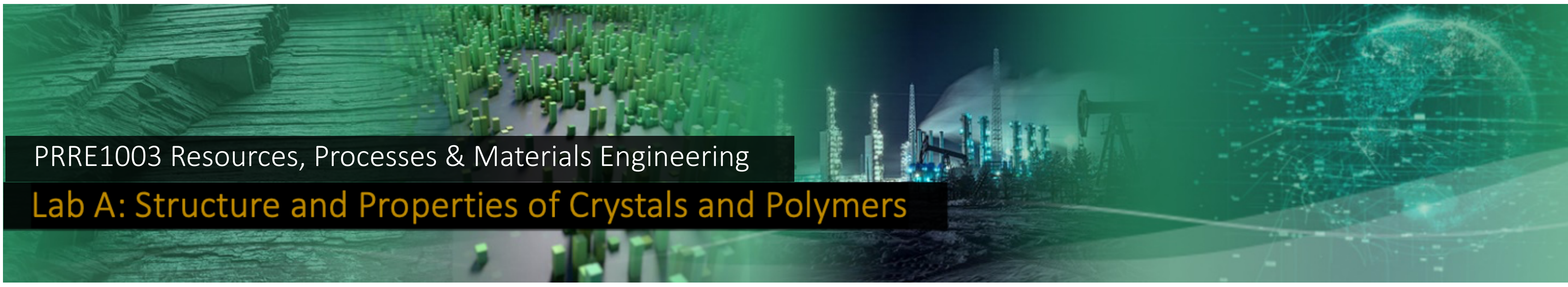


Lab A: Structure and Properties of Crystals and Polymers

AIMS

- To understand the basic structure of crystals and polymers
- To calculate the theoretical density of a crystalline solid based on its structure
- To differentiate between thermoplastic and thermosetting polymers

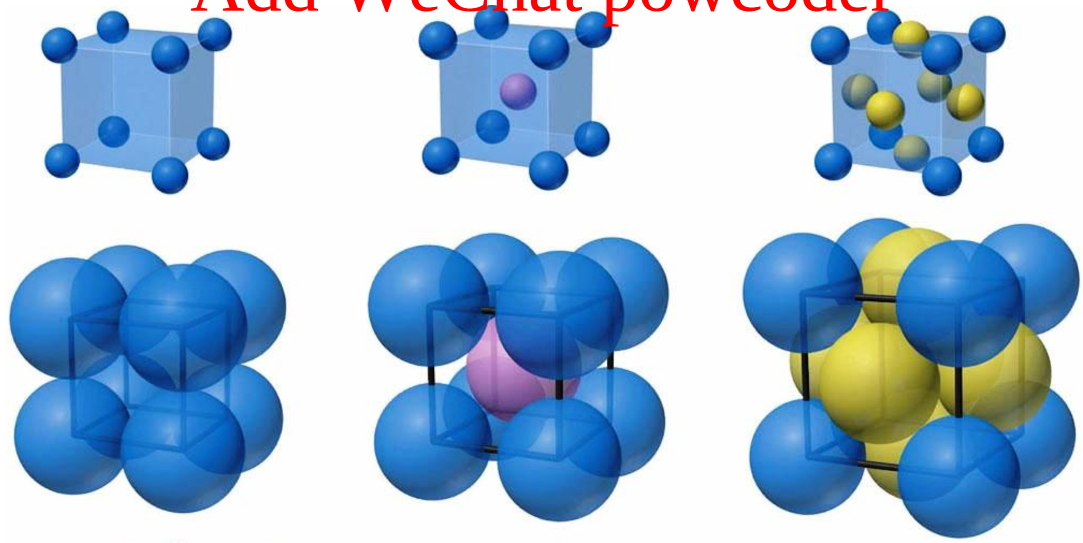
INTRODUCTION

Metals and *ceramics* exist as *crystalline* solids, which means that the atoms are packed in a regular and repeated fashion, unlike *amorphous* solids. In *glasses*, a kind of amorphous solid, the packing of atoms or molecules is disordered with no regularity or alignment. *Polymers* are made up of tangled, long-chain molecules.

The unit that characterises a crystal structure is called its unit cell. The most common unit cells are the simple cubic (SC), body-centred cubic (BCC) and face-centred cubic (FCC) as shown in Figure 1. The theoretical density of a metal is related to the structure of the unit cell, which also determines

- the ratio of lattice parameter to atomic radius (a/R),
- the number of atoms per cell (APC),
- the coordination number (CN) and
- the atomic packing factor (APF).

For cubic unit cells, the lattice parameter is the length of a side of the unit cell.



Simple cubic (SC) Body-centred cubic (BCC) Face-centred cubic (FCC)

Figure 1. Common unit cells of crystalline materials. The top row of images shows the atoms separated for clarity.

These parameters enable the volume of a unit cell (V_c) to be calculated, which is then related to its theoretical density (ρ) by

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

where n is the number of atoms associated with each unit cell (that is, APC), A is the atomic weight, and N_A is Avogadro's number (6.022×10^{23} atoms/mole). Some characteristics of the three structures you'll build in this lab are given in Table 1.

