Acta Cryst. (1978). A**34**, 52–54

Strain-Tensor Components Expressed in Terms of Lattice Parameters

By John L. Schlenker

Department of the Geophysical Sciences, University of Chicago, 5734 *Ellis Avenue, Chicago, Illinois* 60637, *USA*

G. V. Gibbs

Department of Geological Sciences, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, *USA*

and Monte B. Boisen Jr

Department of Mathematics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, *USA*

(*Received* 18 *November* 1976; *accepted* 7 *June* 1977)

Expressions are developed for the components of the linear Lagrangian, linear Eulerian, finite Lagrangian (Green's), and finite Eulerian (Almansi's) strain tensors in terms of a crystal's lattice parameters before and after a deformation. The development has been undertaken with the concepts and notations of linear algebra.

Introduction

When the particles of a material medium (like a crystal) are displaced relative to each other, the medium is said to undergo a deformation. This deformation can be viewed as a mapping T from three-dimensional space (three-space) on to three-space such that if $\mathbf{X}$ denotes the position of a point in space before deformation, then $T(\mathbf{X})$ denotes the position of that same point after deformation. To aid in the discussion, we will often refer to $T(\mathbf{X})$ as $\mathbf{x}$. If we impose a Cartesian coordinate system C on three-space, we have for $\mathbf{X}$ and $\mathbf{x}$ the addresses $\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$ and $\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$, respectively, where X_1, X_2, X_3, x_1, x_2 and x_3 are real numbers. In this case we denote $\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$ by $[\mathbf{X}]_C$ and $\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ by $[\mathbf{x}]_C$. The vector $\mathbf{u} = \mathbf{x} - \mathbf{X}$ determines the displacement of a particle positioned at $\mathbf{X}$ prior to deformation. Since $\mathbf{u}$ is determined either by T and $\mathbf{X}$ or by T and $\mathbf{x}$, $\mathbf{u}$ can be viewed as a function of either $\mathbf{X}$ or $\mathbf{x}$. Consequently, the components of $[\mathbf{u}]_C = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$ can be expressed either in a Lagrangian form as functions of the particle's initial coordinates, *i.e.* as $u_i = u_i(X_1,X_2,X_3)$, or in an Eulerian form as a function of the particle's final coordinates, *i.e.* as $u_i = u_i(x_1,x_2,x_3)$. It can be shown that (Bhagavantam, 1966) the state of deformation (strain) of a body can be characterized by a symmetrical second-rank tensor termed a strain tensor. Several tensors of this type have been defined. Those of interest to us are the linear Lagrangian strain tensor defined as

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

the linear Eulerian strain tensor defined as

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right);$$

the finite Lagrangian (Green's) strain tensor 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 the finite Eulerian (Almansi's) strain tensor defined as

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

The conditions under which one kind of strain tensor rather than another should be used is a subject dealt with in continuum-mechanics texts (Mase, 1970) and will therefore not be discussed here. Our goal is the systematic development of expressions that give l_{ij}, e_{ij}, L_{ij}, and E_{ij} in terms of the lattice parameters of a crystal measured before $\{a_0,b_0,c_0,\alpha_0,\beta_0,\gamma_0\}$ and after

