

## Thermal Expansion Coefficients for Monoclinic Crystals: A Phenomenological Approach

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### Abstract

A phenomenological treatment of the thermal expansion of a monoclinic crystal is presented. The components of the thermal expansion tensor are expressed in differential form as functions of the unit cell parameters. Two sets of expressions are developed from the Lagrangian and the Eulerian definitions of deformation. These correspond in form to the "instantaneous linear thermal expansion coefficient" and the "true linear thermal expansion coefficient" discussed by Kempter and Elliott (1959). The relation of these forms to the Ohashi and Burnham (1973) equations is also discussed.

### Introduction

With the development of techniques for collecting precision intensity data from single crystals at high temperatures, a considerable amount of data has been obtained for a number of minerals (Bloss and Papike, 1973). This has not only resulted in a better understanding of the thermal properties of materials in terms of individual bond length and angle variations, but has also provided valuable insight into the nature of the cohesive forces between bonded atoms. Ohashi and Burnham (1973) have developed expressions for obtaining thermal expansion coefficients from these data. We have since developed a set of similar expressions in differential form. The mean values of these are very similar to the equations given by Ohashi and Burnham. Our approach is an extension of a method discussed by Stokes and Wilson (1941) which was used by them to evaluate the thermal expansion coefficient of lead metal. We have extended their approach to crystals with monoclinic symmetry. The thermal expansion coefficients which result are continuous functions of temperature rather than mean values over some temperature range.

### Types of Thermal Expansion

The thermal expansion coefficient of a material in a given direction may be defined as the rate of change

of strain in that direction per unit temperature change. For each type of strain which has been defined there is a corresponding type of thermal expansion coefficient obtained by taking the derivative of that strain with respect to temperature. Among the types of one-dimensional strain that are used (Mase, 1970) are the "conventional engineering strain" defined as

$$e = (l - l_0)/l_0 \quad (1)$$

and the "natural (logarithmic) strain" defined as

$$\epsilon = \ln(l/l_0) \quad (2)$$

where  $l_0$  and  $l$  represent the length of a given line segment in the medium at temperatures  $T_0$  and  $T$ , respectively. The corresponding thermal expansion coefficients are therefore

$$e' = \frac{de}{dT} = \frac{1}{l_0} \frac{dl(T)}{dT} \quad (3)$$

and

$$\epsilon' = \frac{d\epsilon}{dT} = \frac{d(\ln l(T))}{dT} = \frac{1}{l(T)} \frac{dl(T)}{dT} \quad (4)$$

To describe strain in a three dimensional body a second rank tensor is required. Each of the nine components,  $l_{ij}$ , of this second rank strain tensor is a

function of the applied stress (a second rank tensor whose components are denoted by  $\sigma_{ij}$ ), and the temperature  $T$  (Nye, 1957). Accordingly,

$$l_{ij} = l_{ij}(\sigma_{11}, \sigma_{12}, \dots, \sigma_{33}, T) \quad (5)$$

or in differential form

$$dl_{ij} = (\partial l_{ij} / \partial \sigma_{kl})_T d\sigma_{kl} + (\partial l_{ij} / \partial T)_\sigma dT = S_{ijkl}^T d\sigma_{kl} + \lambda_{ij}^\sigma dT \quad (6)$$

where by definition the  $S_{ijkl}^T = (\partial l_{ij} / \partial \sigma_{kl})_T$  are isothermal elastic compliance coefficients (a fourth rank tensor) and  $\lambda_{ij}^\sigma$  represents the elements of the thermal expansion tensor at constant stress. The subscripts  $k$  and  $l$  in Equation 6 are dummy (running) indices. The Einstein summation convention is being used. There are nine equations of this type, each of which contains a total of ten terms. Since the crystal is not being subjected to a stress, *i.e.*,  $\sigma_{ij} = 0$ , and therefore  $d\sigma_{ij} = 0$ , the  $l_{ij}$ 's are functions of  $T$  alone and the first nine terms of Equation (6) vanish. Therefore, we write

$$dl_{ij} = \lambda_{ij}^\sigma dT = \lambda_{ij} dT \quad (7)$$

(the superscript  $\sigma$  has been deleted to simplify the notation).