Table 1. Characteristic parameters of cubic unit cells.

Structure	*a/R*	APC	CN	APF
SC	2	1	6	0.52
BCC	4/√3	2	8	0.68
FCC	2√2	4	12	0.74

Polymers have a very different structure to metals (Figure 2). Polymers are made up of a chain of carbon atoms to which side groups are attached. Polymer molecules bond together to form solids. Each chain consists of covalent C-C bonds and weak hydrogen bonds that bond each chain to the other. *Thermoplastic* polymers are amorphous, and because the weak hydrogen bonds melt easily, these polymers can be moulded and will retain a new shape on cooling. However, when chains of polymers are cross-linked by replacing some of the weaker hydrogen bonds by stronger covalent C-C bonds, a large cross-linked network is created. *Thermosetting* polymers, have several cross-links and are therefore stiffer and stronger than thermoplastic polymers.

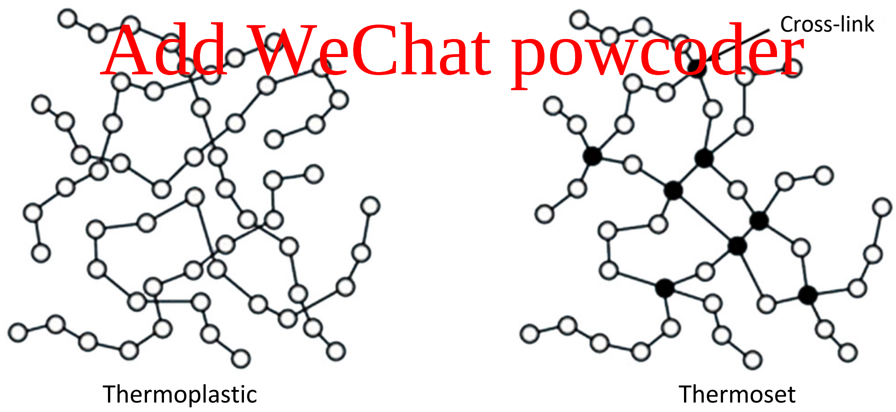


Figure 2. Schematic structures of polymers.

Please note that parts of this assessment are submitted as a group report, while other parts are to be entered in the Lab A Results area on Blackboard and will be marked automatically.

EXPERIMENTAL PROCEDURE

Experiment 1: Structure of crystals and estimation of density

Note: It may be helpful to have the **Lab A Results** *link open and enter data into it as you do your lab, so that you can get immediate feedback on whether your data and calculations are correct. Please enter your data individually onto the Blackboard. Your report should be written in your allocated LAB group.*
Some questions and feedback on answers will help guide you through the worksheet, so if you are doing this Lab online, it is highly recommended that you gain the maximum benefit of the **Lab A Results** *link.*

In this experiment, you will be provided with polystyrene balls and toothpicks. Your task is to construct models of the various cubic structures by following the steps carefully. They will guide you first to obtain the measured values of your unit cells' characteristics and then to compare them with the theoretical values for each crystal structure.
Online students: Watch LabA_V1 to see how a Vernier calliper works.

1. Measure the atomic radius of a sphere (***online:*** *watch LabA_V2*) and record it in the table below and also in **Lab A Results** on Blackboard.
2. The polystyrene balls and toothpicks are used to build each of the three cubic models as shown in the bottom row of images in Figure 1. Build each model (***online:*** *watch the videos LabA_V3 SC, LabA_V3 BCC and LabA_V3 FCC*) and record the lattice parameter in the table below and also in **Lab A Results** on Blackboard.
3. For each cubic model, calculate a/R, V_s, V_c and APC, and deduce coordination number (CN) and APC (***online:*** *LabA_V4 demonstrates how to work out the CN*). Record them in the table and in **Lab A Results** on Blackboard. Show a sample calculation for one structure in your report. *Hint: You will need to remember how to calculate the volume of a cube (a^3), and a sphere ($4/3\pi R^3$).*

Table 2. Summary of data and calculations for Q1-Q3

Structure	Atomic radius (R) cm	Lattice parameter (a) cm	(a/R)	Coordination number (CN)	Atoms per cell (APC)	Total sphere volume (V_s) cm³	Cell volume (V_c) cm³	Atomic packing factor (APF = V_s/V_c)
SC								
BCC								
FCC								

Based on the experimental observations and the results obtained, as well as important concepts of crystallography, please give short answers to the following questions in your lab report:

4. Compare your measured and calculated values with the theoretical values listed in Table 1. Your values most likely do not fully agree with the theoretical ones. Why do you think that occurred? Cite possible causes for the differences.

5. If you were to repeat the experiment using polystyrene balls of a different size, would you obtain the same or different values for the structural parameters (R, a, CN, APC and APF) of the cubic crystal structures? Please justify your answer.

