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LAMMPS Module

A3. Approach to Equilibrium

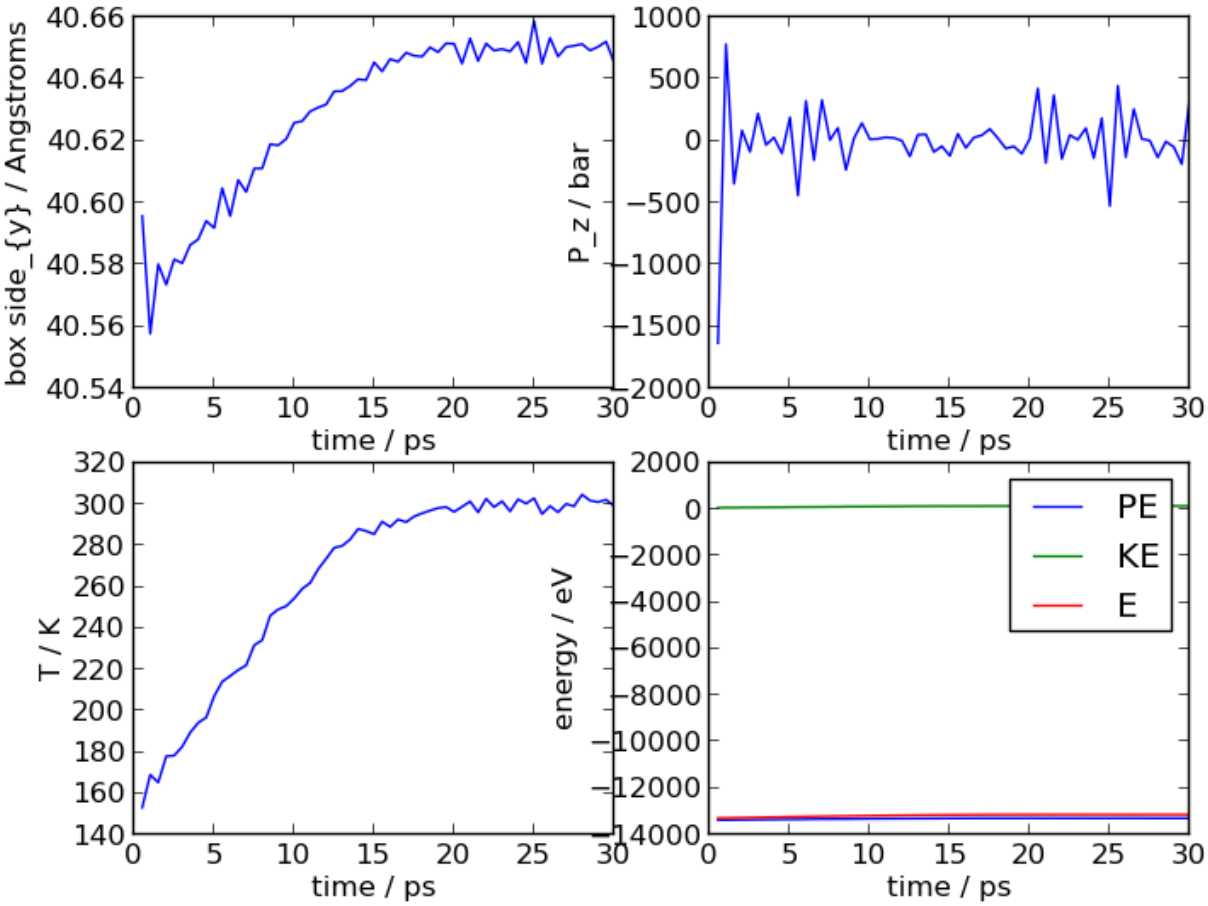

Figure 1. This shows convergence for (i) box side length, (ii) pressure, (iii) temperature and (iv) kinetic potential and total energy at around 30ps.

- Based on the plots produced, the system does converge to points at around 30ps. This can be seen as the plots seem to converge to a point in energy, temperature, box side length and pressure as time approaches the 30ps mark.

