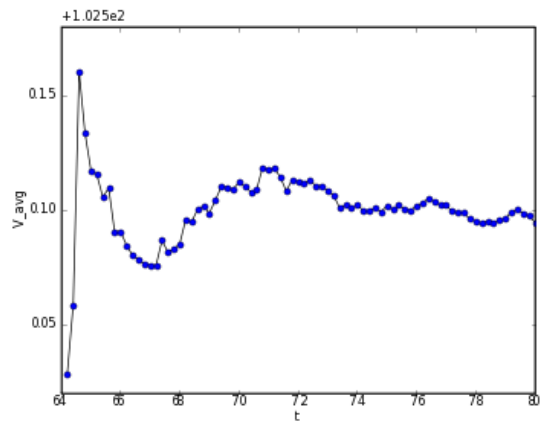


Figure 12: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1200$ K (new080506).

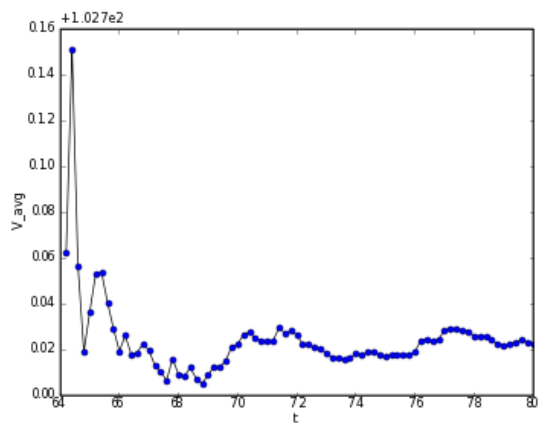


Figure 13: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1300$ K (new080506).

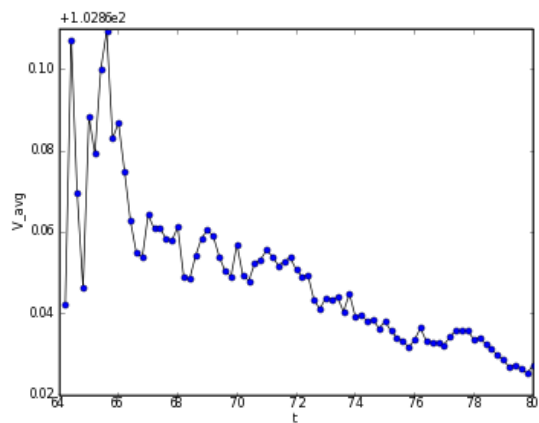


Figure 14: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1400$ K (new080506).

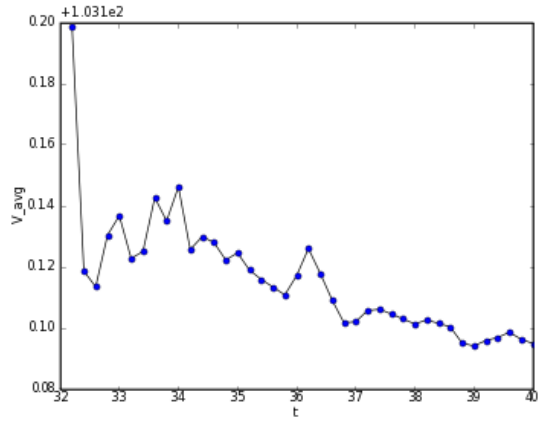


Figure 15: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=1500 K (new080506).

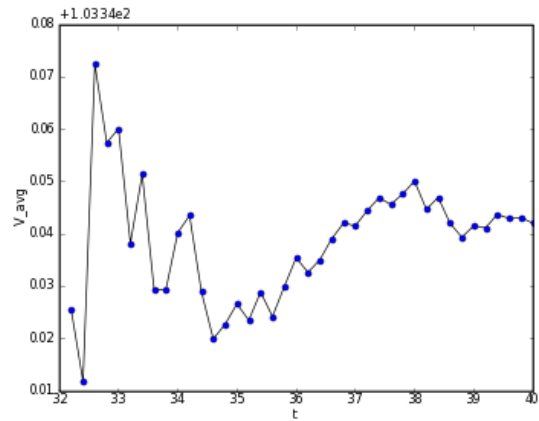


Figure 16: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=1600 K (new080506).