6. Listed in the table below are the atomic weight, density and atomic radius for three hypothetical alloys. For each, determine whether its crystal structure is SC, BCC or FCC, indicate it in the table and also in **Lab A Results** on Blackboard. Show a sample calculation for one alloy in your report. *Hint: use the equation on page 2.*

Table 3. Data and summary of result for Q6

Alloy	Atomic weight (g/mol)	Density (g/cm^3)	Atomic radius (nm)	Crystal structure
A	43.1	6.40	0.122	
B	184.4	12.30	0.146	
C	91.6	9.60	0.137	

Experiment 2: Structure of polymers and classification

In this experiment, you will use some simple tests to classify a range of polymers as either *thermoplastic* or *thermosetting*. Watch this video (4:40 mins) to refresh your understanding of basic polymer chemistry: https://youtu.be/rhFc477fs6s.

Take each polymer sample and carry out a few simple physical tests (**online:** Watch LabA_V5 and LabA_V6) to try and identify it as either a thermoplastic or a thermosetting polymer. Bear in mind that thermoplastics can be moulded and welded (that is, they soften and melt when heated), while thermosets form a rigid network when they are synthesised. Use your observations to help you fill in the first two columns of the table on the next page as you go.

A. Attempt to cut a thin slice off the edge of the sample (check with your demonstrator for instructions on the correct way to do this).
B. Drop the sample onto a hard surface.
C. Attempt to flex and/or stretch the sample.
D. Warm the sample a little with hot water and try to flex or stretch the sample again.

When you have decided whether each sample is a thermoplastic or a thermoset, show the table to your demonstrator. Match the names of the polymers with sample and fill out the rest of the table, with the polymers listed here:

- Phenol formaldehyde
- Polystyrene
- Polyethylene
- Nylon 6,6

Hints:

- *Phenol is a benzene ring with an –OH group on the side*
- *Ethylene is an alkene with formula C_2H_4*
- *Styrene is also known as phenyl ethylene, which is ethylene with a H replaced by an aromatic ring*

Based on the observations and your identification on the samples, please complete the Experiment 2 question in **Lab A Results** on Blackboard. Experiment 2 is not to be included in the group report.

Sample #	Observations on performing experiments A, B, C and D on sample	Polymer name	Structure of repeating unit	Thermoplastic or thermosetting
				
				
				
				

REPORT

You need to write a group report about **Experiment 1 only**. This is a formative assessment.

Please use the Lab A Report Template available on Blackboard. The template contains some further guidance about what your report should contain. Please refer to the Workshop 1 materials for information about technical report writing, including presenting sample calculations.

REPORT MARKING

Criteria	Big idea	Needs improving	Meets expectations	Exceeds expectations
Introduction (4 marks)	*What hypothesis are we testing?*	The introduction is essentially copied from the lab worksheet. It does not seem like the group has used much judgment about the contents. It is very long or very short. (0–2 marks)	The introduction is similar to what was covered in the lab worksheet, but there is evidence of some independent thought about the content. (2–3 marks)	The introduction covers the required content and shows clear evidence of independent research and thinking about the significance and theory. (3–4 marks)
Experimental Materials, Apparatus and Method (4 marks)	*What did you do?*	The information is essentially copied from the lab worksheet, but important information is missing or incorrect. (0–2 marks)	Information is paraphrased from the lab worksheet; almost all the important information is present, may be too long. (2–3 marks)	The information is clearly written; it is concise, yet retains all important details and does not make unneeded assumptions. (3–4 marks)
Results and Discussion (9 marks)	*What did you observe? What does it mean?*	The explanations are not clear or contain serious flaws; there is little justification. One of the sample calculations is missing or contains mistakes. (0–4 marks)	The explanations are mostly clear and correct with some justification provided. Both sample calculations are correct. Experimental uncertainty is considered briefly. (5-7 marks)	Insightful, correct explanations are given with credible justifications. Both sample calculations are clear and correct, and include uncertainty. Some extra, relevant points are made. (8–9 marks)
Conclusions and Recommendations (4 marks)	*What conclusions can we draw? What follow-up work is needed?*	Conclusions are missing or are actually a summary. Recommendations are missing or are unrelated to the experiment. (0–2 marks)	Some reasonable conclusions are given. One or two recommendations given but they may lack usefulness or practicality. (2–3 marks)	Concise conclusions show a thorough understanding of the work. Two or more relevant, valuable and practical recommendations are given. (3–4 marks)
Report writing (4 marks)		Spelling and grammatical mistakes are common. There is poor or inconsistent formatting. It is over the page limit. Overall, it seems that the group is not aware of report writing standards or has not applied them carefully. (0–2 marks)	There are a handful of spelling and grammatical mistakes. The writing is mostly understandable and brief. Formatting is generally consistent and appropriate. The group seems to be aware of report writing standards and has made a good effort to use them. (2–3 marks)	The report is essentially free from spelling and grammatical mistakes. The writing is clear, concise and easy to read. Formatting is consistent and professional. Overall, the report appears to have been compiled carefully; it is near industry quality. (3–4 marks)

RESOURCES

There are many credible sources of information about materials, including:

- Callister, William, D., Jr. and Rethwisch, David G. 2014. *Materials Science and Engineering: An Introduction*. 9th ed. Hoboken, NJ: John Wiley and Sons.
- Carter, Giles F., and Paul, Donald E. 1991. *Materials Science & Engineering*. Materials Park, OH: ASM International.

Ver. 1.3 (July 2022)