The recent treatment by Ohashi and Burnham (1973) assumes the  $\lambda_{ij}$  terms in Equation (7) to be constants. It then becomes possible to integrate between the temperatures  $T_0$  and  $T$  if the reference state of zero strain is taken at  $T_0$  (*i.e.*,  $l_{ij}(T_0) = 0$ ). Thus

$$l_{ij}(T) = \int_0^{l_{ij}(T)} dl_{ij} = \int_{T_0}^T \lambda_{ij} dT = \lambda_{ij}(T - T_0) = \lambda_{ij} \Delta T \quad (8)$$

or

$$\lambda_{ij} = l_{ij} / \Delta T. \quad (9)$$

The  $l_{ij}$  are then formulated in terms of the initial and final cell parameters. A more general theory recognizes that the  $\lambda_{ij}$  terms can vary with temperature. The expression corresponding to Equation (8) then becomes

$$l_{ij}(T) = \int_{T_0}^T \lambda_{ij}(T) dT \quad (10)$$

and the mean value of  $\lambda_{ij}(T)$  between temperatures  $T_0$  and  $T$  is

$$\langle \lambda_{ij} \rangle = \frac{1}{T - T_0} \int_{T_0}^T \lambda_{ij}(T) dT \quad (11)$$

The essential characteristic of all deformations resulting from a change in temperature is that they are homogeneous (often called affine, *i.e.*, deformations in which straight lines remain straight, planes remain planes, and spheres are transformed into triaxial ellipsoids). Such a deformation may be formulated mathematically as

$$\mathbf{u}_i = l_{ij} X_j \quad (12)$$

where  $\mathbf{X} = X_1 \mathbf{i} + X_2 \mathbf{j} + X_3 \mathbf{k}$  refers to the initial coordinates of a "material point" before any deformation, *i.e.*, at  $T_0$ , and  $\mathbf{u} = u_1 \mathbf{i} + u_2 \mathbf{j} + u_3 \mathbf{k}$  indicates the amount of displacement which that point has undergone upon reaching the final state at  $T$ . The final position of the material particle is

$$\mathbf{x} = x_1 \mathbf{i} + x_2 \mathbf{j} + x_3 \mathbf{k} = \mathbf{X} + \mathbf{u}. \quad (13)$$

As a consequence of Equation (12), it can be shown that there exists a second rank tensor  $[e_{ij}]$  such that

$$u_i = e_{ij} x_j. \quad (14)$$

Equations (12) and (14) are referred to as the Lagrangian and Eulerian formulations of the deformation, respectively. For pure strain the tensor  $[l_{ij}]$  is called the linear Lagrangian strain tensor while  $[e_{ij}]$  is the linear Eulerian strain tensor. The components of  $[l_{ij}]$  and  $[e_{ij}]$  are defined by

$$l_{ij} = \frac{1}{2} \left[ \frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} \right] \quad (15a)$$

and

$$e_{ij} = \frac{1}{2} \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right], \text{ respectively.} \quad (15b)$$

Since it follows from these definitions that  $l_{ij} = l_{ji}$  and  $e_{ij} = e_{ji}$ , both strain tensors are symmetric (Frederick and Chang, 1969). The corresponding thermal expansion tensors are

$$\lambda_{ij}(T) = dl_{ij}(T)/dT \quad (16a)$$

and

$$\epsilon_{ij}(T) = de_{ij}(T)/dT. \quad (16b)$$

We will refer to these as the Lagrangian and Eulerian thermal expansion tensors. Note that  $\lambda_{ij}(T)$  and  $\epsilon_{ij}(T)$  also correspond respectively to the "instantaneous linear thermal expansion coefficient" and the "true linear thermal expansion coefficient" given by Kempter and Elliott (1958). These terms are somewhat misleading and hence the terms Lagrangian and Eulerian thermal expansion coefficients are used here.

Starting from Equation (12)<sup>1</sup> it can be shown that for a given line segment in the medium with initial length  $l_0$ , initial direction cosines ( $n_1, n_2, n_3$ ), final length  $l$ , and final direction cosines ( $\bar{n}_1, \bar{n}_2, \bar{n}_3$ ), the following is true:

$$\frac{l - l_0}{l_0} = \frac{2l_{ij}n_i n_j + l_{ij}l_{ik}n_i n_k}{1 + \sqrt{1 + 2l_{ij}n_i n_j + l_{ij}l_{ik}n_i n_k}} \approx l_{ij}n_i n_j \quad (17)$$

since  $l_{ij}l_{ik}n_i n_k \ll 2l_{ij}n_i n_j \ll 1$  (the  $l_{ij}$  values are usually of the order of  $10^{-6}$ ). Similarly, from Equation (14) one can show

