# Final Project: Prediction of solute effects on dislocation motion

## Goals

For the final project, your goal is to predict the changes in plastic response of aluminum with a solid solution of magnesium using empirical potentials. You will develop data that can be used in larger-length scale modeling. You will quantify (a) changes to the dislocation core, (b) changes to the Peierls stress, and (b) changes to the cross-slip stress from the introduction of solutes. You will also consider how to include these changes in a discrete dislocation dynamics simulation.

Successful completion of this work will demonstrate competence in using MD software to analyze material plastic response, and the ability to design your own computational study.

## Deliverables

You will produce a detailed (5–8) page report that includes an Abstract, Introduction, Methods, Results and Discussion, Conclusions, and Bibliography. This will be graded on your

1. design of computational materials research project (20%),
2. appropriate and competent use of computational tools (50%), and
3. clarity of the report (30%)

Your report should be formatted as a single pdf document comprising your report. You may wish to write your report in latex and convert using `pdflatex`, or in markdown and convert using `pandoc report.text --to latex --out report.pdf`. (`module load pandoc` and `module load texlive` to have the most up-to-date versions of each).

You should creating a subdirectory called `/class/mse404pla/sp25/<your_net_id>/FinalProject` and copying your work into that directory by **11:59pm on 15 May 2025.** ***Late submissions will not be accepted*****; let me know in advance if you will have difficulty with completion.**

## 1. Al screw and edge dislocations with and without Mg

You will need to compute the $T = 0$ relaxed structure of a screw and edge dislocation in Al at three different Mg concentrations: 5at.%, 10at.%, 25at.%. You should work with the Mendelev Al-Mg EAM potential available at the NIST repository information. In the directory `/class/mse404pla/FinalProject`, you will find an initial dislocation geometry for an edge and a screw dislocation. You will also find three files of pseudorandom sequences that you can use to construct your solid solutions: `randnum-5.txt`, `randnum-10.txt`, and `randnum-25.txt`. These sequences were generated by incrementing numbers starting at 1, and with a 5, 10, or 25% probability, printing the number. For example, the start of `randnum-25.txt` looks like

```
3
9
10
15
16
```

```
17
22
28
35
51
```

There is also the python script `Random-sequences.py` if you would like to generate your own sequences. These sequences run up to approximately $10^6$. You will also find an edge and screw dislocation geometry for Al.

You will need to construct relaxed edge and screw dislocation geometries containing 0, 5%, 10%, and 25% Mg to determine the changes in the dislocation core splitting, and the difference between edge and screw dislocations.

### 2. Room temperature Peierls stress with and without Mg

You will investigate the effect of solute on the motion of dislocations by determining the Peierls stress for edge and screw dislocations at 300K with 5%, 10%, and 25% Mg.

### 3. Room temperature Cross-slip stress with and without Mg

In addition, for the screw dislocation, you should determine the *cross-slip stress*, which is the shear stress in the *alternate* $\{111\}$ *plane* that causes the screw dislocation to move on that plane. For example, a $\frac{a}{2}[101]$ screw dislocation can glide on either the $(\bar{1}11)$ plane or the $(11\bar{1})$ plane. If the dislocation core has split onto the $(\bar{1}11)$ plane, then a shear stress applied in the *other* plane can cause the two partial cores to recombine and then split on the $(11\bar{1})$ plane and glide: this is called cross-slip. You should determine the stress for this process without Mg, and then with 5%, 10%, and 25% Mg.

Conclude your assessment with a recommendation of how this materials data could be used in discrete dislocation dynamics simulations to model the effects of solutes on work-hardening.