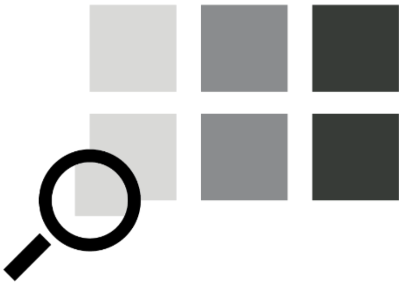
GRANTA EduPack MicroProjects with Solutions:
Structures and Properties



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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. The charts shown in the responses are reproduced here exactly as produced by GRANTA EduPack.

Example Use: In-class activities, homework assignments, activity to introduce students to functionalities of GRANTA EduPack

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Phase Diagram Teaching Package Files:

- Lecture PowerPoint
- Student Lecture Notes
- Exercises
- Quiz Questions (Word and GIFT Format)
- Concept Maps
- Misc.

GRANTA EduPack Introductory MSE Teaching Package Topics:

- Bonding and Material Families
- Crystallography and Crystal Defects
- Mechanical Properties
- Phase Diagrams

Structures & Properties MicroProject 1

Which elements form extensive solid-solutions with Cu?

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
3. The components have the same crystal structure
4. The components have the same valence within ± 1

(Items 1–2: Strong influence; items 3–4: 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 (requiring wider investigation or thought):

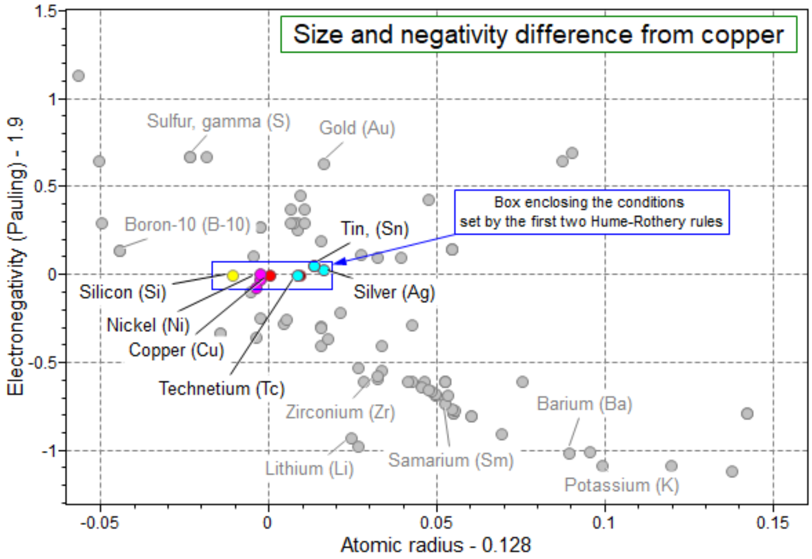
What is the entropy of mixing? What is its value for a mole of an alloy with a concentration *c* of atoms A and *(1-c)* of atoms B?

Answers and Sample Responses

Satisfying the first two Hume-Rothery criteria

Copper has an atomic radius of 0.128 nm and an electronegativity of 1.9 on the Pauling scale. The chart showing the difference between the radius and electronegativity of copper and the other elements looks like this. Copper is at the point (0,0). The blue selection box encloses the conditions set by the first two of the Hume Rothery rules. The elements captured in the box are listed below.

Cobalt (Co)
Iron, alpha (Fe)
Nickel (Ni)
Rhenium (Re)
Silicon (Si)
Silver (Ag)
Technetium (Tc)
Tin, (Sn)



Which elements should form complete solid-solutions with copper?

Of the elements in the list above, only two have the same valence and crystal structure: nickel and silver. Both do form full solid-solutions with copper.

Maximum solid solubility for Cu-Ni, Cu-Zn and Cu-Sn

Phase diagram	Max solid solubility	Comment
Cu-Ni	100 wt%	All four H-R criteria are met
Cu-Zn	39 wt%	Three criteria satisfied; crystal structures differ
Cu-Sn	15 wt%	First two criteria satisfied; crystal structure and valence differ