$$\frac{l - l_0}{l} = \frac{2e_{ij}\bar{n}_i \bar{n}_j - e_{ij}e_{ik}\bar{n}_i \bar{n}_k}{1 + \sqrt{1 + e_{ij}e_{ik}\bar{n}_i \bar{n}_k - 2e_{ij}\bar{n}_i \bar{n}_j}} \approx e_{ij}\bar{n}_i \bar{n}_j \quad (18)$$

since  $e_{ij}e_{ik}\bar{n}_i \bar{n}_k \ll 2e_{ij}\bar{n}_i \bar{n}_j \ll 1$  (the  $e_{ij}$  values are also usually of the order of  $10^{-6}$ ). On differentiating Equations (17) and (18) with respect to temperature we obtain

$$\lambda_{ij}(T)n_i n_j = \frac{dl_{ij}(T)}{dT} n_i n_j \approx \frac{1}{l_0} \frac{dl(T)}{dT} \quad (19)$$

and

$$\begin{aligned} \epsilon_{ij}(T)\bar{n}_i \bar{n}_j &= \frac{de_{ij}(T)}{dT} \bar{n}_i \bar{n}_j \\ &= \sqrt{1 + e_{ij}e_{ik}\bar{n}_i \bar{n}_k - 2e_{ij}\bar{n}_i \bar{n}_j} \\ &\quad \cdot \frac{1}{l(T)} \frac{dl(T)}{dT} - 2e_{ij}(T)\bar{n}_i \frac{d\bar{n}_j}{dT} \\ &\approx \frac{1}{l(T)} \frac{dl(T)}{dT}. \end{aligned} \quad (20)$$

We now consider at temperature,  $T_0$ , a line segment perpendicular to the plane ( $hkl$ ) with length  $l_0$  equal to  $d_{hkl}$ . Let ( $n_1, n_2, n_3$ ) denote the direction cosines of this line segment. At temperature  $T$  the deformed line, with direction cosines ( $\bar{n}_1, \bar{n}_2, \bar{n}_3$ ), is perpendicular to the deformed ( $hkl$ ) plane and its length is given by  $l$ , equal to  $d_{(hkl)}$  for the deformed plane (Bouvaist and Weigel, 1970). We obtain from Equations (19) and (20) the following:

$$\lambda_{ij}(T)n_i n_j \approx \frac{1}{d_{0(hkl)}} \frac{d[d_{(hkl)}(T)]}{dT} \quad (21)$$

and

$$\epsilon_{ij}(T)\bar{n}_i \bar{n}_j \approx \frac{1}{d_{(hkl)}(T)} \frac{d[d_{(hkl)}(T)]}{dT} \quad (22)$$

Equations (19) and (20) may be used to calculate the principal thermal expansion coefficients of any crystal with orthogonal axes because these are known from symmetry considerations to coincide with the unit cell edge vectors  $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ . Accordingly, for an orthogonal crystal we write<sup>2</sup>

$$\lambda_{11}(T) = \frac{1}{a_0} \frac{da(T)}{dT}, \quad (23)$$

$$\lambda_{22}(T) = \frac{1}{b_0} \frac{db(T)}{dT}, \quad (24)$$

$$\lambda_{33}(T) = \frac{1}{c_0} \frac{dc(T)}{dT}, \quad (25)$$

$$\epsilon_{11}(T) = \frac{1}{a(T)} \frac{da(T)}{dT}, \quad (26)$$

$$\epsilon_{22}(T) = \frac{1}{b(T)} \frac{db(T)}{dT}, \quad (27)$$

and

$$\epsilon_{33}(T) = \frac{1}{c(T)} \frac{dc(T)}{dT} \quad (28)$$

for the Lagrangian and Eulerian forms respectively. The purpose of this paper is to develop similar expressions for the monoclinic case. The approach may be extended to the triclinic case.

In order to use Equations (23) through (28), the cell parameters must first be expressed as functions of temperature. Owen and Roberts (1936), Stokes and Wilson (1941), and Kempter and Elliott (1959) utilized a power series expansion in  $T$  for this purpose. For example, we can write the length of the  $a$  cell edge as

$$a(T) = d_a + f_a T + g_a T^2 + h_a T^3 + \dots \quad (29)$$

and hence from Equation (25)

$$\lambda_{11} = \frac{f_a + 2g_a T + 3h_a T^2 + \dots}{a_0} \quad (30)$$

There are circumstances when power series expansions of cell constants as functions of temperature are not appropriate. Deshpande and Mudholker (1961) point out, for example, that power series approximations yield thermal expansion coefficients that do not approach zero as temperature approaches zero, contrary to behavior predicted by the Grüneisen relation. Other functional forms can be devised (Skinner, 1957), but because the number of possibilities is large,

<sup>1</sup> See appendix for alternative derivations of Equations (17) and (18).

