

## 3.60 Symmetry, Structure and Tensor Properties of Materials

### Problem Set 12

1. Point out the fallacy, if any, in the following arguments.

(a) The dipole moment of charges  $+q$  and  $-q$  separated by distance,  $d$ , is a vector quantity defined as  $\vec{p} = q\vec{d}$  (the direction of  $\vec{d}$  is defined as extending from the negative charge to the positive). Atoms subjected to an electric field,  $\vec{E}$ , undergo charge deformation which results in an induced dipole moment. The dipole moment is related to the applied field by the ionic electrical polarizability tensor  $p_i = \alpha_{ij}E_j$ .

Second-rank tensors are isotropic for cubic crystals.

Atoms in many cubic crystals are found to have anisotropic polarizability.

This is a violation of Neumann's Principle.

(b) The ability of a crystal to diffract x-rays is a property of a crystal. Neumann's Principle states that the symmetry of any property depends on the point group of a crystal, and that the symmetry of a property must be at least that of the point group.

X-ray diffraction patterns, however, are commonly used to determine the space group of crystals.

Neumann's Principle therefore does not apply to x-ray diffraction.

2. The Cartesian coordinates of a point,  $X_i$ , transform upon a change of coordinate system according to

$$X_i' = c_{ij}X_j$$

where  $c_{ij}$  is the direction cosine scheme which relates the axes of the two coordinate systems. We have stated that if one can, by inspection, write down a relation between the axes of the two coordinate systems  $x_i$  and  $x_j$  (e.g.,  $x_1' = -x_1$ ,  $x_2' = -x_2$ ), that this provides a convenient method for extracting the direction cosine scheme (e.g.,  $c_{11} = -1$ ,  $c_{12} = 0$ ,  $c_{13} = 0$  etc.).

The above statement is rather cavalier, however, and not strictly correct: The first equation involves coordinates of a point, while the later equations, written by inspection, involve a vector relationship between reference axes in the two coordinate systems.

Demonstrate (by means of a sketch or otherwise) that the procedure is correct--that is, that the coordinates of a point transform in exactly the same way as the axes of the reference system.