

결정학개론 445.206 003

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Final Exam

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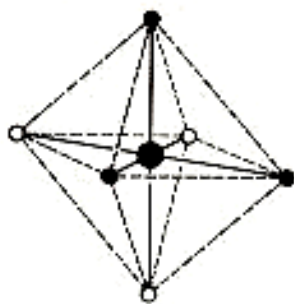
1.(15점) a)(5점) Show that the piezoelectric modulus  $d_{36}$  in point group 4 is zero.

b)(5점) The electrical conductivity tensor of a certain crystal has the following components referred to axes  $x_1, x_2, x_3$ :

$$[\sigma_{ij}] = \begin{bmatrix} 25 \times 10^7 & 0 & 0 \\ 0 & 16 \times 10^7 & 0 \\ 0 & 0 & 4 \times 10^7 \end{bmatrix}$$

in m.k.s. units ( $\text{ohm}^{-1}\text{m}^{-1}$ ). Draw a section of the conductivity ellipsoid (representation quadric) in the plane  $x_1=0$ . Express the relative size of the axes. Assume that an electric field is established in the direction whose cosines are  $(0, \frac{1}{2}, \frac{\sqrt{3}}{2})$ . Calculate the conductivity in that direction.

c)(5점) Determine the point group of the following molecule,  $\text{SF}_3\text{X}_3$ .



2.(35점) The symmetry diagrams for a space group is given below as projections on  $x, y, 0$ .

a)(5점) Enter on the diagram in a general site  $x, y, z$ , and allow the symmetry to operate on it (use the symbol in the International Tables for

X-ray Crystallography ).

b)(5점) Give the coordinates of the points equivalent to x, y, z.

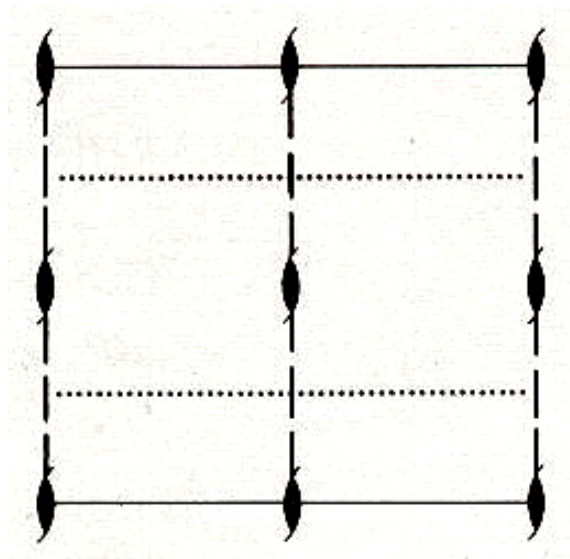
c)(5점) What are the space group symbol and point group.

d)(5점) Indicate a special position-if there are any-and give its multiplicity.

e)(5점) What is crystal system this space group belongs to?

f)(5점) Is the crystal, which has the above space group, is pyroelectric? If it is, what is the direct of the polarization?

g)(5점) How many independent coefficients are required to describe the second rank tensor properties such as electrical conductivity in this material?



3.(30점) In a 2-D rectangular crystal with  $a=4\text{ \AA}$  and  $b=2\text{ \AA}$ ,

a)(10점) Plot the corresponding reciprocal lattice and index the lattice points (indicate the scale).

b)(10점) When the incident X-ray beam ( $\lambda=\frac{4}{\sqrt{5}}\text{ \AA}$ ) is directed normal to

(11) plane, superpose the Ewald circle on the reciprocal lattice using the same scale of (a). Mark the incident beam direction, location of crystal (C), and origin of the reciprocal lattice (O).

c)(10점) Which reciprocal lattice points intersect the Ewald circle?

What is the diffraction angle  $2\theta$ ?

( in 2-D, interplanar spacing  $d_{hk} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2}}}$  )

4.(20점) a)(5점) When there is a screw axis parallel to **b** axis of the crystal, find the condition for systematic absence.

b)(5점) Can you identify the inversion center within the crystal from the diffraction pattern? What is this law? If no, how can you determine the absence of the inversion center?

c)(5점) Represent the amplitude function of a crystal using the amplitude functions of motif, infinite lattice, and shape function, and express the diffraction pattern amplitude based on the above representation. What information can be inferred from each term on the expression.

d)(5점) Prove that the reciprocal lattice vector

$$\overline{G}_{hkl} = h\overline{a}^* + k\overline{b}^* + l\overline{c}^*$$

is perpendicular to the (hkl) set of planes in the real lattice.