A4. Stress Strain Behavior

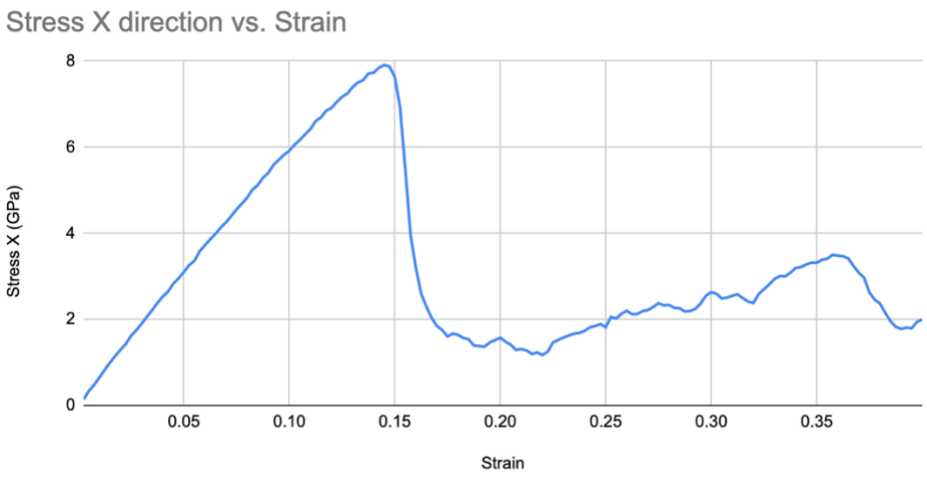

Figure 2. Stress in the x-direction vs strain graph. Here Hookean behavior is observed

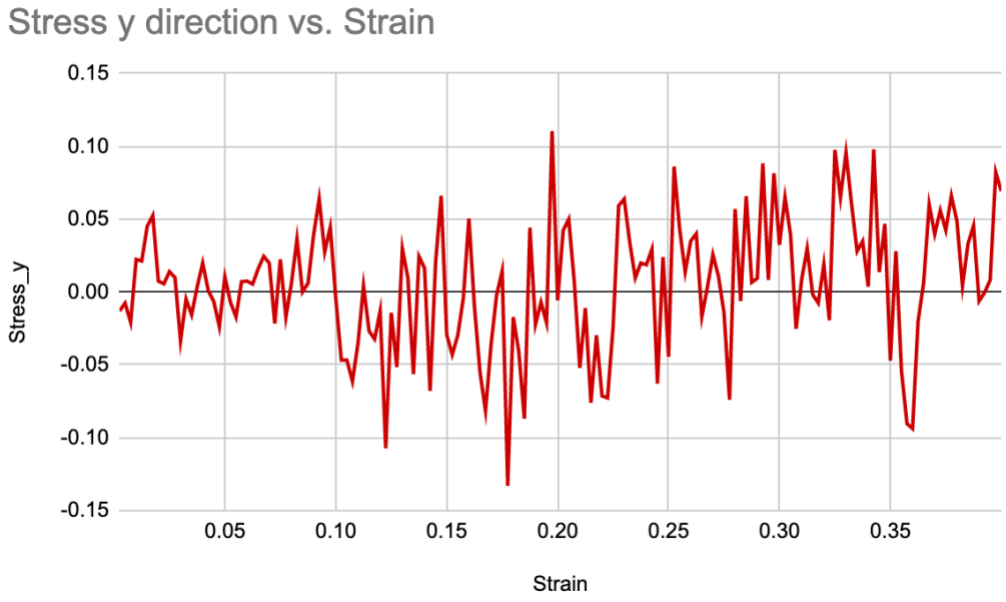

Figure 3. Stress in the y-direction vs strain graph. Hookean behavior is not observed.

