CHAPTER 2 -- PROBLEMS AND EXERCISES

1. Explain the difference between tensor notations and Voigt matrix notations in the writing of the compliance and stiffness matrices

Solution

The tensor notations write the compliance and stiffness coefficients as 4th order tensors, i.e., indexed coefficients that depend on four independent indices. Each of these indices takes values 1 through 3, according to the three independent directions of the three-dimensional space. The reason for the compliance and stiffness matrices having four independent indices is that the strain and stress are shown as 2nd order tensors, i.e., variables that depend on two independent indices each. On this argument, one arrives at the tensor equations (2.1) and (2.2). However, through symmetry arguments, it can be shown that the strain and stress matrices only have six independent variables each. For example, the strain matrix has three direct strains and three shear strains. This observation permits simplification of notations, which leads to the Voigt matrix notations. The six independent strains and stresses are presented in columns, i.e. single-index variables. For example, $S_1, S_2, \ldots, S_6$. Hence, the 4th order compliance and stiffness tensors reduce to 2nd order tensors, i.e., matrices, as illustrated in Equations (2.22) through (2.27).

2. Explain the following difference in subscripts usage: the (1,3) term in the compliance matrix is denoted s_{13}, whereas the (1,3) term in the piezoelectric coefficient matrix is denoted d_{31}

Solution

The difference in subscript usage originates in the definition of the two physical constants. Reference is made to Equations (2.22) and (2.23). On one hand, the compliance matrix $[\mathbf{s}]$ is defined directly by Equation (2.22) as strain columns obtained when a unit stress is applied one at a time in each of the six major directions. On the other hand, the piezoelectric coefficient matrix $[\mathbf{d}]$ is defined by Equation (2.23) as electric displacement columns obtained when a unit stress is applied one at a time in each of the six major directions. The piezoelectric coefficient matrix that appears in Equation (2.22) is the transpose of the piezoelectric coefficient matrix defined in Equation (2.23). This fact is apparent in Equation (2.26), which is the matrix equivalent of Equation (2.22); this equation shows the term $[\mathbf{d}]^t$. For these reasons, the (1,3) term in Equation (2.22) is denoted d_{31}.

3. Calculate the spontaneous strain, S_S, and the spontaneous polarization, P_S, for the barium titanate lattice shown in Figure 2.10.

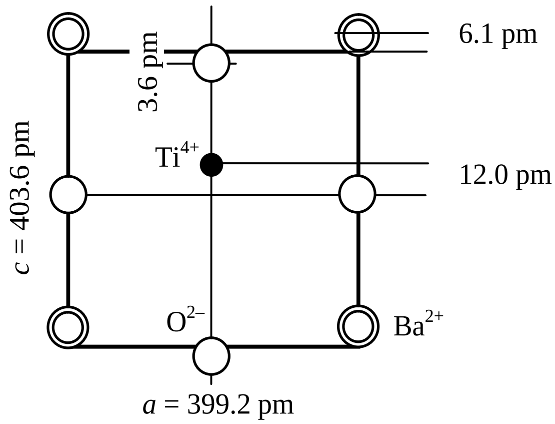

Figure 2.9 Ionic shifts inducing spontaneous strain and spontaneous polarization in barium titanate

Solution

(a) Spontaneous strain is the calculating by assuming that the undistorted cell height was a, while the distorted cell height is c. Hence,

$$S_S = \frac{c-a}{a} = \frac{403.6-399.2}{399.2} \simeq 0.01 = 1\%$$

(b) Spontaneous polarization is defined as the polarization per unit volume. The polarization is calculated as the sum of the dipole moments of each ion, weighted according to their contribution to the unit cell. Thus,

For the Ba^{2+} cations, $p_{\mathrm{Ba}^{2+}} = 8\frac{2e}{8}6.1 = 12.2\,e\,\mathrm{pm}$

For the Ti^{4+} cations, $p_{\mathrm{Ti}^{4+}} = 4e\times 12.0 = 48.0\,e\,\mathrm{pm}$

For the O^{2-} anions, $p_{\mathrm{O}^{2-}} = 2\frac{-2e}{2}\times(-3.6) = 7.2\,e\,\mathrm{pm}$

where $e = 1.602\times 10^{-19}$ C is the value of the unit charge and $1\ \mathrm{pm} = 10^{-12}$ m.

The total polarization is

$$p = p_{Ba^{2+}} + p_{Ti^{4+}} + p_{O^{2-}} = 67.4\,e\,\mathrm{pm} = 1.080\times 10^{-29}\ \mathrm{Cm}$$

Thus, the spontaneous polarization is

$$P_S = \frac{p}{a^2 c} = \frac{1.080\times 10^{-29}}{\left(399.2\times 10^{-12}\right)^2\left(403.6\times 10^{-12}\right)} = 0.170\ \mathrm{C/m^2}$$

This predicted value is not too far off from the experimental value of $0.250\ \mathrm{C/m^2}$.