LABORATORY OF MATERIALS DESIGN AND SIMULATION

MSE-483 ADVANCED PHASE TRANSFORMATIONS
FALL 2025

QUESTION 1

Consider the lattice and cell shown in fig. 1a. The structure is comprised of 4 sublattices. The sublattice composition of the A chemical specie on each of the sublattices is denoted as x_1, x_2, x_3, x_4. An ordered phase that is often found to occur in catalytic and electrochemical applications is comprised of alternating rows of A and B atoms as shown in fig. 1b. A atoms are drawn in red while B atoms are drawn in blue in the figure. Order parameters to distinguish the ordered and disordered phases are given by:

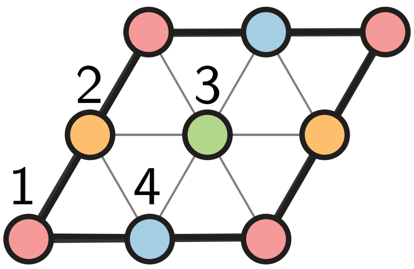
$$\eta_0 = \frac{x_1 + x_2 + x_3 + x_4}{4}$$

$$\eta_1 = \frac{x_1 + x_2 - x_3 - x_4}{4}$$

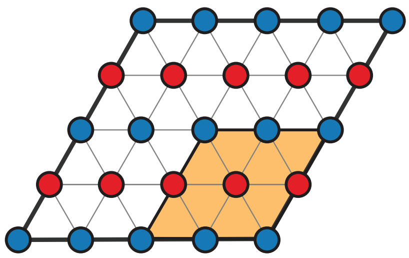
$$\eta_2 = \frac{x_1 - x_2 + x_3 - x_4}{4}$$

$$\eta_3 = \frac{x_1 - x_2 - x_3 + x_4}{4}$$

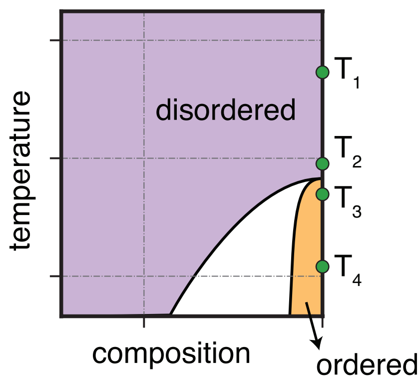
1. Sketch the crystal structures of all variants of the ordered phase shown in fig. 1b?
2. Compute the values of the order parameters for each variant.
3. Identify the locations of the ordered and disordered phases in the three dimensional space spanned by $\eta_1 - \eta_2 - \eta_3$
4. Sketch $G(\eta_1, T)$ vs η_1 for the material at a composition of 0.5 at the four temperatures shown in fig. 1c.



(a)



(b)



(c)

QUESTION 2

The body-centered cubic (bcc) crystal structure can be transformed to the hexagonal close-packed (hcp) crystal structure along a pathway described by Burgers. In the Burgers transformation, $\{110\}$ planes of bcc are

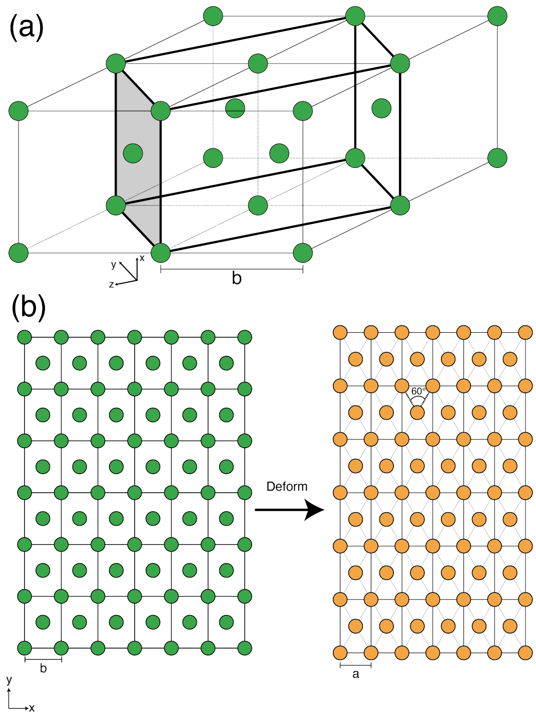


Figure 2: Burgers transformation

transformed into the triangular lattices of hcp. Figure 2a shows the three dimensional unit cell of bcc (as solid dark black lines) that must be strained to obtain the hcp crystal structure. The transformation of a $\{110\}$ plane (highlighted in gray in fig. 2a) of bcc to the triangular lattice of hcp is shown in fig. 2b. An additional strain is required along the z direction to convert the bcc lattice vector to have a length of c - corresponding to twice the length between close-packed planes in hcp. Alternate triangular planes need to be shuffled to obtain the perfect hcp stacking, however you can neglect these shuffles for this problem..

1. Write down the lattice vectors of the supercell of bcc shown in solid dark lines and the lattice vectors of hcp. The orientation of the Cartesian coordinate system is shown in fig. 2. The edge length of the conventional bcc cell is b, while the edge length of the triangular layers in hcp is a and the distance between adjacent close-packed planes is $\frac{c}{2}$.
2. Find the deformation matrix $\boldsymbol{F}$ of the bcc$\rightarrow$hcp structural phase transition. Express your answer in terms of the lattice parameters of the bcc and hcp phases.
3. Assuming the $\frac{c}{a}$ ratio corresponds to the ideal value for an hcp crystal structure, is there a plane that is invariant under the Burgers transformation? What is the normal vector to this plane?
4. Under what condition could the invariant plane cease to exist?