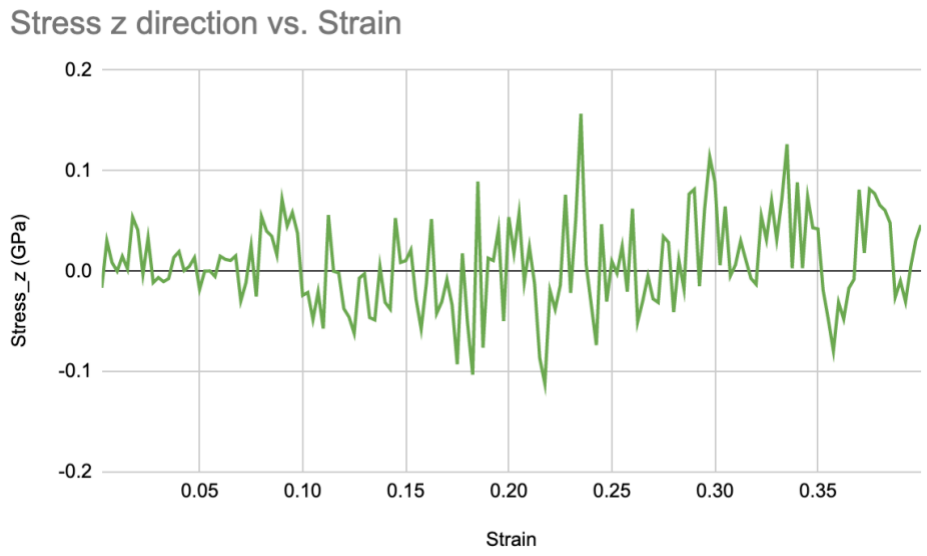

Figure 4. Stress in the z-direction vs strain graph. Hookean behavior is not observed.

- The physical rationalization for the different behaviors in the x, y, z direction exemplifies that stress is being applied in the x-direction. Directions of x and y seem like random noise as the stress is not loaded in these directions.

- The range of strains where Hookean stress-strain behaviors is observed is between 0-0.15

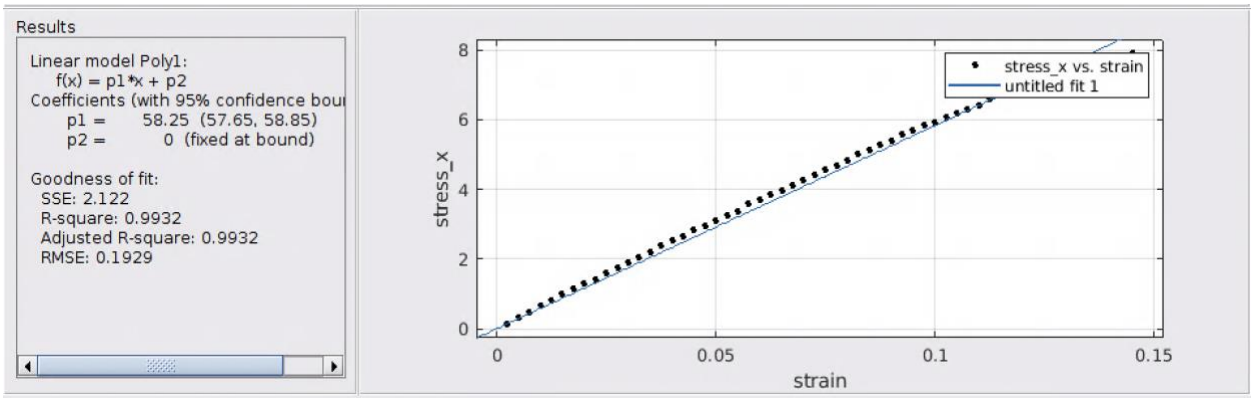

Figure 5. Linear fit on Stress in X direction vs strain graph to find Young's Modulus.

- Based on the produced fit using Matlab, the Young's Modulus extrapolated by the linear fit was 58.25GPa with a 95% confidence interval (57.65, 58.85).
- An experimental measure of aluminum's Young's Modulus is 68.3 GPa [1]. Comparing this to the obtained value of 58.25 we have a percent error of 17.25%.
- The yield strength of Al from the simulation was found to be 7.3972 GPa
- A referenced yield strength was found to be 276 MPa which is magnitudes below the found yield strength which is because the simulation runs on the microscopic level

assuming a perfect lattice and thus accounts for no defects in the material. The percent error can be seen as large due to the magnitude differential resulting in a percent error of 2580%.

