

Please construct a simulation box oriented along $[01\bar{1}] - [\bar{2}11] - [111]$ parallel to x-y-z frame with a size of 22 atoms x 100 atoms x 50 atoms employing W potential under periodic boundary conditions at 10 K. Create a hole at a coordinate of (y,z) = (30,45) with a radius of 4 Angstroms and centerline parallel to x axis. After relaxation and energy minimization procedures as introduced in the class, apply a positive sign shear deformation yz at an engineering strain rate of 0.01 for 40000 steps and generate the shear stress vs shear strain plot. Similarly repeat the same simulation by reorienting the simulation box along $[\bar{1}10] - [\bar{1}\bar{1}2] - [111]$. Please comment on the dislocation nucleation stress in two cases by comparing the shear stress- shear strain plots. Provide your input files and include screenshots from Ovito.

Hint :

Please insert these two lines in the input file for W potential:

```
pair_style eam/fs
```

```
pair_coeff ** W.eam.fs W
```

The crystal structure of W is bcc and has an equilibrium lattice constant of $a = 3.165$ Angstroms.

Ans.