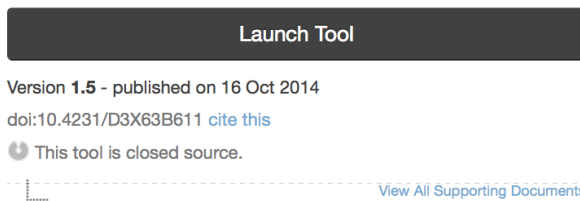


nanoHUB Materials Simulation Homework: Engineering the Yield Stress of a Material by Controlling Grain Size

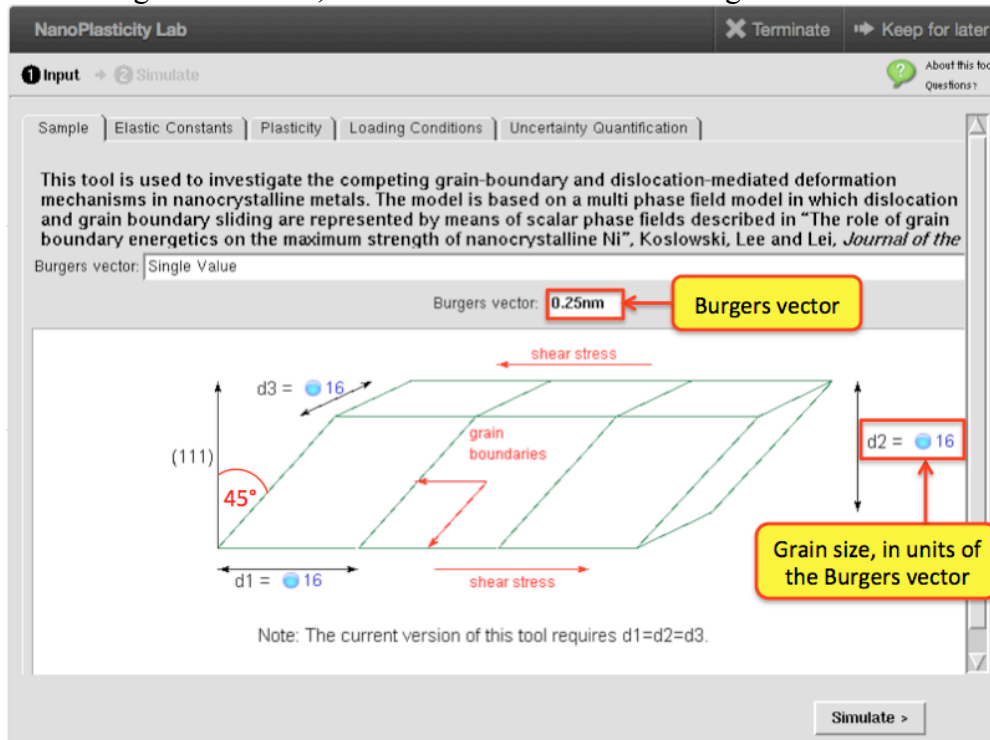
It may seem that the yield stress of a sample is a fundamental materials property, but it can be engineered by controlling the grain size. This phenomenon, often called the “Hall-Petch effect”, is used to obtain materials with a high yield stress. To see this effect, you can run a dislocation dynamics simulation¹ in nanoHUB.org that compares nickel samples with grain sizes of 4 nm and 16 nm.

First, create a free account at <https://nanohub.org>. This account will give you access to many tools, seminars and classes. Then, follow the simulation steps listed below.

1. Go to the **nanoplasticity lab** simulation tool at <https://nanohub.org/resources/nanoplasticity>, and click the *Launch Tool* button. You may have to install the latest version of Java in your browser to run the simulation. Most browsers should work, except Chrome, which does not work with Java.



2. Below is the screen that you will see when you launch the tool. The sample is a repeating array of grains, tilted at 45° as shown in the figure. To specify the grain size, change the values of the grain dimensions d1, d2, and d3, which are given as multiples of the Burgers vector. The default Burgers vector length is 0.25 nm, so use d1 = d2 = d3 = 16 for a grain size of 4 nm.



¹ Marisol Koslowski, Dong-Wook Lee and Lei Lei, Role of the grain boundary energetics on the maximum strength of nanocrystalline Nickel, *Journal of the Mechanics and Physics of Solids*, **59** 1427-1436, 2011.

- Click the *Elastic Constants* tab. Choose **Single Value** and set the **Young Modulus** to $E = 200 \text{ GPa}$. Set the **Poisson's ratio** to a **Single Value** of **0.3**.

The screenshot shows the NanoPlasticity Lab interface. At the top, there are buttons for 'Terminate' and 'Keep for later'. Below that, there are tabs for 'Input' and 'Simulate'. The 'Elastic Constants' tab is selected. Under this tab, there are two dropdown menus: 'Young's modulus' and 'Poisson's ratio'. Both are set to 'Single Value'. Below each dropdown, the specific values are entered in text boxes: '200GPa' for Young's Modulus and '0.3' for Poisson's ratio.

- Open the *Plasticity* tab. Choose **Single Value** and set the **Dislocation Glide Peierls Energy Barrier** to 0.6 J/m^2 . This is the activation energy for dislocation motion. The **Grain Boundary Sliding Energy Barrier** should be set to **Single Value** with an **Energy** of 0.35 J/m^2 . This describes the energy needed for grain boundaries to slide past one another.

The screenshot shows the NanoPlasticity Lab interface with the 'Plasticity' tab selected. There are two dropdown menus: 'Dislocation Glide: Peierls Energy Barrier (J/m^2)' and 'Grain Boundary Sliding: Energy Barrier (J/m^2)'. Both are set to 'Single Value'. Below each dropdown, the specific values are entered in text boxes: '0.6' for Peierls energy and '0.35' for Energy.

- Press **Simulate**. The parameters you entered are sent to the server, and you can monitor the progress of the simulation, which should take just few seconds.
- When the simulation finishes choose **Stress-Strain curve** in the *Result* Tab. The 0.01% strain offset method is used to draw a blue line alongside the simulated results that allows you to determine the yield stress of the sample.
- Repeat this procedure for a larger grain size of **16 nm**.
- Print the two stress strain curves and discuss the obtained results. How does grain size affect the yield strength of this material? You may run additional simulations to test your hypothesis.
- Change the **Grain Boundary Sliding Energy Barrier** to 0.15 J/m^2 and run the simulation again with grain sizes of 4 nm and 16 nm. What do you observe? Hint: this is called the “inverse Hall-Petch effect”. Explain your observation in terms of the relative energies of the two competing plastic deformation processes of dislocation motion and grain boundary sliding.