$\{a_1,b_1,c_1,\alpha_1,\beta_1,\gamma_1\}$ it has been subjected to a deformation. The ease with which such lattice parameters may be obtained by means of routine X-ray diffraction techniques make such formulations particularly useful. Expressions of the type developed here are useful in a variety of crystallographic problems involving topotaxy and exsolution (Morimoto & Tokonami, 1969), solid-solution series (Ohashi & Burnham, 1973) and thermal expansion (Schlenker, Gibbs & Boisen, 1975). Before we can develop these expressions, we must first examine the properties of the mapping T. In the study of deformation, we are only interested in the relative distances between pairs of points before and after deformation. Consequently, translations are irrelevant and we may assume that the origin $\mathbf{O}$ of our Cartesian coordinate system remains fixed. Hence, without loss of generality, we may assume that $T(\mathbf{O}) = \mathbf{O}$. If we denote the natural basis of the crystal before deformation by $B_0 = \{\mathbf{a}_0,\mathbf{b}_0,\mathbf{c}_0\}$ and if we denote $T(\mathbf{a}_0)$, $T(\mathbf{b}_0)$ and $T(\mathbf{c}_0)$ by $\mathbf{a}_1$, $\mathbf{b}_1$ and $\mathbf{c}_1$ respectively, then $B_1 = \{\mathbf{a}_1,\mathbf{b}_1,\mathbf{c}_1\}$ is the natural basis of the crystal after deformation. In fact, if $\mathbf{v} = r_1\mathbf{a}_0 + r_2\mathbf{b}_0 + r_3\mathbf{c}_0 \left\{ i.e.\ [\mathbf{v}]_{B_0} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} \right\}$ is any vector before deformation, then the deformed vector $T(\mathbf{v})$ equals the *same* linear combination of $\{\mathbf{a}_1,\mathbf{b}_1,\mathbf{c}_1\}$, *i.e.* $T(\mathbf{v}) = r_1\mathbf{a}_1 + r_2\mathbf{b}_1 + r_3\mathbf{c}_1$ (Born & Huang, 1968). Therefore, $[\mathbf{v}]_{B_0} = [T(\mathbf{v})]_{B_1}$. Since B_0 and B_1 have a common origin [since we may assume $T(\mathbf{O}) = \mathbf{O}$], the above observations imply that T is a linear transformation [*i.e.* $T(\mathbf{X} + \mathbf{Y}) = T(\mathbf{X}) + T(\mathbf{Y})$ for all vectors $\mathbf{X}$, $\mathbf{Y}$ in three-space and $T(r\mathbf{X}) = rT(\mathbf{X})$ for all real numbers r and all $\mathbf{X}$ in three-space]. Consequently, as is always the case for a linear transformation, T can be represented by a matrix. It is therefore apparent that the equations giving the displacement in the Cartesian system must be of the form $u_i = I_{ij}X_j = J_{ij}x_j$ where the I_{ij} and J_{ij} are constants. Since $I_{ij} = \partial u_i/\partial X_j$ and $J_{ij} = \partial u_i/\partial x_j$, it is also evident that $[l] = \frac{1}{2}(I + I^T)$, $[e] = \frac{1}{2}(J + J^T)$, $[L] = \frac{1}{2}(I + I^T + I^TI)$, and $[E] = \frac{1}{2}(J + J^T + J^TJ)$.

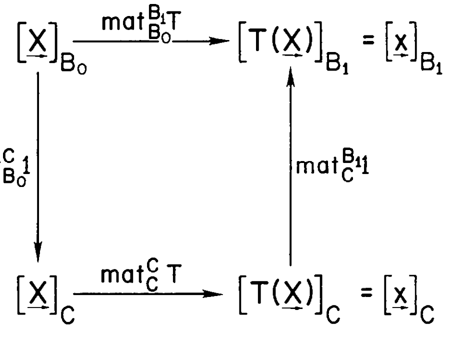

Fig. 1. Matrix representation of T with respect to the bases B_0 and B_1.

The linear Lagrangian and Eulerian strain tensors

The conventional [Institute of Radio Engineers (IRE) convention, Mason, 1950] orientation of a crystallographic coordinate system relative to a Cartesian coordinate system is to place the **c** cell edge of the crystal along the z axis of the Cartesian system and the **b** cell edge in the yz plane of the Cartesian system so that $\mathbf{a}^*$ is oriented along the x axis. Hence, the change of basis matrix from the basis B_i, $i = 0,1$, to the Cartesian basis $C = \{\mathbf{i},\mathbf{j},\mathbf{k}\}$, symbolized by $\mathrm{mat}^C_{B_i}\,1$ (*i.e.* $\mathrm{mat}^C_{B_i}\,1$ is the matrix representation of the identity map with respect to the basis B_i and C), is

$$\mathrm{mat}^C_{B_i}1 = \begin{bmatrix} a_i \sin\beta_i \sin\gamma_i^* & 0 & 0 \\ -a_i \sin\beta_i \cos\gamma_i^* & b_i \sin\alpha_i & 0 \\ a_i \cos\beta_i & b_i \cos\alpha_i & c_i \end{bmatrix}. \qquad (1)$$

Note that $\mathrm{mat}^C_{B_i}1$ has the property that $(\mathrm{mat}^C_{B_i}\,1)[\mathbf{X}]_{B_i} = [\mathbf{X}]_C$. Also, $(\mathrm{mat}^C_{B_i}\,1)^{-1} = \mathrm{mat}^{B_i}_C\,1$. As the diagram in Fig. 1 indicates, the matrix representation of T with respect to the bases B_0 and B_1, symbolized $\mathrm{mat}^{B_1}_{B_0}$, can be decomposed as

$$\mathrm{mat}^{B_1}_{B_0}T = (\mathrm{mat}^{B_1}_C\,1)(\mathrm{mat}^C_C\,T)(\mathrm{mat}^C_{B_0}\,1). \qquad (2)$$

