

# Materials for Devices: Problem Set 1

1. A capacitor is made of two parallel plates of surface area  $A$  and separated by a distance  $L$ . It supports a charge  $Q$  on each plate (positive on one and negative on the other) and an associated voltage difference  $V$  across the plates. The capacitance  $C$  of the capacitor is defined as:

$$C = \frac{Q}{V}. \quad (1)$$

For a parallel plate capacitor, the charge density  $\sigma = \frac{Q}{A}$  on each plate is related to the displacement field of the dielectric material between the plates through:

$$\sigma = |\mathbf{D}|. \quad (2)$$

- (i) Show that:

$$C = \epsilon \frac{A}{L}, \quad (3)$$

where  $\epsilon$  is the permittivity of the dielectric material between the parallel plates.

- (ii) What is the capacitance of an *empty* parallel plate capacitor with plates of surface area  $500 \text{ mm}^2$  and separated by  $2.5 \text{ mm}$ ? If a potential difference of  $10 \text{ V}$  is applied across the plates, what is the magnitude of the charge stored on each plate? And the surface charge density?
  - (iii) Consider the insertion of  $\text{SiO}_2$  ( $\kappa = 4.52$ ) between the plates. For the same applied potential difference of  $10 \text{ V}$ , calculate the capacitance, the magnitude of charge stored on each plate, and the surface charge density.
  - (iv) What is the polarisation of  $\text{SiO}_2$  in the setup above? With reference to the empty parallel plate capacitor, explain why the total charge density on the plates is not the same as the polarisation of the dielectric.
  - (v) What would be the surface area of a new capacitor of the same capacitance and thickness as the  $\text{SiO}_2$  capacitor above, but made from a ferroelectric material with a dielectric constant one hundred times greater than that of  $\text{SiO}_2$ ?
2. A ceramic material has a piezoelectric coefficient of  $250 \text{ pC N}^{-1}$  and a dielectric constant of 500. A compressive stress of  $5 \text{ MPa}$  is applied across a  $1 \text{ cm}$  thick sample of the material. Calculate the voltage that will develop across the sample.
  3. Goldschmidt postulated that materials that adopt the perovskite structure arrange so that “the number of anions surrounding a cation tends to be as large as possible, subject to the condition that all anions touch the cation”. In this problem, we use this principle to derive the Goldschmidt tolerance factor.

- (i) Sketch a unit cell of a cubic perovskite  $\text{ABX}_3$  structure, placing the  $B$  cation at the centre of the cell.
- (ii) Let the lattice parameter of the cubic cell be  $a$ . Show that according to Goldschmidt’s statement above, then:

$$a = 2(r_B + r_X), \quad (4)$$

where  $r_B$  and  $r_X$  are the ionic radii of ions  $B$  and  $X$ , respectively.

(iii) Show that according to Goldschmidt's statement above, then:

$$\sqrt{2}a = 2(r_A + r_X), \quad (5)$$

where  $r_A$  and  $r_X$  are the ionic radii of ions A and X, respectively.

(iv) Therefore, show that for an ideal cubic perovskite, the Goldschmidt tolerance factor:

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}, \quad (6)$$

is equal to 1.

(v) For  $\text{BaTiO}_3$ , the ionic radii are  $r_{\text{Ba}^{2+}} = 1.75 \text{ \AA}$ ,  $r_{\text{Ti}^{4+}} = 0.75 \text{ \AA}$ , and  $r_{\text{O}^{2-}} = 1.21 \text{ \AA}$ . Calculate the Goldschmidt tolerance factor for  $\text{BaTiO}_3$  and discuss the result in terms of the stability of cubic  $\text{BaTiO}_3$ .

4. Consider a ferroelectric material whose free energy is given by:

$$\mathcal{F}(P, T) = a(T - T_c)P^2 + \frac{b}{2}P^4, \quad (7)$$

where  $P$  is the polarisation,  $T$  the temperature, and  $a$ ,  $b$ , and  $T_c$  are positive scalar parameters. This free energy provides a universal characterisation of ferroelectric-to-paraelectric phase transitions.

- (i) Find the extrema of the free energy with respect to  $P$  in the case when  $T > T_c$  and sketch the resulting function.
- (ii) Find the extrema of the free energy with respect to  $P$  in the case when  $T < T_c$  and sketch the resulting function.
- (iii) Calculate the polarisation  $P$  as a function of temperature  $T$ . What is the role of  $T_c$ ?