LAMPIRAN

Lampiran 1 :*script input* proses amorfisasi c-Si

```
units           real
boundary        p p f
atom_style      charge

lattice         diamond 5.4307 orient x 1 1 0
orient y -1 1 0
region          space block 0.0 5.0 0.0 5.0
0.0 14.0
create_box      3 space
create_atoms    1 box

region          vacuum block 0.0 5.0 0.0 5.0
10.0 14.0
delete_atoms    region vacuum

pair_style      reax
pair_coeff      * * ffield.reax 6 6 6

mass            1 28.086
mass            2 28.086
mass            3 28.086

region          r_surf block  0.0 5.0 0.0 5.0
9.7 10.0
region          r_heat block  0.0 5.0 0.0 5.0
0.5  9.7
region          r_fix  block  0.0 5.0 0.0 5.0
0.0  0.5

group           g_surf region r_surf
group           g_heat region r_heat
group           g_fix  region r_fix
group           g_Film union  g_surf g_heat

set group       g_fix  type 1
```

```
set group       g_heat type 2
set group       g_surf type 3

compute         peratom all pe/atom
compute         pe_atom all reduce ave
c_peratom
compute         Film_temp g_Film temp

thermo          100
thermo_style    custom step c_Film_temp temp
c_pe_atom pe ke etotal vol press
thermo_modify   lost ignore norm yes

neighbor   2 bin
neigh_modify    every 1 delay 0 check yes

dump            mindump all custom 1
mini_*.dat id type  xs ys zs x y z q type
minimize   1.0e-4 1.0e-6 1000 10000
undump          mindump

velocity   g_Film create 300.0 4726959 rot yes
dist gaussian loop geom

reset_timestep  0
fix             1 g_fix nve/noforce

############ heating ###########

fix        2 g_Film nve
fix        3 g_heat temp/rescale 100 300.0
3500.0 1.0 0.9
#fix       4 all reax/bonds 100000 bonds.dat

compute    crdf g_Film rdf 100
fix        5 g_Film ave/time 50000 1 50000
c_crdf file rdf_heating.dat mode vector
```

```
timestep   0.025
dump       heating all custom 200
heating_*.dat id type  xs ys zs x y z q type

run   400000 #10ps

unfix      5
unfix 3
unfix 2
undump          heating
reset_timestep   0
######### melted #######

fix        6 g_Film nvt temp 3500.0 3500.0
25.0
compute    mrdf g_Film rdf 100
fix        7 g_Film ave/time 50000 1 50000
c_mrdf file rdf_melted.dat mode vector

timestep   0.025

dump       melted all custom 100 melted_*.dat
id type  xs ys zs x y z q type

run        40000 #1ps 3.2 10^15 K/s

unfix      6
unfix      7
undump          melted
reset_timestep   0
############### cooling ###############

fix        8 g_Film nvt temp 3500.0 300.0 25.0

timestep   0.025

dump       cooling   all custom 100
cooling_*.dat id type  xs ys zs x y z q type
run        60000   # 1.5ps
```

```
unfix      8
undump           cooling
reset_timestep   0

########## cooled ############

fix        9 g_Film nvt temp 300.0 300.0 25.0
fix        10 all reax/bonds 10000
bonds_amorf.dat

timestep   0.025

dump       amorf all custom 100 amorf_*.dat id
type  xs ys zs x y z q type

compute    amorf_rdf g_Film rdf 100
fix        11 g_Film ave/time 50000 1 50000
c_amorf_rdf file rdf_amorf.dat mode vector

run        140000 #4ps

unfix      9
unfix      10
unfix      11
undump           amorf
reset_timestep   0
```

Lampiran 2 :*script input* proses Nitrogenasi a-Si

```
units           real
boundary        p p f
atom_style      charge
read_data       amorf.data

pair_style      reax
pair_coeff      * * ffield.reax 6 6 4

group           g_fix  type 1
group           g_Film type 2 3

compute         peratom all pe/atom
compute         pe_atom all reduce ave
c_peratom
compute         Film_temp g_Film temp

thermo          100
thermo_style    custom step c_Film_temp temp
c_pe_atom pe ke etotal vol press
thermo_modify   lost ignore norm yes

neighbor        2 bin
neigh_modify    every 1 delay 0 check yes

fix        walls all wall/reflect zhi 130.0


fix        1 g_fix setforce 0.0 0.0 0.0

velocity   all create 300.0 432732 rot yes
dist gaussian loop geom

fix        2 g_Film nvt temp 300.0 300.0 100

fix        4 all reax/bonds 20000 bonds.dat
```

```
compute    rdf g_Film rdf 100 2 2 2 3

fix        5 g_Film ave/time 20000 1 20000
c_rdf file rdf.dat mode vector

timestep   0.05
dump       datdump  all custom 80 a-
SiN300_*.dat id type  xs ys zs x y z q  type


restart    10000 restart6.*

run   400000 ## 20 ps
write_restart   restart6.*
```

