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No.8

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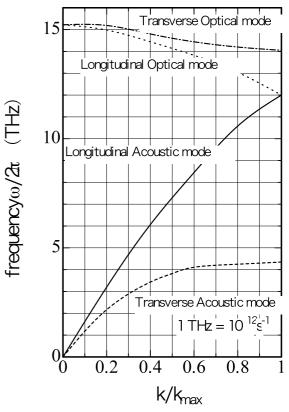
8. Consider the relationship between the lattice vibration and the elastic properties.

 $\omega_k - k$ dispersion relation of [100] direction in Si is indicated in the right figure.

8-1 Explain the six modes of the lattice vibration in Si [100] direction.

8-2 Explain the relationship between three elastic waves and the lattice vibration in Si [100] direction.

Si[100] direction $\omega/2\pi$ -k/k_{max} dispersion relation



8-3 Give the velocities of three elastic waves of Si [100] direction from the figure of $\omega_k - k$ dispersion.

Here $k_{\text{max}} = 2\pi / a$, and $a = 5.4 \times 10^{-10} \text{m}.$



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9. Consider the elastic waves in cubic crystals in the [110] direction.

Here, ρ is the density [kg/m³], u, v, w are the displacement in the x, y, z directions, respectively. C_{ij} is elastic stiffness constants [N/m²]. Equations of motion in the x, y, z directions are given by

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial^2 u}{\partial x^2} + C_{44} \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \left(C_{12} + C_{44} \right) \left(\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 w}{\partial x \partial z} \right),$$

$$\rho \frac{\partial^2 v}{\partial t^2} = C_{11} \frac{\partial^2 v}{\partial y^2} + C_{44} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial z^2} \right) + \left(C_{12} + C_{44} \right) \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 w}{\partial y \partial z} \right), \text{ and }$$

$$\rho \frac{\partial^2 w}{\partial t^2} = C_{11} \frac{\partial^2 w}{\partial z^2} + C_{44} \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) + \left(C_{12} + C_{44} \right) \left(\frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 v}{\partial y \partial z} \right).$$

9-1 Consider elastic waves that propagate in the xy plane with the particle motion in the xy plane as $u = u_0 \exp[i(k_x x - k_y y - \omega t)]$, and $v = v_0 \exp[i(k_x x - k_y y - \omega t)]$.

Derive the propagating direction of this elastic wave, and calculate the values of k_x and k_y . where, $k^2 = k_x^2 + k_y^2$, $k_x = k_y > 0$.

9-2 Calculate the velocities $\frac{\omega}{k}$ of longitudinal and transverse waves.



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10-1-1 Illustra	te the	"new"	coordi	nate vectors	\boldsymbol{e}_1 , \boldsymbol{e}_2 and	e_3 which	n are trans	formed	from
e_{1}, e_{2} ,	and	e_3 t	y the	following	symmetries.	Then,	describe	the u	nitary

transformation matrices a for the symmetry elements. Note that 4 represents anticlockwise rotation of 90°:

a) $\overline{1}$, b) 2_z , c) 4_z , d) $\overline{4}_z$

10-1-2 Find the inverse unitary matrix $a^{-1}(4_z)$, by transposing (with respect to the matrix diagonal axis) the elements of the matrix $a(4_z)$ [note that $a^{-1}(4_z) = a^{T}(4_z)$].



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- 11-1. i) Rewrite Eq. (4.1b) in conventional summation notation (instead of dummy suffix notation).
 - ii) Show that $\boldsymbol{B} = (B_1, B_2, B_3)$ and $\boldsymbol{D} = (D_1, D_2, D_3)$ are transformed by $\overline{2}_{i}$ as described in Eq. (4.4) as $\mathbf{B'} = |\mathbf{a}|\mathbf{a}\mathbf{B}$ and $\mathbf{D'} = \mathbf{a}\mathbf{D}$

iii) Using Eq. (4.1a), show that **B** is kept unchanged by $\overline{1}$. Also show D' by using D.

11-2. Gyration tensor $g(g_{ij})$ gives optical rotation (i.e. rotates azimuth angle of polarization of light).

