MicroProject Prompts

Fundamentals of Crystallography with Ansys Granta EduPack Software

Mike Ashby[1] and Kaitlin Tyler[2]

[1]Department of Engineering, University of Cambridge
[2]Ansys Academic Program

Edited by the Ansys Academic Program

education@ansys.com

Ansys Software Used

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

Summary

These MicroProjects are short investigations of an aspect of Materials Science and Engineering that can be completed in less than an hour. Each poses a set of questions that can be answered using the Granta EduPack Material Science and Engineering (MS&E) database. All start at a level that is readily accessible, using the SEARCH function to find records, creating charts using the CHART/SELECT function, and extracting relevant data from a Record and its linked SCIENCE NOTES. Hints in gray help with any difficult step.

Each MicroProject has an attached Discussion Point – a challenge to go further – highlighted in red and separated from the MicroProject by this separator:

The Discussion Point poses a question linked to or arising from the MicroProject. Responding to the Discussion point requires independent thought and research, takes longer, but is rewarding if followed. It is an add-on for more advanced study.

Each MicroProject and its Discussion point has a fully worked Sample Response, available to the instructor.

Crystallography MicroProject #1

Zirconia, a ceramic that thinks it's a metal

Database: Materials Science and Engineering

- What is Zirconia? (Use the Search facility to find the record. To copy and reuse text and images from a record: right click on the opened record, select Copy, then open WORD and Paste. The entire record is pasted into WORD. You can then copy and re-paste the bits you want for a report.)

- What makes it special among ceramics? (Explore the record to find out.)

- What is the value of its Fracture Toughness?

- How does this compare with the Fracture toughness of other ceramics? Make a bar-chart of Fracture toughness for Technical ceramics to find out. (When you open the "Materials" data-table of the MS&E DB, a set of panels, each labeled with a sub-set of materials, appears on the right. One panel says "Technical Ceramics". Clicking on that limits the selection and charts to technical ceramics.)

- Reset the scale from log to linear and adjust its range to run from 0 to 10. (To make the changes, double click on the axis name to re-open the Axis Settings box, select "Linear" and adjust the range.)

- What does "Fracture toughness" measure? (Try the information ("i") link next to the property name on any materials record to access Science notes.)

Discussion Point

What gives Zirconia its unusual Fracture toughness?

Crystallography MicroProject #2

Which elements form extensive solid-solutions with Cu?

Database: Materials Science & Engineering

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

1. Atom size difference less than 15%
2. Electronegativity difference less than 0.2
   } Strong Influence
3. The components have the same crystal structure
4. The components have the same valence within ± 1
   } Less strong Influence

The Elements data-table of the MS&E database contains data for all of these. Which elements would you expect to form an extensive solid -solution with copper?

- Select the ELEMENTS data-table from the Home page. Make a chart with atomic radius difference from copper (Atomic radius – Atomic radius of copper) on one axis and electronegativity difference from copper (Electronegativity – Electronegativity of copper) to find elements that are close to copper. (First look up the atomic radius and electronegativity of copper in the Copper record, then use the Advanced axis facility to make the functions in brackets above. Chose linear scales for both axes – double click on the axis name and select "linear" instead of "log".)

- Apply a selection box centered on Copper with a width that is 15% of the atomic radius of copper on either side and differs from copper by an electronegativity of 0.075 above and below. List the elements appearing in the Results window. These meet the first two H-R criteria and will form extensive solid-solutions with copper.

- Complete solid-solubility across the entire composition range from 0 to 100% requires that the remaining two conditions are also met. Which of the elements in your list fulfill these additional requirements?

- The Phase Diagram data-table has diagrams for three copper alloys: Cu-Ni, Cu-Zn and Cu-Sn. What is the maximum solid solubility at the copper-rich side of each diagram? Are they consistent with the Hume-Rothery rules?

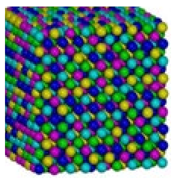
Discussion Point

What is the entropy of mixing? What is its value for a mole of an alloy with a concentration c of atoms A and (1-c) of atoms B?

Crystallography MicroProject #3

Designing high-entropy alloys

Database: Materials Science & Engineering



Model of Co-Cr-Fe-Mn-Ni (Wikipedia)

High entropy alloys are solid-solutions with five or more components each with concentrations above 5%. The cumulative entropy of mixing reduces the free energy of the alloy, stabilizing it and enhancing mechanical properties. The Hume-Rothery rules give guidance in selecting components that will form extensive solid-solutions:

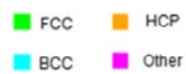
The Hume-Rothery rules set out criteria for the formation of extensive solid-solution:

1. Atom size difference less than 15%
2. Electronegativity difference less than 0.2 } Strong Influence
3. The components have the same crystal structure
4. The components have the same valence within ± 1 } Less strong Influence

The Elements data-table of the MS&E database contains data for all of these. Make a chart for selecting promising component-sets for high-entropy alloys.

- Make a chart for selecting promising component-sets for high-entropy alloys. Plot Electronegativity on the y-axis and Atomic radius on the x-axis. Use a linear scale for Electronegativity but retain the default Log scale for Atomic radius. (To change an axis from log to linear, double click on the axis name, then click on "linear" in the Axis settings box.)

- Recolor the elements to identify their crystal structure.



(The best way to do this is to use a limit stage to select all the elements with a "Cubic, face centered" structure, highlight the resulting list, right click and select Record color, chose color, then repeat for the other structures.)

- Create a selection box with a width that corresponds to 15% change in atomic radius and a height that corresponds to a difference of 0.075 in electronegativity. Use this box to track across the array of elements on the chart, placing it over clusters to identify promising components. (Feel free to relax the constraints a little – we are only looking for a solubility greater than 5%, not total solid solubility.)

- Enclose each cluster with a line using the Curve tool in the tool-bar across the top of the chart. Label the encircled clusters, listing the elements they contain, using the Text label tool in the same tool-bar. How many promising clusters do you find?

Discussion Point

High-entropy alloys are a relatively new and currently-active field of research. Research "High-entropy alloys" on the world-wide web. What are their characteristics, properties and potential applications?

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Document Information

This case study is part of a set of teaching resources to help introduce students to topics related to fluids.

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ANSYS, Inc.
Southepointe
2600 Ansys Drive
Canonsburg, PA 15317
U.S.A.
724.746.3304
ansysinfo@ansys.com