Lampiran 3 :*Read_data* atom N

```
LAMMPS readable file from
(number,type,charge,x,y,z)

           4208 atoms
           0 bonds
           0 angles
           0 dihedrals
           0 impropers

           3 atom types
           0 bond types
           0 angle types
           0 dihedral types
           0 improper types

      0.000000 38.400800 xlo xhi
      0.000000 38.400800 ylo yhi
      0.000000 130.000000 zlo zhi
Masses

           1 28.0860
           2 28.0860
           3 14.0067

Atoms

1 1 5.84657e-08 0 3.84008 0.933993
2 1 -2.67395e-07 1.92004 3.84008 2.22549
3 2 6.3584e-07 1.90799 5.7592 3.5347
4 1 5.84658e-08 3.84008 3.84008 0.933993
5 1 -2.67395e-07 5.76013 3.84008 2.22549
6 1 -2.67395e-07 5.76013 0 2.22549
7 1 -2.67395e-07 1.92004 0 2.22549
8 2 6.35841e-07 5.21075 1.93443 3.44108
9 2 6.35841e-07 3.46906 1.8779 5.43223
10 2 6.35841e-07 2.86987 1.89225 3.15012
11 2 6.35841e-07 5.75625 5.84778 3.54332
```

12 2 6.35841e-07 6.35787 2.07185 5.56544
13 2 -1.35446e-06 -0.0247695 5.56353 5.10361
14 1 5.84661e-08 7.68017 3.84008 0.933993
15 2 -1.35446e-06 7.65595 5.87856 4.77093
16 2 -1.35446e-06 8.16351 0.653741 5.08053
17 1 -2.67394e-07 9.60021 3.84008 2.22549
18 2 6.35842e-07 9.67713 1.88584 3.56146
19 2 -1.35446e-06 11.5765 1.7912 4.65633
……
……
4204 3 0 31.235 30.79589 87.708
4205 3 0 9.0111 10.0957 77.5637
4206 3 0 17.2283 2.0104 97.159964
4207 3 0 18.290854 20.2365121 85.7938
4208 3 0 19.29085 21.236514 86.793800

Lampiran 4: Data grafik 4.2 RDF *(Radial distribution function)*

Radius (Å)	**Kondisi**		
	quenching	***melting***	***ekuilibrium***
0,05	0	0	0
0,15	0	0	0
0,25	0	0	0
0,35	0	0	0
0,45	0	0	0
0,55	0	0	0
0,65	0	0	0
0,75	0	0	0
0,85	0	0	0
0,95	0	0	0
1,05	0	0	0
1,15	0	0	0
1,25	0	0	0
1,35	0	0	0
1,45	0	0	0
1,55	0	0	0
1,65	0	0	0
1,75	0	0,0124531	0,0126346
1,85	0	0,0594321	0,0602982
1,95	0	0,330995	0,329034
2,05	0,0030693	1,17681	1,14792
2,15	0,692038	2,56887	2,5784
2,25	7,35348	3,85247	3,88313
2,35	9,06049	4,30978	4,35623
2,45	2,33599	3,06709	3,13757
2,55	0,321375	1,86536	1,9342
2,65	0,0771506	1,0827	1,11685
2,75	0,0272923	0,541368	0,557786
2,85	0,026999	0,485263	0,48757
2,95	0,220869	0,566887	0,575148
3,05	0,880579	0,794123	0,802922
3,15	1,41451	0,9726	0,977673
3,25	1,33369	1,15563	1,16393
3,35	1,2725	1,40491	1,41849
3,45	1,60191	1,79149	1,80134
3,55	2,46595	2,17124	2,19673

3,65	3,18288	2,66568	2,70453
3,75	3,55848	2,88167	2,89797
3,85	3,50485	2,9561	2,99396
3,95	3,05761	2,8776	2,93276
4,05	2,46333	2,7016	2,73861
4,15	2,15879	2,44156	2,48163
4,25	1,82699	2,2013	2,25338
4,35	1,72964	2,10261	2,1387
4,45	1,71402	1,87369	1,90425
4,55	1,58841	1,76275	1,78782
4,65	1,47369	1,60307	1,63121
4,75	1,43288	1,45063	1,47234
4,85	1,3936	1,38872	1,40951
4,95	1,39104	1,30879	1,31891
5,05	1,50951	1,29686	1,31323
5,15	1,66791	1,33137	1,34785
5,25	1,78893	1,36094	1,37844
5,35	1,85203	1,40473	1,41934
5,45	1,99405	1,55486	1,56579
5,55	2,01289	1,63763	1,66023
5,65	2,053	1,74986	1,76768
5,75	2,13478	1,80875	1,83511
5,85	2,13103	1,91279	1,93878
5,95	2,03377	1,94888	1,974
6,05	1,85853	2,01839	2,04922
6,15	1,88113	1,97144	1,9913
6,25	1,84817	2,05698	2,08893
6,35	1,90272	2,12483	2,1558
6,45	1,96264	2,07902	2,1118
6,55	2,06796	2,17341	2,20117
6,65	2,02811	2,21291	2,24341
6,75	2,05907	2,15257	2,17998
6,85	2,08408	2,03707	2,06868
6,95	2,106	2,0381	2,07315
7,05	2,16452	1,97711	2,01086
7,15	2,10087	1,99458	2,01935
7,25	2,0816	1,96751	1,99717
7,35	2,09221	1,92917	1,9537
7,45	2,08361	1,9657	1,99412
7,55	2,05322	1,9432	1,9645
7,65	2,08609	2,03266	2,06118

