

The deform keyword

From GPUMD

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Purpose

This keyword is used to deform the simulation box, which can be used to do tensile tests.

Grammar

It requires 4 parameters:

```
deform strain_rate deform_x deform_y deform_z
```

Here, strain rate specifies the speed of the increase of the box length, which is in units of A/step. For example, suppose the box length (in a given direction) in the beginning of a run is 100 Å and this parameter is 10^{-5} Å/step, then a run with 10^6 steps will change the box length by 10%. This gives a strain rate of 10^8 s^{-1} if the time step is 1 fs. The second parameter deform_x can be 0 or 1, where 0 means do not deform the x direction and 1 means deform the x direction. The last two parameters have similar meanings for the y and z directions.

Examples

Example 1

- For uniaxial tensile test, one can first equilibrate the system and then deform the box:

```
# The equilibration stage
ensemble npt_ber 300 300 0.1 0 0 0 0.0005
run 1000000

# The production stage
ensemble npt_ber 300 300 0.1 0 0 0 0.0005
neighbor 1
deform 0.00001 1 0 0
run 1000000
```

- Currently, one must use the NPT ensemble when using this keyword. That is, the code assumes that the pressure components in the directions which are not deformed will be controlled.
- Also note that we have chosen to update the neighbor list. When the system is deformed, the neighbor list might need to be updated.

- In the equilibration stage, it is also recommended to use the NPT ensemble to obtain the zero strain state before applying the deformation.

Caveats

- See the example above.

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