<sup>2</sup>  $a_0, b_0, etc$  are the cell parameters at some reference temperature,  $T_0$ .

explicit examples will not be further discussed in this paper. The approach adapted here assumes simply that it is possible to express the cell parameters accurately as continuous functions of temperature. For this reason there should be no phase changes in the temperature range under consideration.

### Lagrangian Thermal Expansion Coefficients for Monoclinic Crystals

It is readily established from symmetry considerations (Nye, 1957) and Neumann's principle that the thermal expansion coefficient tensor for a monoclinic crystal in the second setting is of the form

$$\begin{bmatrix} \lambda_{11} & 0 & \lambda_{13} \\ 0 & \lambda_{22} & 0 \\ \lambda_{13} & 0 & \lambda_{33} \end{bmatrix} \quad (31)$$

If we adopt the rectangular coordinate system employed by Ohashi and Burnham (1973) with  $\mathbf{c}$  oriented along  $Z$ ,  $\mathbf{b}$  along  $Y$ , and  $\mathbf{a}^*$  along  $X$ , then by means of Equation (21), we obtain

$$\begin{aligned} \lambda_{11}(T) &= \frac{1}{d_{0(100)}} \frac{d[d_{(100)}(T)]}{dT} \\ &= \frac{1}{a_0 \sin \beta_0} \frac{d[a(T) \sin \beta(T)]}{dT} \end{aligned} \quad (32)$$

The expressions for  $\lambda_{22}(T)$  and  $\lambda_{33}(T)$  are the same as those given in Equations (24) and (25). The off-diagonal element,  $\lambda_{13}(T)$ , is somewhat more difficult to obtain. The thermal expansion along the  $a$  cell edge in the Lagrangian formulation is given by

$$\lambda_a(T) = \frac{1}{a_0} \frac{da(T)}{dT} \quad (33)$$

Since the initial direction cosines ( $n_1, n_2, n_3$ ) for  $\mathbf{a}$  are  $(\sin\beta_0, 0, \cos\beta_0)$ , we use Equation (19) to obtain

$$\begin{aligned} \frac{1}{a_0} \frac{da(T)}{dT} &= \lambda_{11}(T) \sin^2 \beta_0 \\ &+ \lambda_{13}(T) \sin 2\beta_0 + \lambda_{33}(T) \cos^2 \beta_0. \end{aligned} \quad (34)$$

Replacing  $\lambda_{11}(T)$  and  $\lambda_{33}(T)$  by Equations (32) and (25) and solving for  $\lambda_{13}(T)$  yields

$$\begin{aligned} \lambda_{13}(T) &= \frac{1}{a_0 \sin 2\beta_0} \frac{da(T)}{dT} - \frac{1}{2} \left[ \frac{1}{a_0 \cos \beta_0} \right. \\ &\left. \frac{d[a(T) \sin \beta(T)]}{dT} + \frac{\cot \beta_0}{c_0} \frac{dc(T)}{dT} \right]. \end{aligned} \quad (35)$$

Note that Equations (35) and (32) reduce to those obtained for orthogonal crystals when  $\beta = \beta_0 = 90$ . We

may utilize Equation (11) to obtain the following mean values for  $\lambda_{11}$ ,  $\lambda_{22}$ ,  $\lambda_{33}$ , and  $\lambda_{13}$ :

$$\langle \lambda_{11} \rangle = \frac{1}{T - T_0} \left[ \frac{a_1 \sin \beta_1}{a_0 \sin \beta_0} - 1 \right], \quad (36)$$

$$\langle \lambda_{22} \rangle = \frac{1}{T - T_0} \left[ \frac{b_1}{b_0} - 1 \right], \quad (37)$$

$$\langle \lambda_{33} \rangle = \frac{1}{T - T_0} \left[ \frac{c_1}{c_0} - 1 \right], \quad (38)$$

and

$$\begin{aligned} \langle \lambda_{13} \rangle &= \frac{1}{2(T - T_0)} \\ &\cdot \left[ \frac{a_1}{a_0} \left( \frac{1 - \sin \beta_1 \sin \beta_0}{\sin \beta_0 \cos \beta_0} \right) - \frac{c_1 \cos \beta_0}{c_0 \sin \beta_0} \right]. \end{aligned} \quad (39)$$

It is readily apparent that these equations are quite similar in form to the Ohashi and Burnham (1973) equations.