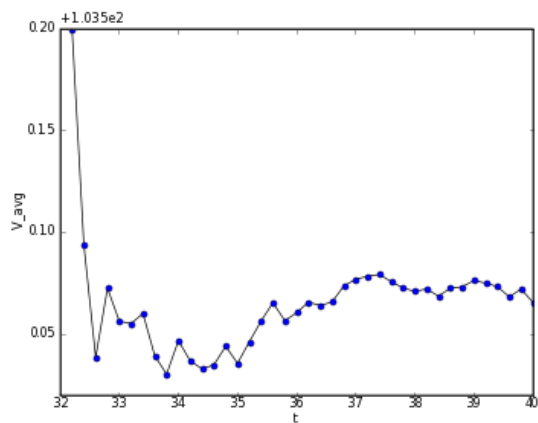


Figure 17: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1700$ K (new080506).

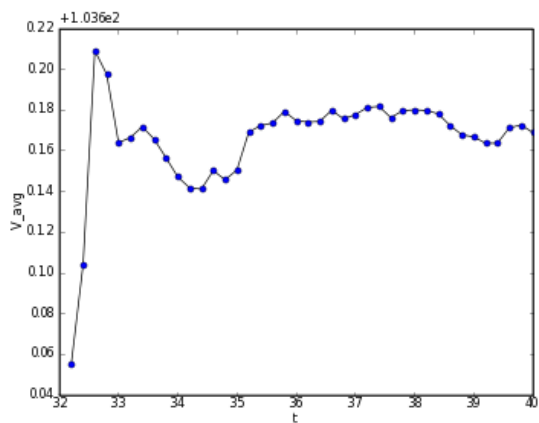


Figure 18: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature $T=1800$ K (new080506).

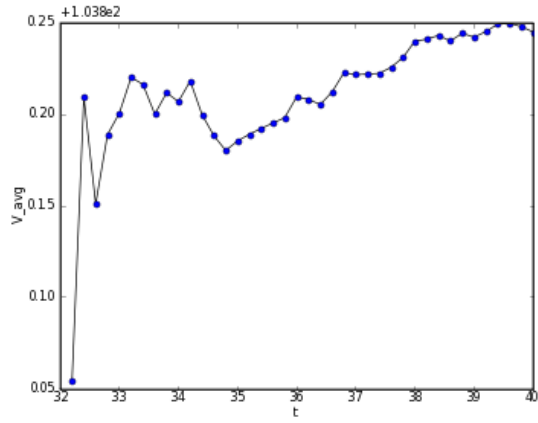


Figure 19: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=1900 K (new080506).

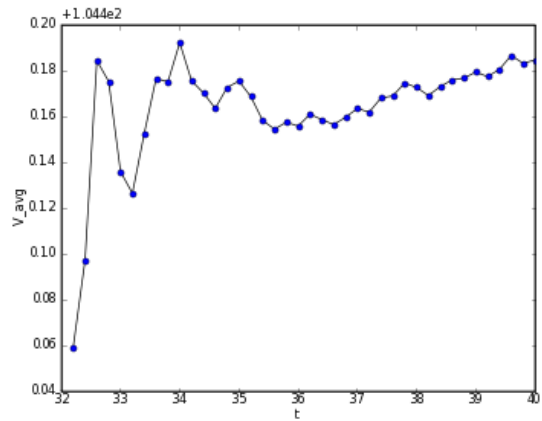


Figure 20: Temperature, Pressure, Volume, Polarization verse time for MD simulation of LiNbO3 at target temperature T=2000 K (new080506).