7,75	2,05322	2,0195	2,04549
7,85	1,99517	1,98818	2,01862
7,95	1,97204	1,91192	1,93509
8,05	1,94127	1,98304	2,01473
8,15	1,94403	1,90692	1,93471
8,25	1,95216	1,84528	1,87786
8,35	2,01948	1,8267	1,8511
8,45	1,96329	1,83287	1,85578
8,55	2,02493	1,82782	1,85304
8,65	2,02942	1,76728	1,79338
8,75	2,04936	1,79189	1,81732
8,85	2,05585	1,79513	1,82244
8,95	2,05703	1,81779	1,84943
9,05	2,03939	1,8387	1,86124
9,15	2,05901	1,87057	1,89906
9,25	2,05981	1,91906	1,94341
9,35	2,09612	1,98282	2,00891
9,45	2,08826	2,10895	2,13723
9,55	2,1483	2,15746	2,18621
9,65	2,15748	2,27383	2,29893
9,75	2,16937	2,34714	2,37538
9,85	2,1637	2,35071	2,38563
9,95	2,15653	2,35687	2,38744

Lampiran 5 : Data Hasil dan Pembahasan

1. Grafik 4.4 Jumlah atom N berdasarkan kedalaman

Kedalaman	Jumlah atom N			
	300K	600K	900K	1200K
0 – 2.5	27	17	18	9
2.5 – 5	32	50	50	46
5 – 7.5	23	46	59	88
7.5 – 10	0	3	2	14
jumlah	82	116	129	157

2. Grafik 4.5 Fraksi jumlah atom N berdasarkan kedalaman

Kedalaman	Fraksi Jumlah atom N			
	300K	600K	900K	1200K
0 – 2.5	32,93%	14,66%	13,95%	5,73%
2.5 – 5	39,02%	43,10%	38,76%	29,30%
5 – 7.5	28,05%	39,66%	45,74%	56,05%
7.5 – 10	0,00%	2,59%	1,55%	8,92%
jumlah	100,00%	100,00%	100,00%	100,00%

3. Grafik 4.6 Jumlah ikatan n-*fold* atom Si sebelum dan sesudah nitrogenasi

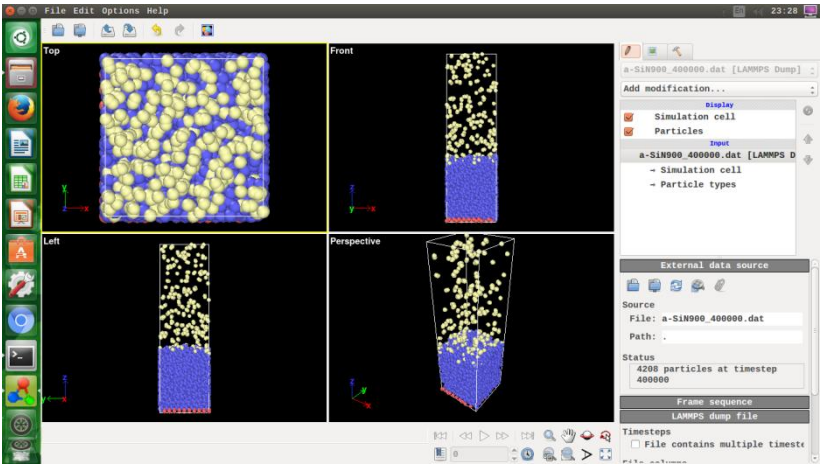
n-fold	Kondisi				
	Awal	300 K	600 K	900 K	1200 K
2	1	1	1	2	2
3	51	36	36	27	26
4	801	382	275	230	569
5	102	87	151	197	257
6	0	2	22	53	98
7	0	0	1	1	3

4. Grafik 4.7 Jumlah ikatan n-*fold* atom N

n-fold	Kondisi			
	300 K	**600 K**	**900 K**	**1200 K**
0	138	70	36	23
1	174	220	250	268
2	20	16	10	6
3	19	32	22	25
4	4	38	75	98
5	1	5	10	20
6	0	0	1	0

Lampiran 5 : Tampilan Perangkat Visualisasi

1. Tampilan Perangkat OVITO saat memvisualkan hasil nitrogenasi 600K



2. Tampilan atom Eye saat memvisualkan hasil nitrogenasi 1200K