### Eulerian Thermal Expansion Coefficients for Monoclinic Crystals

The form of the thermal expansion tensor remains the same as in the Lagrangian case. Using Equation (22) we obtain

$$\begin{aligned} \epsilon_{11}(T) &= \frac{1}{d_{(100)}(T)} \frac{d[d_{(100)}(T)]}{dT} \\ &= \frac{d[\ln(a \sin \beta)]}{dT} = \frac{1}{a} \frac{da}{dT} + \cot \beta \frac{d\beta}{dT} \end{aligned} \quad (40)$$

The expressions for  $\epsilon_{22}(T)$  and  $\epsilon_{33}(T)$  remain as given in Equations (27) and (28). The expression for  $\epsilon_{13}(T)$  is obtained by expanding Equation (22) and realizing that the instantaneous direction cosines, ( $\bar{n}_1, \bar{n}_2, \bar{n}_3$ ) of  $\mathbf{a}$  are  $(\sin\beta(T), 0, \cos\beta(T))$ . On solving the expanded form of Equation (20) for  $\epsilon_{13}(T)$  one obtains

$$\begin{aligned} \epsilon_{13}(T) &= \frac{\cot \beta(T)}{2} \left[ \frac{1}{a(T)} \frac{da(T)}{dT} \right. \\ &\left. - \frac{1}{c(T)} \frac{dc(T)}{dT} \right] - \frac{1}{2} \frac{d\beta(T)}{dT} \end{aligned} \quad (41)$$

Equations (40) and (41) reduce correctly to the orthogonal case. Using Equation (11) one obtains

$$\begin{aligned} \langle \epsilon_{11} \rangle &= \frac{1}{T - T_0} \ln \left[ \frac{a_1 \sin \beta_1}{a_0 \sin \beta_0} \right] \\ &\approx \frac{1}{T - T_0} \left[ \frac{a_1 \sin \beta_1}{a_0 \sin \beta_0} - 1 \right], \end{aligned} \quad (42)$$

$$\langle \epsilon_{22} \rangle = \frac{1}{T - T_0} \ln \left[ \frac{b_1}{b_0} \right] \approx \frac{1}{T - T_0} \left[ \frac{b_1}{b_0} - 1 \right], \quad (43)$$

and

$$\langle \epsilon_{33} \rangle = \frac{1}{T - T_0} \ln \left[ \frac{c_1}{c_0} \right] \approx \frac{1}{T - T_0} \left[ \frac{c_1}{c_0} - 1 \right] \quad (44)$$

where we have utilized the approximation

$$\ln(x) = (x - 1) \quad (45)$$

which is the linear approximation to  $\ln(x)$  at  $x = 1$ . Since the change in  $a$ ,  $b$ ,  $c$ , and  $\beta$  is very small in comparison to their initial dimensions, the quotients involved in Equations (42), (43), and (44) are very close to 1 and hence, for these values, the linear approximation is quite accurate.

Since  $\beta(T)$  is unspecified and not part of a perfect differential, an exact integration of Equation (11) in the case of  $\epsilon_{13}(T)$  is not possible. If, however, we assume that  $\beta(T)$  is a constant function, *i.e.*,  $\beta(T) = \beta_0$ , then

$$\begin{aligned} \langle \epsilon_{13} \rangle &= \frac{\cot \beta_0}{2(T - T_0)} \left[ \ln \left( \frac{a_1}{a_0} \right) - \ln \left( \frac{c_1}{c_0} \right) \right] \\ &\approx \frac{\cot \beta_0}{2(T - T_0)} \left[ \frac{a_1}{a_0} - \frac{c_1}{c_0} \right] \end{aligned} \quad (46)$$

in the case where  $\beta(T)$  varies significantly in the interval  $[T_0, T]$ , the approximation given in Equation (46) may not yield an accurate estimate of  $\langle \epsilon_{13} \rangle$ . Hence, a numerical approximation to the integral using, for example, the trapezoidal rule may be more desirable. We note that the approximate value of  $\langle \epsilon_{13} \rangle$  given in Equation (46) is the same as obtained by Ohashi and Burnham (1973; Eq. A-10, p. 848) if  $\beta(T)$  is assumed to be a constant function.

### Conclusions

Once functions have been found which permit  $a$ ,  $b$ ,  $c$ , and  $\beta$  to be expressed accurately as functions of temperature, Equations (24), (25), (32), and (35) or (27), (28), (41), and (42) may be used to obtain values for the thermal expansion coefficients at any desired temperature. The orientation of the representation quadric with respect to the crystallographic axes may also be calculated (Eq. A-13, Ohashi and Burnham, 1973).

