

Indentation code by Yongjian 2017/6/18

1. Special indenter implementation with friction

lammps version: lammps-4Feb14

Triangular indenter with rounded tip: see attached indenter implementation

Indenter fix example:

```
fix 100 all indent $k triangle z v_halfx v_y ${rad} angle ${tip_angle} orient y minus side out frict ${cof}
```

```
approach ${svel} units box
```

explanation: \$k is the spring constant between indenter and atom; z means the indenter is in the

plane of xy; v_halfx is the x position and v_y is the y position of the indenter; rad is the tip radius;

tip_angle is the triangle tip angle; orient y means the indentation direction is along y; cof is the friction

coefficient between the indenter and atoms; “approach” means the indenter is approaching the surface,

otherwise, it should be “retract”; svel is the indentation velocity.

2. Indentation simulation

(1) Input code: s

You can control the temperature, velocity, load, adhesion, etc on the first

2~15 lines inside the input file.

(2) Readdata file: olivia.T-0.036.readdata sample relaxed at Temp=0.036

(3) Output:

lata4olivia_indent: atom configuration during the indentation.

log.lammps, log.sliding, format:

step temp pe etotal press vol f_100[2] f_200[1] v_displ

f_100[2] and f_200[1] is the force on the indenter in indenting directions and the force on the wall in indenting directions.

v_displ is the indenter's displacement

indent- stress-dist: stress distribution of the sample in xy plane

3. Convert indent- stress-dist to .xyz file

Correct syntax: stress2xyz-version2.pl file (e.g indent-stress-dist)

element_size (coarse grain size, e.g.5)

The above code would search for log.lammps file for the 2.5D sample's thickness. If it does not exist, a default value 10.3581 would be used for the thickness.

Output: .xyz file, format:

Id x y z number_of_atom_in_this_grid sigma_xx sigma_yy sigma_zz sigma_xy sigma_xz sigma_yz,
hydrostatics_pressure