Exercise Prompts

Fundamentals of Crystallography with Ansys Granta EduPack Software

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Ansys Software Used

This resource uses Ansys Granta EduPack™ teaching software for materials education.

Instructions

Use the Granta EduPack Materials Science & Engineering database to explore crystallography-related topics.

Exercise 1: Exploring Theoretical vs. Measured Density

Density is a highly used material property, as it helps us determine if a product will be light or heavy depending on its volume.

The theoretical equation for density is:

$$\rho = \frac{nA}{V_c N_A}$$

Where n=the number of atoms per unit cell, A=the atomic weight, V_c=the unit cell volume, and N_A =Avogadro's number.

- Using the Elements data-table, find the lattice parameter, atomic weight, and crystal structures for Tungsten, Aluminum, and alpha Titanium and put them in a table
- Use these variables to calculate the theoretical densities for the three elements and add it to the table
- Using the Add Record (other, select Elements table) function in the Tools menu of the main toolbar, create three records for the theoretical density values of Tungsten, Aluminum, and Cobalt. Create a custom subset using the Element records for each element and your custom records. Create a bar chart of density. How do the numbers compare?
- Now create three custom records in the MaterialUniverse for the theoretical density. Create another custom subset in the MaterialUniverse using the added records and the bulk material records for the three metals and recreate the density bar chat. How do the numbers compare? Is there a difference for each unit cell? (use Cast aluminum as the bulk Al record)

Exercise 2: Calculating Atomic Packing Factor

Atomic packing factor (APF) is sphere volume inside a unit cell and is represented by the equation below:

APF=volume of the atoms within a unit cell/total unit cell volume

Calculate the APF for the FCC and BCC unit cell. How do they differ? Why? How does this impact details like the closest packed plane within each unit cell?

Exercise 3: Solid solutions and High entropy alloys.

The Hume-Rothery rules set out criteria for the formation of extensive solid solution:

- Atom size difference less than 15%
- Electronegativity difference less than 0.075
- The components have the same crystal structure
- The components have the same valence within ± 1

Make a chart of Electronegativity against Atomic radius. If you choose a log scale for the Atomic radius and a linear one for Electronegativity you can plot a selection box meets the first two of these rules. If, in addition, you re-color-code the element-by crystal structure the chart allows the third criterion to be applied. To do this, add a Limit stage, sequentially select; Crystal structure “Cubic: face centered”, “Hexagonal close packed” etc. isolating materials of a single structure, high-light the list that appears in the Results window, right-click on high-lighted list and select “Recolor”, giving a choice of color; finally clear the Limit stage and proceed to the next structure. It is now easy to pick pairs of materials that will form extensive solid solutions. The final valence criterion can be applied if desired by adding another Limit stage.

High entropy alloys are solid solutions with four or more components each with concentrations above 5%. The cumulative entropy of mixing as the components mix reduces the free energy of the alloy, stabilizing the alloy and enhancing mechanical properties. The Hume-Rothery rules give guidance in selecting components to make such alloys. Use your chart to Identify some clusters of elements that might form high entropy alloys.

Exercise 4: Make yourself a structure table.

There are many other things you can do with the Elements data-table. Here is one that will illustrate the method.

- Open the Elements data-table. Apply a limit stage. Select “Structure – Cubic, face-centered. “Click Apply”.
- A list of all the elements in the Periodic table with the FCC structure appears in the “Results” window.
- Highlight the list and copy and paste into WORD as the first column of a 4-column table.
- Open any one of the selected records. Copy and paste into WORD. Copy and resize the crystal structure image. Paste it into the top of Column 1 of the table
- Clear the limit stage, and repeat the process for Hexagonal close packed, Cubic, body-centered and Cubic, diamond type, thereby filling the remaining 3 columns.

The result: a useful single-sheet look-up table for the elements with the most important crystal structures.

Exercise 5: Explore Soldi Solution Strengthening

Defects in crystal structures can be used to our advantage during processing to alter the properties of various materials. Open the Structure science notes located on the homepage of the MS&E database to answer the following questions

Open the solid solution strengthening science note.

1. What four parameters are crucial for determining solid solubility?
2. How does solid solution strengthening impact dislocation motion?
3. Is there a limitation to the degree of strengthening that can be achieved through this mechanism?
4. How does the jewelry industry take advantage of solid solution strengthened alloys?

Exercise 6: Explore Precipitation Strengthening

Defects in crystal structures can be used to our advantage during processing to alter the properties of various materials. Open the Structure science notes located on the homepage of the MS&E database to answer the following questions

1. Open the precipitation strengthening science note. How does precipitation strengthening differ from solid solution strengthening?
2. How do the precipitates impact dislocation motion?
3. What is one practical limitation of precipitation strengthened alloys?

Exercise 7: Copper alloys: strengthening mechanisms.

Copper can be strengthened by work hardening, solution hardening and precipitation hardening. Explore these using the “Alloying and working copper alloys” module of the Property-Process Profiles data-table. To do so make a chart of Yield strength plotted against Copper content (chose a linear, not log, scale for the copper content). What are the characteristics of each strengthening mechanism? At what copper content is the strength contribution from solution hardening in Cu-Ni alloys a maximum?

Exercise 8: Aluminum alloys: Thermal conductivity and Strength.

Like copper alloys, aluminum alloys can be strengthened by work hardening, solution hardening and precipitation hardening. As always, there are trade-offs. Increasing strength tends to reduce elongation, toughness and thermal and electrical conductivities. An aluminum alloy is sought for the heat-exchanger of a domestic air-conditioning unit. Good thermal conductivity is essential, but since the unit is pressurized, a strength of at least 100 MPa is specified. Use the “Alloy and heat treatment of aluminum alloys” module of the Property-Process Profile data-table to make a chart with Thermal conductivity on the y-axis and Yield strength on the x-axis and use it to select a candidate for the job.

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