When a crystal is heated, an arbitrarily chosen line segment in the crystal changes in both length and orientation. As before, let  $l(T)$  denote the length of the line segment at temperature  $T$ . The Eulerian expression for the thermal expansion is the change of  $l(T)$  per unit temperature change divided by  $l(T)$ . On the other hand the corresponding Lagrangian expression for the thermal expansion is the change of  $l(T)$  per unit temperature change divided by  $l(T_0)$  where  $T_0$  is an arbitrarily chosen reference temperature. The

values of the thermal expansion coefficients obtained from the Lagrangian expressions are therefore not unique but rather dependent upon the choice of  $T_0$ . Since it is never necessary to choose a reference temperature,  $T_0$ , in the case of the Eulerian formulation, the values obtained for the components of  $[\epsilon_{ij}]$  are unique. While the Eulerian expressions appear to provide a more accurate description of thermal expansion, the Lagrangian values are more easily computed. Furthermore, the Lagrangian expressions have a distinct advantage in that statistical procedures for obtaining error estimates are much simpler in the Lagrangian than in the Eulerian case. In addition  $\lambda_{13}$  can be integrated exactly in its general form over a given temperature interval, while  $\epsilon_{13}$  cannot. It should be pointed out that in the limit of an infinitesimal displacement gradient these two formulations become equivalent (Frederick and Chang, 1965).

### Appendix

Equations (17) and (18) may also be obtained by considering the deformation of a material particle initially located at  $\mathbf{X} = l_0(n_1\mathbf{i} + n_2\mathbf{j} + n_3\mathbf{k})$ , where  $|\mathbf{X}| = l_0$ . If the particle is displaced  $\mathbf{u} = u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k}$  (where  $u_i = l_{ij}X_j = l_{ij}n_jl_0$ ) during formation, then

$$\frac{\mathbf{u} \cdot \mathbf{X}}{\mathbf{X} \cdot \mathbf{X}} = \frac{l_{ij}n_jl_0 \cdot l_0n_i}{l_0^2} = l_{ij}n_jn_i$$

But, according to Equation (13),  $\mathbf{u}$  is defined to be  $\mathbf{u} = \mathbf{x} - \mathbf{X}$  so that  $u_i = x_i - X_i = l_i\bar{n}_i - l_0n_i$ . Hence,

$$\frac{\mathbf{u} \cdot \mathbf{X}}{l_0^2} = \frac{(l_i\bar{n}_i - l_0n_i)l_0n_i}{l_0^2} = \frac{\bar{n}_i n_i l - n_i n_i l_0}{l_0}$$

so that  $(\bar{n}_i n_i l - l_0)l_0 = l_{ij}n_jn_i$ .

Since the deformation is small, we may make the approximation that  $n_i \cong \bar{n}_i$  from which it follows that

$$\frac{l - l_0}{l_0} \cong l_{ij}n_jn_i$$

Inherent in this approximation is the assumption that the line segment from  $\mathbf{O}$  to the material particle is unrotated during deformation. By using the same arguments but starting with  $\mathbf{u} \cdot \mathbf{x}/\mathbf{x} \cdot \mathbf{x}$ , we obtain Equation (18).

Some authors write Equation (17) using an equals rather than an approximately equals sign (Nye, 1960). This is correct provided it is realized that the expression is exact only in the limit of an infinitesimal displacement gradient, *i.e.*, exact within the context of the assumptions incorporated into the theory of linear strain.

*Note Added in Proof*

Equations (17) and (18) may also be written in the form

$$\frac{l - l_0}{l_0} = \frac{2L_{ij}n_jn_i}{1 + \sqrt{1 + 2L_{ij}n_jn_i}} \approx l_{ij}n_jn_i$$

and

$$\frac{l - l_0}{l} = \frac{2E_{ij}\bar{n}_i\bar{n}_j}{1 + \sqrt{1 - 2E_{ij}\bar{n}_i\bar{n}_j}} \approx e_{ij}\bar{n}_i\bar{n}_j$$

where  $L_{ij}$  and  $E_{ij}$  are the finite Lagrangian and Eulerian strain tensors. These are defined as

$$L_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \frac{\partial u_k}{\partial X_i} \frac{\partial u_k}{\partial X_j} \right)$$

and

$$E_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} \right)$$

respectively.

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