

Problem sheet 1: Bravais lattice and symmetry

11.10.2023

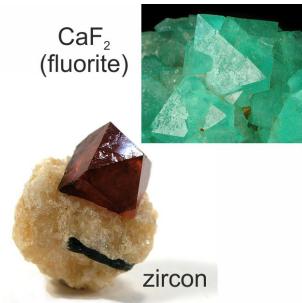
1.1. Shortcut to lattice parameters (2 P)

- (a) The density of fcc nickel is $8.908 \times 10^3 \text{ kg/m}^3$. Determine the lattice constant.
- (b) Determine the effective radius (metallic radius) of the nickel atom.

1.2. How big is the primitive cell? (3 P)

- (a) Calculate the dimensions and angles of the primitive unit cell for fluorite, CaF_2 (fcc structure).
- (b) Calculate the dimensions and angles of the primitive unit cell for zircon, a common gemstone (ZrSiO_4 , body-centered tetragonal structure).

You can find lattice parameters at Wikipedia, or wait until lecture 3 where we will discuss how to retrieve them generically



1.3. Packing tutorial (6 P)

- (a) 2D: Determine packing fractions for the square lattice and triangular lattice.
- (b) 3D: Determine packing fractions for the primitive cubic lattice, bcc lattice, and fcc lattice.
- (c) Consider orange fruit as the sphere with the diameter of 10 cm and the weight of 130 g. Oranges should be packed into boxes with the dimensions of $80 \times 50 \times 40 \text{ cm}$. The weight of the box can not exceed 23 kg so that one docker would be able to lift it and carry it around. How should the oranges be packed?



1.4. Neumann-imposed constraints (6 P)

- (a) Show that Neumann's principle can be formulated as $\sigma = \mathbb{R} \sigma \mathbb{R}^{-1}$ where σ is tensor property of the crystal and \mathbb{R} is the symmetry operation.
- (b) Use the above expression to analyze symmetry constraints for tetragonal crystals (symmetry group: $4/m = C_{4h}$)
- (c) Do the same for a monoclinic crystal (symmetry group: $2/m = C_{2h}$)

Hint: feel free to use the expression from (a) even if you do not know how to derive it. Apply this equation to a generic 3×3 tensor and realize that some of these components must be equal to each other, or vanish. This will leave less than 6 independent components of σ depending on the crystal symmetry.

1.5. Hexagonal structure (3 P)

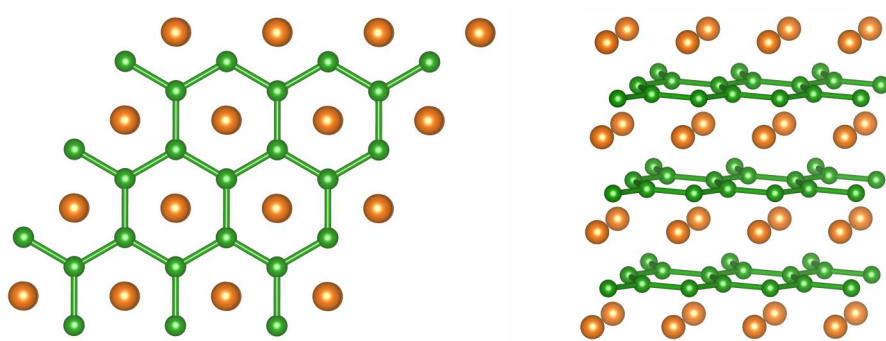
The figure below shows the crystal structure of the MgB_2 superconductor.

- (a) Indicate the unit cell (you can draw it directly on the figure).
- (b) How many atoms (N) and formula units (Z) does the unit cell contain? Indicate which atom is Mg and which atom is B. Why?
- (c) List symmetry elements of the crystal structure and show them on the figure.

If you feel it difficult to assess symmetry from these two drawings, wait until lecture 3 (18.10) where you will

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learn how to plot crystal structures yourself

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- oranges – JJ Harrison (CC-BY-SA)