The matrices $\mathrm{mat}^C_{B_0}\,1$ and $\mathrm{mat}^{B_1}_C\,1$ are given by (1). Since $(\mathrm{mat}^{B_1}_{B_0}T)[\mathbf{X}]_{B_0} = [T(\mathbf{X})]_{B_1}$ and since, as noted above $[\mathbf{X}]_{B_0} = [T(\mathbf{X})]_{B_1}$, $\mathrm{mat}^{B_1}_{B_0}\,T$ must be the identity matrix I_3. We now write $\mathrm{mat}^C_C\,T$ in terms of I and solve. Since $[u]_C = I[\mathbf{X}]_C$ and $[u]_C = [T(\mathbf{X})]_C - [\mathbf{X}]_C$, we have $[T(\mathbf{X})]_C = [\mathbf{X}]_C + I[\mathbf{X}]_C = I_3[\mathbf{X}]_C + I[\mathbf{X}]_C = (I_3 + I)[\mathbf{X}]_C$. Therefore, $\mathrm{mat}^C_C T = (I_3 + I)$. Equation (2) now becomes

$$I_3 = (\mathrm{mat}^C_{B_1}\,1)^{-1}(I_3 + I)(\mathrm{mat}^C_{B_0}\,1).$$

Therefore, $I = (\mathrm{mat}^C_{B_1}\,1)(\mathrm{mat}^C_{B_0}\,1)^{-1} - I_3$. On letting S_i^T denote $(\mathrm{mat}^C_{B_i}\,1)$, it is apparent that $I = S_1^TS_0^{-T} - I_3$. The linear Lagrangian strain tensor then takes the form

$$[l] = \tfrac{1}{2}[I + I^T] = \tfrac{1}{2}[(S_0^{-1}S_1)^T + S_0^{-1}S_1] - I_3.$$

On carrying out the indicated operations the following expressions are obtained for the elements of $[l]$:

$$l_{11} = \frac{a_1 \sin\beta_1 \sin\gamma_1^*}{a_0 \sin\beta_0 \sin\gamma_0^*} - 1,$$

$$l_{22} = \frac{b_1 \sin\alpha_1}{b_0 \sin\alpha_0} - 1,$$

$$l_{33} = \frac{c_1}{c_0} - 1,$$

$$l_{12} = l_{21} = \frac{1}{2}\left[\frac{b_1 \sin\alpha_1 \cos\gamma_0^*}{b_0 \sin\alpha_0 \sin\gamma_0^*} - \frac{a_1 \sin\beta_1 \cos\gamma_1^*}{a_0 \sin\beta_0 \sin\gamma_0^*}\right],$$

$$l_{13} = l_{31} = \frac{1}{2}\left[\frac{a_1 \cos\beta_1}{a_0 \sin\beta_0 \sin\gamma_0^*} + \frac{\cos\gamma_0^*}{\sin\gamma_0^*} \times \left(\frac{b_1 \cos\alpha_1}{b_0 \sin\alpha_0} - \frac{c_1 \cos\alpha_0}{c_0 \sin\alpha_0}\right) - \frac{c_1 \cos\beta_0}{c_0 \sin\beta_0 \sin\gamma_0^*}\right],$$

$$l_{23} = l_{32} = \frac{1}{2}\left[\frac{b_1 \cos\alpha_1}{b_0 \sin\alpha_0} - \frac{c_1 \cos\alpha_0}{c_0 \sin\alpha_0}\right].$$

Equation (3) was previously developed by Ohashi & Burnham (1973). It is not clear from their derivation that the strain tensor (3) is identical with the linear Lagrangian strain of classical continuum theory. The above expressions for the monoclinic case have been developed by Morimoto & Tokonami (1969) in their study of the oriented exsolution of augite in pigeonite, however, no derivation was given.

The elements of the linear Eulerian strain tensor, $[e]$, may be obtained as follows. From a discussion analogous to that presented above it can be shown that $[\mathbf{X}]_C = (I_3 - J)[T(\mathbf{X})]_C$ from which it follows that $\text{mat}_C^C T = (I_3 - J)^{-1}$. On employing (2) we obtain $I_3 = S_1^{-T}(I_3 - J)^{-1} S_0^T$ which, on solving for J, yields $J = I_3 - S_0^T S_1^{-T}$. From the definition of the Eulerian strain tensor it is apparent that

$$[e] = \tfrac{1}{2}[J + J^T] = I_3 - \tfrac{1}{2}[(S_1^{-1}S_0)^T + S_1^{-1}S_0].$$

