

Supporting Information

Carbon nanotube triaxial woven films with high mechanical property for impacting protection

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Input code of bilayer films impacting simulation for MD simulation.

```
units      metal
dimension   3
atom_style  full
boundary    s s s
atom_modify map yes
read_data   san7.0ro0.data
read_data   plaindata add append
mass        * 12.017
pair_style  airebo 3.0 1 1
pair_coeff  * * CH.airebo C
timestep    0.001
thermo_style custom step temp pe ke epair etotal press pxx pyy pzz vol lx ly lz
thermo      100
neighbor    2.0 nsq
neigh_modify every 1 delay 0 check yes
compute     ke all ke/atom
compute     s all stress/atom NULL virial
compute     peratom all pe/atom
variable    mises atom "0.707106781 * sqrt( (c_s[1] - c_s[2])^2 + (c_s[2] - c_s[3])^2 + (c_s[1] - c_s[3])^2 + 6*(c_s[4]^2 + c_s[5]^2 + c_s[6]^2) )"
velocity    all create 10 4928459 sum no dist gaussian loop local
velocity    all zero linear
dump       1 all custom 10000 mini.*.lammpstrj id type x y z
min_style  cg
minimize   0 0 1000000 10000000
fix        1 all nve
fix        2 all temp/berendsen 1.0 1.0 0.5
run       10000
```

```

undump    1
unfix    1
unfix    2
write_restart minimize*.restart
region    left    block INF INF INF INF 150 INF INF
region    stre    block INF INF 1400 INF INF INF
region    up      block INF INF INF INF 150 INF
region    bottom   block INF INF INF INF INF 1400
group     up      region up
group     bottom   region bottom
group     left    region left
group     stre    region stre
fix       6 up setforce 0 NULL 0
velocity  up set 0.0 NULL 0.0 units box
fix       7 bottom setforce 0 NULL 0
velocity  bottom set 0.0 NULL 0.0 units box

fix       4 left setforce 0 0 0
velocity  left set 0.0 0.0 0.0 units box
fix       8 stre setforce 0 NULL 0
velocity  stre set 0.0 NULL 0.0 units box
variable  stre1 equal -pyy
variable  stressy equal v_stre1*lx*lz/(PI*6.7*3.4*10000*4*sin(PI*60/180))
variable  1 equal xcm(stre,y)
variable  3 equal xcm(left,y)
variable  initial_y equal v_1-v_3
variable  iniy equal ${initial_y}
variable  strainy equal (v_1-v_3-v_iniy)/v_iniy
fix      1 all nve
fix      2 all temp/berendsen 1.0 1.0 0.5
fix      3 all ave/time 1 100 1000 v_strainy v_stressy file stre_stress.txt
fix      ave all ave/atom 1 100 1000 v_mises c_peratom
dump    1 all custom 5000 2layerstre.*.lammpstrj id type xs ys zs f_ave[1] f_ave[2]
unfix    8
fix      5 stre move linear 0.0 0.05 0.0 units box
run      5000000

```

```
write_restart  stre*.restart
undump      1
```