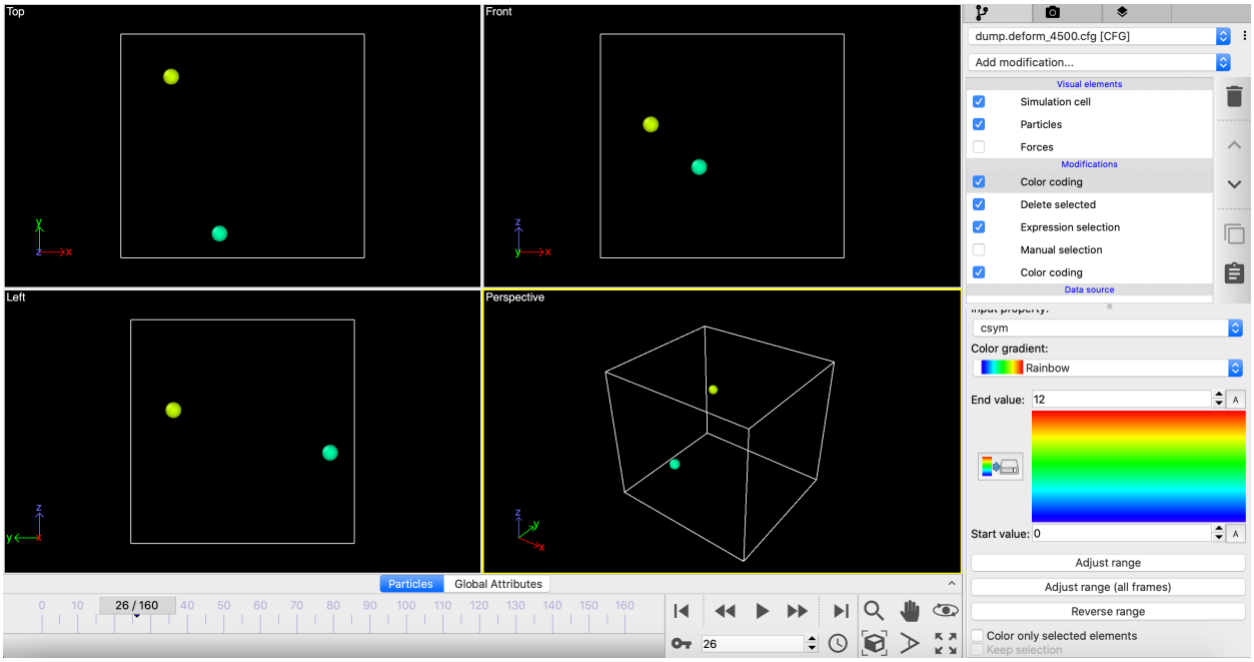

Figure 6. Ovito Imaging of dislocation planes begin to nucleate

B3. Construct Input Script

- This command is to set a variable “strain” equal to a variable expression that would calculate the quantity of strain by multiplying he constant of proportionality between the x-distance of the boundary atom from the centerline of the block and its z-velocity (v_vperAng) with time and instantaneous length in the x-direction (lx) all divided by the instantenous length in the x direction.