***Discussion point:* What is the entropy of mixing?**

When n atoms of element A are mixed with N-n atoms of element B on a mole N (6.02 x 10^{23}) of atomic sites, there is an increase in the entropy of A + B due to the numerous ways in which the two kinds of atoms can be arranged among each other. The total number of ways of doing this is

$$\frac{N!}{n!(N-n)!}$$

The entropy associated with the mixing is

$$S = -k\,ln\left[\frac{N!}{n!(N-n)!}\right]$$

where k is Boltzmann constant (1.38 x 10^{-23} J/K). This simplifies, using the Stirling approximation to

$$S = -Nk\left[c\,ln(c) + (1-c)\,ln(1-c)\right]$$

here $c = n/N$ and $(1-c) = (N-n)/N$. The entropy of mixing reduces the free energy of an alloy, increasing it stability; it is this that keeps the alloy mixed and acts against it separating out into two distinct phases. When c = 1 or 0, S = 0 (no entropy of mixing). When c = (1-c) = 0.5, S = 5.7 J/mol.K

Structures & Properties MicroProject 2

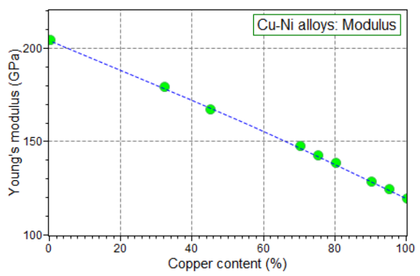
What do Processes do to Properties?

The Process-Property Profile (PPP) data-table in the MS&E database allows charting of the effect of processing on properties. This project uses the PPP facility to explore solid-solutions.

- Open the PPP data-table from the home page and isolate Copper-Nickel alloys for exploration. (Chart/Select – Select from: Custom Define your own subset – Deselect all then open 1. Alloying and work hardening: copper alloys – select Copper-Nickel alloys)

- Make a chart with Young's modulus on the y-axis and Copper content on the x-axis. Use linear scales for both. Set the axis range for Copper content (%) to run from 0 to 100. (To choose linear scales and set axis ranges first make the chart then double click on the axis name on the chart to bring up Axis settings. Click on "Linear" and use "Set" to adjust range.)

- Add a title using the Text label function (T) and draw a curve through the data using the Curve function (C) above the chart. Your modulus chart should now look like this.



- Now step through the mechanical, thermal and electrical properties in the same way, copying and pasting the charts into WORD to allow comparison. Follow the order
  1. Yield strength,
  2. Fracture toughness
  3. Thermal conductivity
  4. Thermal expansion
  5. Heat capacity
  6. Electrical resistivity

- Some properties (like Youngs modulus) vary with composition in an almost linear way. Which behave like this?

- Some, by contrast, show a much stronger dependence, with a maximum or minimum in the middle of the composition range – which are these?

Discussion point (requiring wider investigation or thought):

Why does the Yield strength vary with solute concentration in the way shown in Chart 1? Got to the Home page, locate Science Notes, open Structure Science notes and open "Solid-solution strengthening" to find out.

Why does the Electrical resistivity vary with solute concentration in the way shown in Chart 6? Open the Structure Science note "Electron scattering" to find out.

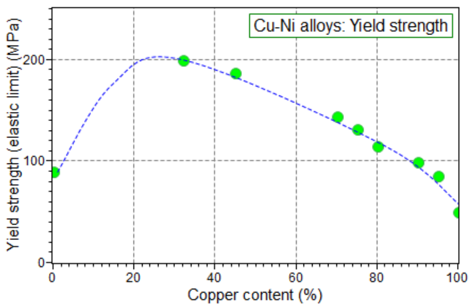
(Text and images can be copied from these Science notes by highlighting, copying and pasting into WORD.)

Answers and Sample Responses

Mechanical properties

The Modulus, as we saw in the statement of the micro-project, varies almost linearly with composition. By contrast, Yield strength, Fracture toughness show a strongly non-linear behavior with a peak or trough towards the middle of the composition range.

(1)



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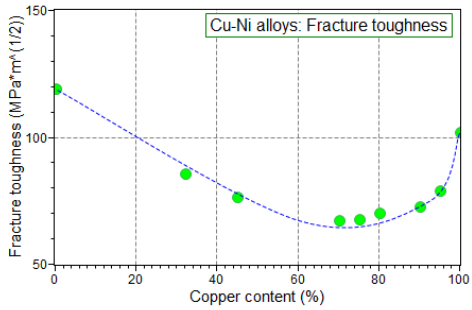

Thermal and Electrical properties

Thermal expansion coefficient and Heat capacity vary almost linearly with composition. Thermal conductivity and Electrical resistivity vary in a strongly non-linear way.

