Hello user：

I am trying to calculate the stress-strain curves during tensile-induced crystallization. My date file containing 200 chains with chain length of 200 UA model and CNTs. Then, I run my system based on the in file, the content of which can also be seen in the following sections.

But the fluctuation of the stress-strain curve has a very strange phenomenon. As can be seen in the following picture, the stress-strain curve (The length of cnt is 36.89 and the number is 4, m=n=7) fluctuates too much. I don't know where is the problem in the in file and how to smooth the stress strain curve. Please give me some advice.

I really appreciate your help.

THANKS.

Here is my stress-strain curve:



Here is my in file:

units metal

dimension 3

boundary p p p

atom\_style molecular

read\_data Poly.data

pair\_style hybrid/overlay airebo 3.0 0 0 lj/cut 10

pair\_modify tail yes

bond\_style harmonic

angle\_style harmonic

dihedral\_style fourier

pair\_coeff 1 1 lj/cut 0.004857 4.01

pair\_coeff 1 2 lj/cut 0.004944 3.71

pair\_coeff \* \* airebo ./CH.airebo NULL C

bond\_coeff 1 15.1795 1.53

angle\_coeff 1 2.6022 109.5

dihedral\_coeff 1 3 0.03513 1 0 -0.01865 2 0 0.07026 3 0

neighbor 2 bin

neigh\_modify every 1 delay 0 check yes

minimize 0.0 4.336e-10 1000 100000

min\_style cg

run\_style verlet

# reset\_timestep 0

timestep 0.001

fix 1 all npt temp 400 400 0.1 y 1 1 1 z 1 1 1 drag 0.5

fix 2 all deform 1 x erate 1e-2 units box remap x

thermo\_style custom step temp etotal pe epair ebond eangle edihed density lx ly lz pxx pyy pzz

thermo 1000

compute 4 all rdf 200 1 1

fix 3 all ave/time 3000 1 3000 c\_4[\*] file temp4.rdf mode vector

variable l\_x equal lx

variable lx0 equal ${l\_x}

variable strain equal (lx-v\_lx0)/v\_lx0

variable stressx equal "-pxx/1000"

variable stressy equal "-pyy/1000"

variable stressz equal "-pzz/1000"

fix 4 all ave/time 1 300 100000 v\_strain v\_stressx v\_stressy v\_stressz file strain\_stress.txt

thermo\_style custom step temp v\_strain v\_stressx v\_stressy v\_stressz pe etotal epair ebond eangle edihed density lx ly lz pxx pyy pzz

thermo 1000

dump lashen1 all custom 100000 lashen1.lammpstrj id type element x y z ix iy iz

dump\_modify lashen1 sort id pad 6

dump lashen2 all custom 10000 LSdump.\*.txt id mol type x y z xu yu zudump\_modify lashen2 sort id pad 8

run 600000

undump lashen1

undump lashen2

unfix 1

unfix 2

write\_restart restartLS.equil

write\_data dataLS.polymer