Use the “nano-Materials Simulation Toolkit” nanoHUB.org to calculate the elastic constants C11, C12, and C44 for platinum at 300K and 1000K. You will be able to define the loading conditions and can plot the stress-strain curves from which you can measure C11 and C12. You can then calculate C44 by measuring C11 at a different orientation. **Complete the following include a sample output from the simulation with calculations:**

a) Using the Pt unit cell, choose the size of the supercell and report the dimensions in nm.
b) Choose your loading parameters and calculate the strain rate.
c) Run the simulation and for a given time report the strain tensor and the stress tensor.
d) Use your result from part-c to find C11 and C12.
e) Use the Pt [111] unit cell and indicate the coordinate system.
f) Repeating the steps above find C'11 for the [111] direction. Be sure to pick the correct loading conditions for your coordinate system.
g) Calculate C44 noting that:

\[ C'_{11} = C_{11} - 2[C_{11} - C_{12} - 2C_{44}](\ell^2 m^2 + m^2 n^2 + n^2 \ell^2) \]

where \( \ell, m, \) and \( n \) are the directional cosine between \(<100>\) and \([hkl]\).

(for example assuming unit vectors: \( m = [0 1 0] \cdot [hkl] \))

h) Compare your results to
TABLE XI. Elastic constants of fcc metals in units of GPa at 0 K. At each entry, the first number gives the experimental result while the second number in round brackets is the static calculation of Sutton and Chen (Ref. 1). Third number is the MD result.

<table>
<thead>
<tr>
<th>Metal</th>
<th>$C_{11}$ (GPa)</th>
<th>$C_{12}$ (GPa)</th>
<th>$C_{44}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>261.13(230.69)231.37</td>
<td>150.59(177.82)176.59</td>
<td>131.36(80.10)79.08</td>
</tr>
<tr>
<td>Cu</td>
<td>176.22(169.81)168.77</td>
<td>124.96(129.76)128.77</td>
<td>81.70(57.87)57.68</td>
</tr>
<tr>
<td>Ag</td>
<td>131.36(140.98)140.98</td>
<td>97.72(96.12)96.02</td>
<td>51.26(59.27)59.10</td>
</tr>
<tr>
<td>Au</td>
<td>187.43(179.42)179.74</td>
<td>155.39(147.38)147.49</td>
<td>44.86(41.64)42.11</td>
</tr>
<tr>
<td>Pt</td>
<td>357.25(313.99)314.02</td>
<td>254.72(257.92)257.70</td>
<td>76.90(73.69)73.54</td>
</tr>
<tr>
<td>Rh</td>
<td>421.33(339.62)340.63</td>
<td>192.24(232.29)232.24</td>
<td>193.84(142.58)142.73</td>
</tr>
</tbody>
</table>
nano-Materials Simulation Toolkit

This MD simulation tool developed by Professor Alejandro Strachan and can be used to access research-grade simulation codes on nanoHUB.org. Professor Strachan teaches an on-line course on molecular dynamics that can be viewed at https://nanohub.org/resources/5838; the first lecture provides an overview of how the method works.

Molecular dynamic simulations using the tools at nanoHUB.org of FCC nanowires
Step 1: Go to the nanohub.org
Step 2: Create an account and Login
Step 3: Click on “All Tools” and select: nano-Materials Simulation Toolkit
Step 4: Enter the conditions and select “simulate”

1) Pick the input model (hoover the mouse over the selection to see the details of the structure)
2) Define a Supercell.
3) Enter in the “loading conditions”

- **Ensemble:** NVE
- **MD time step:** 0.002ps
- **Number of steps:** 2000
- **Temperature:** 100K
- **Temperature increment (K/ps):** 0
- **Strain per MD step:**
  - X direction: 2e-5
  - Y direction: 0
  - Z direction: 0

4) Run the simulation

5) Examine the output plots (for example the “xx stress tensor component vs. Time”). Use the strain rate the strain values.

**Note in this case there is NO strain in the Y and Z directions.**

The structure is constrained in the domain defined by the supercell. You can use the Advanced Options to remove material to remove this constraint for example to create a nanowire.