We can change g by applying electric field E, which is called "electric-field induced optical rotation." We can also change g by applying magnetic field **B**, which is called "magneto-optical Faraday rotation."

The effects are represented as follows using tensors A and B

 $\Delta g = A \cdot E$ and $\Delta g = B \cdot H$.

What kind of tensors are A and B? (Tell rank and whether axial or polar. Refer Table 4.1)



11-3. Tensor whose elements are symmetrical (namely such relation as $T_{ij} = T_{ji}$, $T_{ijk} = T_{jik}$ or $T_{ijkl} = T_{jikl}$ holds are called symmetrical tensor (for suffixes *i* and *j*). What change occurs in Eqs. (4.14) of [Example V] if the tensor $T = \begin{bmatrix} T_{11} & T_{12} & 0 \\ -T_{12} & T_{11} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}$ becomes symmetrical $(T_{ij} = T_{ji})$?

11-4. On BaTiO₃ answer the following questions.

i) In the temperature region I the crystal has a cubic lattice (a = b = c, $\alpha = \beta = \gamma = 90^{\circ}$), which reduces in symmetry in other regions.

The lower-symmetry lattice is called "pseudo cubic lattice." What relations do *a*, *b*, *c*, α , β , and γ of the pseudo cubic lattice satisfy in regions II, III, and IV, respectively? [Hint: Fig. 4.8]

ii) Illustrate the spontaneous polarization p and the unit cell in respective regions II, III, and IV.

iii) In respective regions II \sim IV, show p and the mirror planes that the lattice has.

iv) In the region III, express a', b', and c' (lattice parameters of true lattice) in terms of a, b, c, and α (lattice parameters of pseudo cubic lattice). Also find an approximate relation which holds for a', b', and c'.



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12-1. Rewrite the following matrix elements as tensor elements.

i) The piezoelectric matrix elements d_{12}, d_{25} and d_{34} .

- ii) The stress matrix elements σ_2 and σ_6 .
- iii) The dielectric constant matrix elements ϵ_3, ϵ_5 and ϵ_6 .
- 12-2. Rewrite the four equations given in Table 5.1 in conventional summation notation (rather than dummy suffix notation).

12-3. i) The piezoelectric coefficient of crystals belonging to 32 point group (given in Table 5.2) is expressed in the matrix notations as

$$\begin{bmatrix} d_{ij} \end{bmatrix} = \begin{pmatrix} d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Following this example, express in the matrix notation the piezoelectric coefficient of crystals belonging to $\overline{4}2$ m and 3 point symmetry groups.

ii) Describe the non zero tensor elements d_{ijk} for crystals belonging to $\overline{4}2$ m point group. Also describe the relation holding for these elements.



12-4. A tensor stress σ_{11} is applied to a crystal belonging to point group 3 along the x_1 axis. Find the polarization induced by the piezoelectric effect.

[Hint: $\boldsymbol{P} = \boldsymbol{d\sigma}$ or $P_i = d_{ij}\sigma_j$]

12-5. An electric field E_1 is applied to a crystal belonging to $\overline{4}2$ m point group along the x_1 axis. Find the strain induced by E_1 .

[Hint: Put j=1 in $\varepsilon_i = d_{ij}E_i$]



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- 1. i) Along what direction(s) does a BaTiO₃ crystal exhibit pyroelectricity at -100°C, 0°C, 100°C, and 150°C? Answer on the "pseudo-cubic" lattice. [Hint: Fig. 4.4]
 - ii) Along what direction(s) does a crystal belonging to 4mm point group exhibit pyroelectricity? [Hint: Table 3.3]
- 2. In Table 6.1, find the point group(s) to which the following crystals belong. (Note that some are not existing.)i) Polar crystal(s) with tetragonal symmetry (i.e. belonging to tetragonal system).
 - ii) Cubic crystal(s) exhibiting piezoelectricity.
 - iii) Cubic crystal(s) exhibiting pyroelectricity.
 - iv) Crystal without $\overline{1}$ symmetry, but not exhibiting piezoelectricity.
 - v) Hexagonal crystal(s) allowed by symmetry to exhibit ferroelectricity.
 - vi) Cubic crystals allowed by symmetry to exhibit ferroelectricity.