Therefore the elements of $[e]$ are:

$$e_{11} = 1 - \frac{a_0 \sin\beta_0 \sin\gamma_0^*}{a_1 \sin\beta_1 \sin\gamma_1^*},$$

$$e_{22} = 1 - \frac{b_0 \sin\alpha_0}{b_1 \sin\alpha_1},$$

$$e_{33} = 1 - \frac{c_0}{c_1},$$

$$e_{12} = e_{21} = \frac{1}{2}\left[\frac{a_0 \sin\beta_0 \cos\gamma_0^*}{a_1 \sin\beta_1 \sin\gamma_1^*} - \frac{b_0 \sin\alpha_0 \cos\gamma_1^*}{b_1 \sin\alpha_1 \sin\gamma_1^*}\right],$$

$$e_{13} = e_{31} = \frac{1}{2}\left[\frac{c_0 \cos\beta_1}{c_1 \sin\beta_1 \sin\gamma_1^*} + \frac{\cos\gamma_1^*}{\sin\gamma_1^*} \times \left(\frac{c_0 \cos\alpha_1}{c_1 \sin\alpha_1} - \frac{b_0 \cos\alpha_0}{b_1 \sin\alpha_1}\right) - \frac{a_0 \cos\beta_0}{a_1 \sin\beta_1 \sin\gamma_1^*}\right],$$

$$e_{23} = e_{32} = \frac{1}{2}\left[\frac{c_0 \cos\alpha_1}{c_1 \sin\alpha_1} - \frac{b_0 \cos\alpha_0}{b_1 \sin\alpha_1}\right].$$

The finite Lagrangian and Eulerian strain tensors

Since the expressions for the elements of the finite Lagrangian and Eulerian strain tensors are complicated when given in explicit form, only implicit expressions, given in terms of S_0 and S_1, are presented here. For the finite Lagrangian strain tensor we have

$$\begin{aligned}[L] &= \tfrac{1}{2}[I + I^T + I^T I] \\ &= \tfrac{1}{2}[(S_1^T S_0^{-T} - I_3) + (S_1^T S_0^{-T} - I_3)^T \\ &\quad + (S_1^T S_0^{-T} - I_3)^T (S_1^T S_0^{-T} - I_3)]\end{aligned}$$

which on simplification yields

$$[L] = \tfrac{1}{2}[S_0^{-1} S_1 S_1^T S_0^{-T} - I_3]$$

while for the finite Eulerian strain tensor we have

$$\begin{aligned}[E] &= \tfrac{1}{2}[J + J^T + J^T J] \\ &= \tfrac{1}{2}[(I_3 - S_0^T S_1^{-T}) + (I_3 - S_0^T S_1^{-T})^T \\ &\quad + (I_3 - S_0^T S_1^{-T})^T (I_3 - S_0^T S_1^{-T})]\end{aligned}$$

which yields on simplification

$$[E] = \tfrac{1}{2}[3I_3 + S_1^{-1} S_0 S_0^T S_1^{-T} - 2(S_1^{-1} S_0)^T - 2(S_1^{-1} S_0)].$$

Conclusion

The calculation of strain-tensor components for deformed crystalline materials is a necessary step in the solution of a variety of physical and crystal-chemical problems. In this paper, a mathematical procedure has been used to develop expressions for calculating components of the linear Lagrangian and Eulerian strain tensors from measurements of lattice parameters before and after deformation. Implicit expressions of the same type are presented for the finite Lagrangian and finite Eulerian strain tensors.

We thank the National Science Foundation for supporting this study with Grant DES 571-00486-A03 and Ramonda Haycocks for typing the manuscript.

References

BHAGAVANTAM, S. (1966). *Crystal Symmetry and Physical Properties*. London: Academic Press.

BORN, M. & HUANG, K. (1968). *Dynamical Theory of Crystal Lattices*. Oxford: Clarendon Press.

MASE, G. E. (1970). *Theory and Problems of Continuum Mechanics*. New York: McGraw-Hill.

MASON, W. P. (1950). *Piezoelectric Crystals and their Application to Ultrasonics*. New York: Van Nostrand.

MORIMOTO, N. & TOKONAMI, M. (1969). *Am. Mineral.* **54**, 1101–1117.

OHASHI, Y. & BURNHAM, C. W. (1973). *Am. Mineral.* **58**, 843–849.

SCHLENKER, J. L., GIBBS, G. V. & BOISEN, M. B. JR (1975). *Am. Mineral.* **60**, 828–833.