

Homework 6 Solutions

1. Non-Centrosymmetry and Piezoelectricity. We have stated that the ionic equilateral hexagon shown in Fig. 1(a) is a good example of a non-centrosymmetric unit cell.

- (a) Write down a simple argument for why the ionic hexagon is non-centrosymmetric. Use the built-in dipoles to derive an expression for the built-in electric polarization vector in the coordinate system shown in Fig. 1.

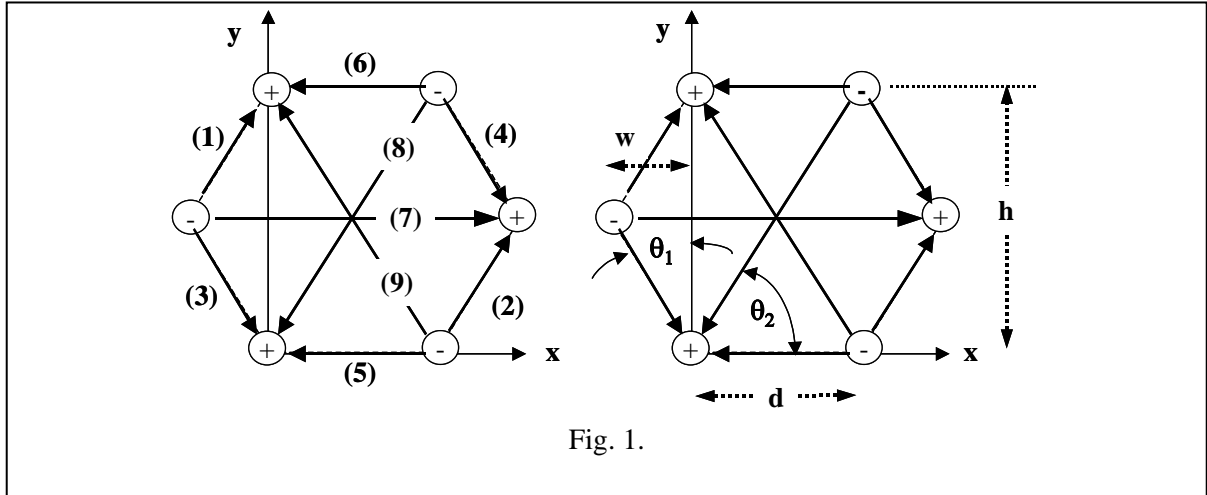


Fig. 1.

The ionic hexagon is non-centrosymmetric because if we draw any line through the center of the hexagon that connects two atoms, the two atoms have opposite charge, which generally means they are different atoms. In the coordinate system given, we can write down the electric polarization vector as a sum over 9 terms, each being a unique pairing of a negative and positive ion. It is helpful to label the 9 dipoles as in Fig. 1, which also shows the key angles and dimensions. From the decomposition into equilateral triangles that the hexagon allows, we see that $\theta_1 = 30^\circ$ and $\theta_2 = 60^\circ$. Therefore, the parallel dipoles (1) and (2) contribute a net dipole moment $e(d\hat{x} + h\hat{y})$, dipoles (3) and (4) $e(2w\hat{x} - h\hat{y}) = e(d\hat{x} - h\hat{y})$, and dipoles (5) and (6) contribute $-2ed\hat{x}$. Clearly the sum of all 6 is zero. Similarly, dipole (7), (8), and (9) are $2ed\hat{x}$, $-e(d\hat{x} + h\hat{y})$, and $e(-d\hat{x} + h\hat{y})$, which collectively also add to zero. *So there is no built-in polarization for the ionic equilateral hexagon.*

- (b) If a compressive strain δd is induced along the y axis, then the dimension h becomes $h' = h(1 - \Delta)$. Before compression, the area of the hexagon is $A = h(d + w) = (3/2)hd$ since $w = d/2$ for the equilateral hexagon. After compression (and referring to the above figure), the new area is $A' = (h - \delta h)(d + \delta d + w + \delta w)$. So if the area is assumed to stay fixed, $(3/2)hd = (h - \delta h)(d + \delta d + w + \delta w) = (h - \delta h)(3d/2 + \delta h + \delta w)$. If δh is small, this can be well approximated as $(3/2)d(1 + \delta h/h) = (3d/2 + \delta d + \delta w)$, or $(3/2)d\delta h/h = \delta d + \delta w$ or $[(3)^{1/2}/2]\delta h = \delta d + \delta w$ since $d/h = 1/(3)^{1/2}$ for the equilateral hexagon.

