Input file :

# 3D peridynamic simulation for traction

units nano

dimension 3

boundary s s s

atom\_style peri

atom\_modify map array

neighbor 0.1 bin

lattice sc 0.3615

 #define all the parts

region beam block 0 36.15 0 2.169 0 2.169 units box

create\_box 1 beam

create\_atoms 1 region beam

region leftbc block 0 1.0845 0 2.169 0 2.169 units box

group leftbc region leftbc

region rightbc block 35.0655 36.15 0 2.169 0 2.169 units box

group rightbc region rightbc

group boundary union leftbc rightbc

region lastbc block 100 100 0 0 0 0

group lastbc region lastbc

region firstbc block 0 0 0 0 0 0 units box

group firstbc region firstbc

group middle\_atoms subtract all boundary

pair\_style peri/eps

pair\_coeff \* \* 37000 27750 1.0846 0.009 0.25 40e3

set group all density 8960e-6

set group all volume 0.047241

run 100

velocity all set 0.0 0.0 0.0 sum no units box

fix 1 middle\_atoms nve

compute peratom middle\_atoms stress/atom NULL

compute sigmaxx middle\_atoms reduce sum c\_peratom[1]

variable sigmavolxx equal c\_sigmaxx/(0.94\*vol)

timestep 0.005e-3

fix 2 rightbc move linear 1.8075 0 0 units box

fix 3 leftbc move linear -1.8075 0 0 units box

thermo 100

thermo\_style custom step v\_sigmavolxx lx temp

dump 1 firstbc custom 100 peri\_nano\_resf.txt id x

dump\_modify 1 append yes

dump 2 lastbc custom 100 peri\_nano\_resl.txt id x

dump\_modify 2 append yes

run 20000

unfix 1

unfix 2

unfix 3

fix 4 middle\_atoms nve

fix 5 rightbc move linear -1.8075 0 0 units box

fix 6 leftbc move linear 1.8075 0 0 units box

dump 3 firstbc custom 100 peri\_nano\_resf.txt id x

dump\_modify 3 append yes

dump 4 lastbc custom 100 peri\_nano\_resl.txt id x

dump\_modify 4 append yes

run 20000