Homework 6

1. **Non-Centrosymmetry and Piezoelectricity.** We have stated that the ionic honeycomb crystal shown in Fig. 1(a) is a good example of a non-centrosymmetric structure.

(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.

(b) Now assume a deformation δd is induced by a uniaxial stress perpendicular to one of the facets of the honeycomb. Assuming the resulting strain to be small enough to apply Hooke's law, calculate the distortion of the dipoles in (a) and use this to write down the new electric polarization. (clue: assume the area of the honeycomb stays constant).

(c) Now assume combine the hexagons with each other to form a honeycomb two-dim crystal lattice (not a Bravais lattice, but a lattice with a two-atom basis). If the resulting 2D sample is in the form of a large square, what will be the *line* charge [Cb/m] be on the two sides perpendicular to the applied stress? What will the piezoelectric stress coefficient be in MKSA ?

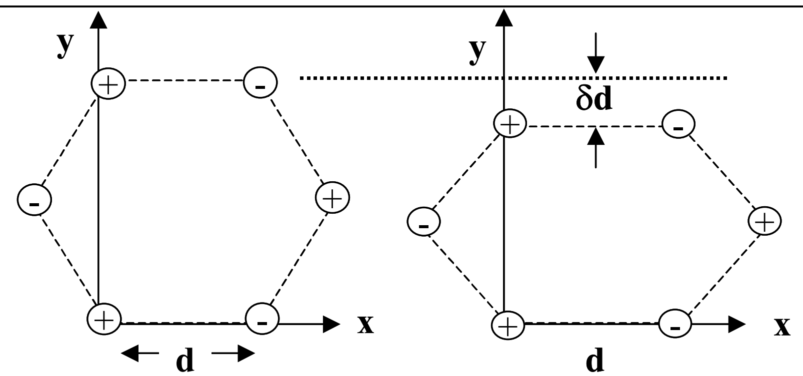

Fig. 1.

2. **AlN as a Piezoelectric Material**. AlN is an emerging piezoelectric material with the advantage of being producible in thin-film form by epitaxial techniques on substrates (e.g., SiC) of very good mechanical (i.e., high stiffness) and electrical (i.e., high resistivity) properties. Suppose you have an AlN film in the x-y plane in a completely "clamped" state (e.g., sandwiched between two stiffer materials) and subjected to a uniform external electric field of E_0 = 10 KV/cm along the z axis.

(a). Write the appropriate connection equations between the stress and E_0 and evaluate all nonzero stress components.

(b) Write and evaluate an expression between the surface charge density in the two interface planes and E_0.

(c) Now suppose you wish to use the AlN film as a MEMS cantilever by unclamping it completely. For the same application of E field, write down the connection equations between the strain and E_0.

(d) Use Matlab or your favorite computational tool to invert the relations and find the values of the first three strain components, η_1, η_2, and η_3 if E_0 = 10 KV/cm.

(clues: "clamped" means all the strain components are zero, "unclamped" means that all stress components are zero; you will want to use the 6x3 form of the piezoelectric stress matrix for this problem; the non-zero stiffness coefficients for AlN are given below).

3. **Common Crystal Structures.** Some of the most commonly occurring crystal structures in nature are: (1) Sodium Chloride, (2) Cesium Chloride, (3) Hexagonal Close Packed, (4) Diamond, and (5) Zincblende

(a) Inspect each of these for noncentrosymmetry and, therefore, piezoelectricity.
(b) Inspect each for a unique polar axis relative to the atomic structure.