Now, if we recalculate the built-in dipole, (1) and (2) contribute

$$e(w'\hat{x} + h'\hat{y}) = 2e[(w + \delta w)\hat{x} + (1/2)(h - \delta h)\hat{y}], \text{ dipoles (3) and (4)}$$

$$e(w'\hat{x} + h'\hat{y}) = 2e[(w + \delta w)\hat{x} - (1/2)(h - \delta h)\hat{y}], \text{ and dipoles (5) and (6) contribute } -2e[d + \delta d]\hat{x}.$$

So the contribution from (1) to (6) is just $2e[2w + 2\delta w - d - \delta d]\hat{x} = 2e[2\delta w - \delta d]\hat{x}$. And the remaining three dipoles (7), (8), and (9) become $e[d + \delta d + 2(w + \delta w)]\hat{x}$,

$-e[(d + \delta d)\hat{x} + (h + \delta h)\hat{y}]$, and $e[-(d + \delta d)\hat{x} + (h + \delta h)\hat{y}]$, which add up to $e[(2\delta w - \delta d)\hat{x}]$. So the overall dipole moment is now the sum of all nine: $\vec{p}_{tot} = 3e[(2\delta w - \delta d)\hat{x}]$. Note: This result becomes zero under the special condition that $2\delta w = \delta d$. But the ratio of $\delta w/\delta d$ is determined by the bonding (i.e., elastic) properties, which are not likely to satisfy this special case.

(c) If the hexagons are combined to form a two-dim (honeycomb lattice) we will get the result from (b) for each hexagon. But the area of each hexagon before compression is just $(3^{3/2}/2)d^2$ so the sheet density is $n_s = 2/(d^2 3^{3/2})$. And the total (line) polarization induced by the stress is $\vec{P} = 6e[(2\delta w - \delta d)\hat{x}]/(3^{3/2} d^2)$ [note the units are correct for two dimensions: Cb/m]. From the direct piezoelectric constitutive relation, we can write $D_x = \epsilon E_x + e_{12}\eta_2$ for a reaction along x from a strain along y, where e_{12} is the piezoelectric stress coefficient. But in the above calculation $\epsilon = \epsilon_0$ (since all calculations were done at the atomic level), so that $e_{12}\eta_2 = D_x - \epsilon_0 E_x = P_x$. So if δh is small compared to h , we can write $\eta_2 = \delta h/h$, and we get the result $e_{12} = P_x/\eta_2 = 6eh[(2\delta w - \delta d)\hat{x}]/(3^{3/2} d^2 \delta h) = 2e[(2\delta w - \delta d)\hat{x}]/(d\delta h)$ in units of [Cb/m] !

2. AlN as a Piezoelectric Material .

(a). By definition, clamped in x and y means that there can be no strain in these axes and the only nonzero strain term will be η_3 . So the connection equation will be the inverse piezoelectric relation $P_j = C_{IJ} \eta_j - e_{ij} E_j$. To use this, we need the 6x3 form of the piezoelectric stress which can be derived from the more commonly used 3x6 form as follows:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix} \Rightarrow \begin{bmatrix} 0 & 0 & e_{31} \\ 0 & 0 & e_{31} \\ 0 & 0 & e_{33} \\ 0 & e_{15} & 0 \\ e_{15} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

We also need the stiffness coefficients and values of the piezoelectric stress coefficients, which are both tabulated here:

AlN Stiffness Coefficients ($\times 10^{10}$ Newton/m ²)						
C11	C12	C13	C14	C33	C44	C66
41	14	10		39	12	13.5

Material	Piezoelectric Constants (Coulomb/m ²)						ϵ_r
	e11	e14	e15	e22	e31	e33	ϵ_r
AlN			-0.48		-0.58	1.55	8.5

The stiffness coefficients go into the general stiffness matrix for solids having hexagonal symmetry:

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ 0 & C_{11} & C_{13} & 0 & 0 & 0 \\ 0 & 0 & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}$$

where $C_{66} = (1/2)(C_{11} - C_{12})$. Now using matrix multiplication, we can write

$$P_1 = C_{13} \eta_3 - e_{31} E_0$$

$$P_2 = C_{13} \eta_3 - e_{31} E_0$$

$$P_3 = C_{33} \eta_3 - e_{33} E_0$$

Where the other possible P components: P_4 , P_5 , and P_6 are necessarily zero because we assumed up front that the only nonzero strain component was η_3 .