B4. Stress-Strain Behavior

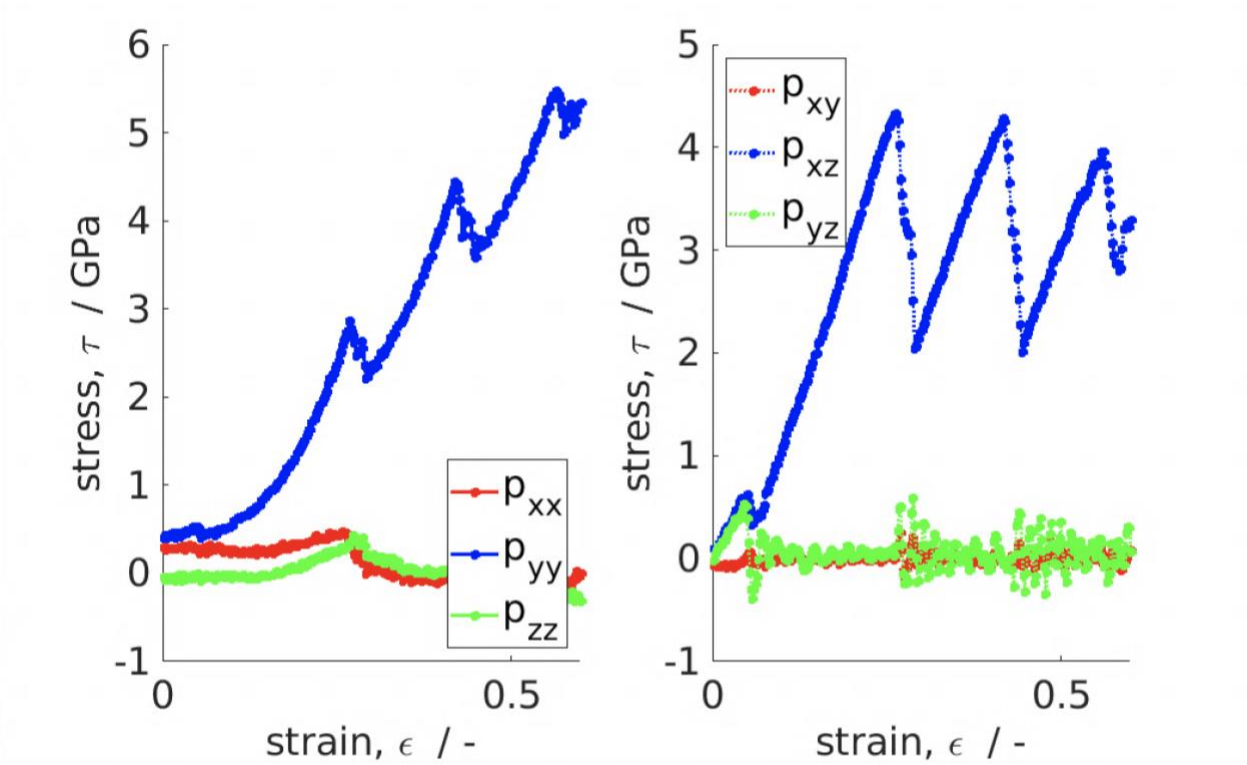

Figure 7. (i) normal stress p_{xx}, p_{yy}, p_{zz} vs strain curve against xz strain (ii) off diagonal components of the stress for p_{xx}, p_{yy}, p_{zz} against xz strain

- The value of the Peierls stress for the irreversible movement of a screw dislocation is fiven by the first peak in the pxx and pzz. Thus it can be estimated as 0.3 GPa.
- The molecular dynamics model is close to the value of 256MPa given. The percent error is given by 17.19% which is reasonable

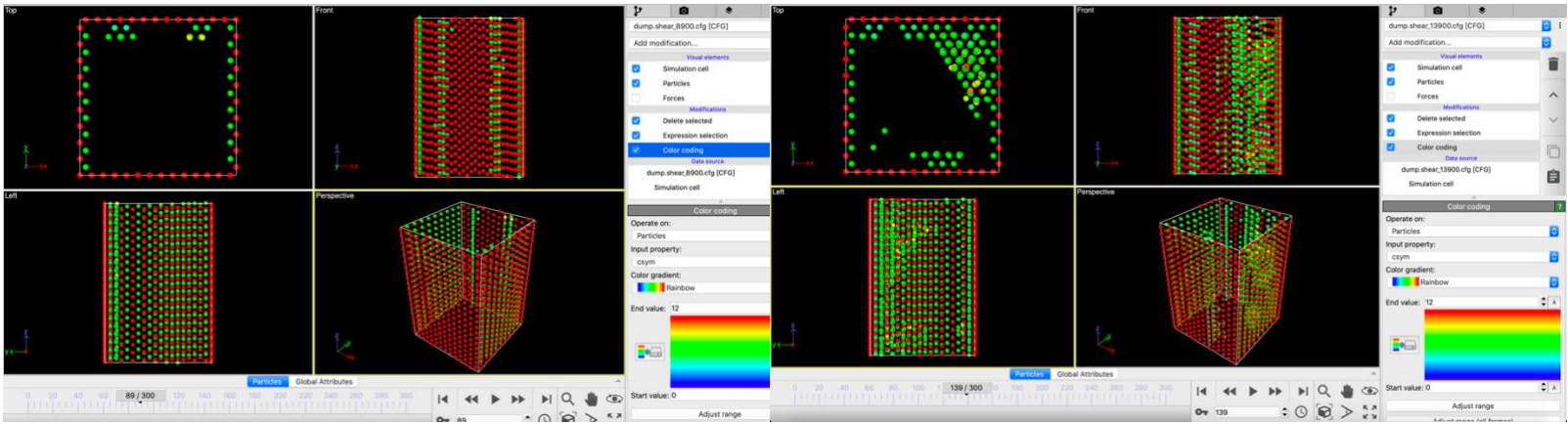

Figure 8. (i) System under initial configuration and (ii) irreversible motion of preexisting dislocations.