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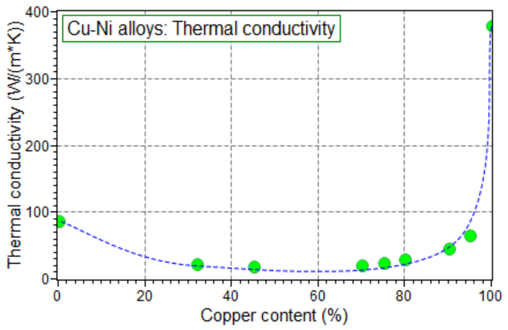

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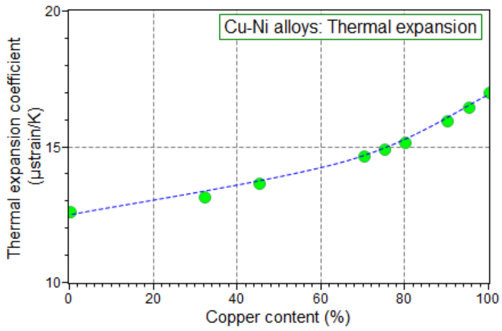

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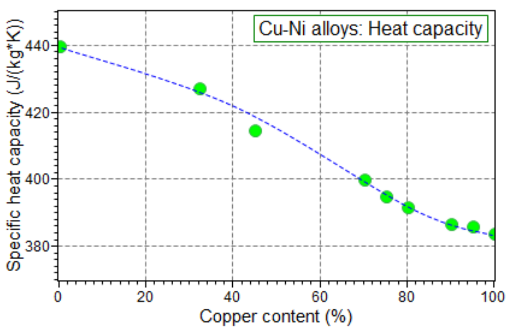
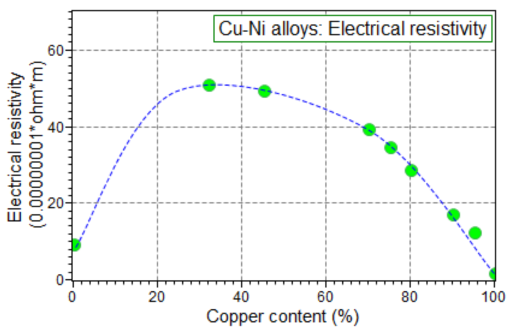


(6)



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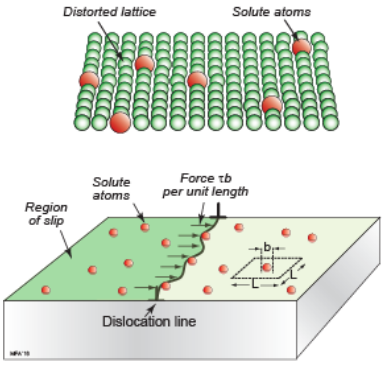
***Discussion point:* The underlying mechanisms.**

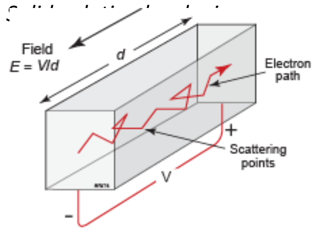
Why does the Yield strength vary with solute concentration in the way shown in Chart (1)? The Structure Science note gives the following insight.

Solute atoms differ in size from those of the host, roughening the planes on which dislocations move, and thus obstructing their motion. The number of such obstacles increases with solute concentration, *c*, leading to a parabolic ($c^{1/2}$) dependence of yield strength on concentration. This dependence is evident in Chart 1, which shows a roughly parabolic rise starting from 0% Ni or from 0% Cu.

Why does the Electrical resistivity vary with solute concentration in the way shown in Chart (6)? The Structure Science note for Electron Scattering gives the following insight.

Electrical conduction in a metal is by the movement of "free" electrons in response to the field *V/d* caused by the potential difference *V*. Impurity or solute atoms act as scattering centers, limiting the mean free path of the electrons, which is why alloys always have a higher resistivity than pure metals.





Electron scattering

Document Information

This exercise unit is part of a set of teaching resources to help introduce students to materials, processes and rational selections.

Accuracy

The author(s) try hard to make sure that these resources are of a high quality. If you have any suggestions for improvements, please contact the author(s) by email. You may also write to the Ansys Granta Education Team with your suggestions at granta-education-team@ansys.com.

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- Lecture presentations with notes
- Case studies
- Exercises with worked solutions
- Microprojects
- Recorded webinars
- White papers
- Solution manuals
- Interactive exercises

Some of the resources are open access and students can access them. Others are only available to educators using GRANTA EduPack.

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