Substitution of the appropriate values leads to

$$P_1 = 10 \times 10^{10} \eta_3 + 0.58 \times 10^6 \quad [\text{N/m}^2]$$

$$P_2 = 10 \times 10^{10} \eta_3 + 0.58 \times 10^6 \quad [\text{N/m}^2]$$

$$P_3 = 39 \times 10^{10} \eta_3 - 1.55 \times 10^6 \quad [\text{N/m}^2]$$

(b) To get the surface charge density in the two interface planes, we start with the direct piezoelectric relation: $D_i = \epsilon_{ij} E_j + e_{ij} \eta_j$. When expressed in terms of the known E_z and η_3 , and using the above 3x6 form of the piezoelectric stiffness matrix, we get $D_z = \epsilon_r \epsilon_0 E_0 + e_{33} \eta_3$. Then from electrostatics, we know $P_z = D_z - \epsilon_0 E_0 = (\epsilon_r - 1) \epsilon_0 E_0 + e_{33} \eta_3 = 6.6 \times 10^{-5} + 1.55 \eta_3$ [Cb/m²]. Until we know the strain, no further evaluation can be done.

(c) If the AlN film is now used as a MEMS cantilever by unclamping it, by definition all the stress coefficients will be zero. So we can write from the piezoelectric inverse relation,

$$P_j = 0 = C_{ij} \eta_j - e_{ij} E_j, \quad \text{which in full matrix form becomes}$$

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \\ \eta_5 \\ \eta_6 \end{bmatrix} = \begin{bmatrix} 0 & 0 & e_{31} \\ 0 & 0 & e_{31} \\ 0 & 0 & e_{33} \\ 0 & e_{15} & 0 \\ e_{15} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ E_z \end{bmatrix}$$

And when written out using the stress coefficients and $E_0 = 10^6$ V/m becomes

$$C_{11} \eta_1 + C_{12} \eta_2 + C_{13} \eta_3 = e_{31} E_z = -0.58 \times 10^6$$

$$C_{12} \eta_1 + C_{11} \eta_2 + C_{13} \eta_3 = e_{31} E_z = -0.58 \times 10^6$$

$$C_{13} \eta_1 + C_{13} \eta_2 + C_{33} \eta_3 = e_{33} E_z = 1.55 \times 10^6$$

This has a simple 3x3 numerical matrix form: $10^{10} \cdot \begin{bmatrix} 41 & 14 & 10 \\ 14 & 41 & 10 \\ 10 & 10 & 39 \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} = \begin{bmatrix} -0.58 \times 10^6 \\ -0.58 \times 10^6 \\ 1.55 \times 10^6 \end{bmatrix}$

(d) One can use MATLAB to invert the 3x3 numerical matrix to get

$$\begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} = 10^{-10} \cdot \begin{bmatrix} 0.0285 & -0.0085 & -0.0051 \\ -0.0085 & 0.0285 & -0.0051 \\ -0.0051 & -0.0051 & 0.0283 \end{bmatrix} \begin{bmatrix} -0.58 \times 10^6 \\ -0.58 \times 10^6 \\ 1.55 \times 10^6 \end{bmatrix}$$

or $\eta_1 = -1.96 \times 10^{-6}$, $\eta_2 = -1.96 \times 10^{-6}$, and $\eta_3 = 4.98 \times 10^{-6}$

- 3. Common Crystal Structures.** Refer to the “Simple Crystal Structures” of Kittel Chapter 1:
- (a) (1) Sodium Chloride is centrosymmetric, (2) Cesium Chloride is centrosymmetric, (3) Hexagonal Close Packed (monatomic) is centrosymmetric, (4) Diamond (monatomic) is centrosymmetric, and (5) Cubic zinc sulfide (Zincblende) is noncentrosymmetric. (note: several of the “hexagonal” materials we have been talking about, such as AlN, are not HCP, but rather Wurtzite. That is why they are noncentrosymmetric).
- (b) None of the simple crystal structures has a unique polar axis except for zincblende, whose polar axis is oriented along the [111] direction of the conventional cubic unit cell.