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Review of relationships between different strain tensors. By N. ZOTOV, *Institute of Applied Mineralogy, Bulgarian Academy of Sciences, Rakovski Street 92, Sofia 1000, Bulgaria*

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Abstract

The relationships between different Lagrangian strain tensors are summarized on the basis of an illustrative tensor diagram emphasizing the equivalence of the definitions of lattice deformation in the crystallographic and the Cartesian reference frames.

Introduction

Several kinds of second-rank tensors characterizing the state of lattice deformation of a solid have been defined. They are usually based on Cartesian rather than crystallographic atomic coordinates. However, in a variety of physical and crystallochemical problems it is necessary to preserve crystallographic presentation of the lattice.

The calculation of the components of the strain tensors is usually restricted to the case of small deformations and is carried out by means of explicit expressions in terms of the unit-cell parameters of the deformed and the undeformed lattices (Morimoto & Tokonami, 1969; Ohashi & Burnham, 1973; Schlenker, Gibbs & Boisen, 1978; Hazen & Finger, 1982; Catti, 1985; Chanh *et al.*, 1988). From a computational point of view, the use of implicit expressions in terms of orthogonalization matrices and metric tensors is more straightforward, and allows one easily to calculate both the linear and the finite strain tensors and to carry out complete error analysis.

This indicates once more the necessity to elucidate and summarize the relationships between the different strain tensors in the crystallographic and the Cartesian reference frames.

Theory

Let us consider a crystal lattice L with covariant basis vectors $\mathbf{a} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ and unit-cell parameters $(a, b, c, \alpha, \beta, \gamma)$.

Let us consider further homogeneous deformation under which the initial lattice L transforms to another lattice L' with covariant basis vectors $\mathbf{a}' = (\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)$ and unit-cell parameters $(a', b', c', \alpha', \beta', \gamma')$. The matrix of the affine transformation can be expressed by the strain tensor \mathbf{S} (Ohashi & Burnham, 1973):

$$\mathbf{a}' = \mathbf{a}(\mathbf{I} + \mathbf{S}), \quad (1)$$

where \mathbf{I} is the unit matrix. Evidently the tensor \mathbf{S} is a mixed contravariant tensor [Ohashi & Burnham (1973) used the transpose matrix of \mathbf{S}].

Let \mathbf{O} and \mathbf{O}' be the orthogonalization matrices which transform L and L' into a fixed Cartesian reference frame with basis vector set \mathbf{e} :

$$\mathbf{e} = \mathbf{a}\mathbf{O}; \quad \mathbf{e} = \mathbf{a}'\mathbf{O}'. \quad (2)$$

Comparison of (1) and (2) produces the following matrix

representation for \mathbf{S} in the crystallographic reference frame:

$$\mathbf{S} = \mathbf{O}\mathbf{O}'^{-1} - \mathbf{I}. \quad (3)$$

In the case of homogeneous deformation the contravariant lattice coordinates remain unchanged (Born & Huang, 1954). The Cartesian coordinates of a general point before (\mathbf{X}) and after (\mathbf{X}') the deformation, however, are connected by the general strain tensor ξ (Murnaghan, 1951; Nye, 1957):

$$\mathbf{X}' = (\mathbf{I} + \xi)\mathbf{X}$$

which may contain both deformation and rigid rotation of the lattice L . Taking into account the invariance of the contravariant coordinates with respect to lattice deformation, it can be shown that (Catti, 1985)

$$\xi = \mathbf{O}'^{-1}\mathbf{O} - \mathbf{I}. \quad (4)$$

The change in the distance between two arbitrary lattice points caused by homogeneous deformation can be expressed in the crystallographic reference frame by the finite Lagrangian strain tensor \mathbf{D} (Sedov, 1983; Catti, 1985; Chanh *et al.*, 1988; Catti, 1989):

$$\mathbf{D} = \frac{1}{2}[\mathbf{g}' - \mathbf{g}],$$

where \mathbf{g}' and \mathbf{g} are the corresponding covariant metric tensors.

With the transformation equation $\mathbf{g}' = (\mathbf{I} + \mathbf{S})^T \mathbf{g} (\mathbf{I} + \mathbf{S})$, the finite Lagrangian strain tensor \mathbf{D} can be expressed by \mathbf{S} and \mathbf{g} :

$$\mathbf{D} = \frac{1}{2}[\mathbf{g}\mathbf{S} + (\mathbf{g}\mathbf{S})^T + \mathbf{S}^T \mathbf{g}\mathbf{S}]. \quad (5)$$

If the deformation is small we obtain the linear Lagrangian strain tensor in the crystallographic reference frame:

$$\mathbf{d} = \frac{1}{2}[\mathbf{g}\mathbf{S} + (\mathbf{g}\mathbf{S})^T]. \quad (6)$$

It can be seen that the strain tensors \mathbf{D} and \mathbf{d} are related to the covariant tensor $\mathbf{g}\mathbf{S}$ by a symmetrization operation. Therefore, we can interpret the $\mathbf{g}\mathbf{S}$ tensor as the affine analogue of the general Cartesian tensor ξ :

$$\xi = \mathbf{O}^T \mathbf{g}\mathbf{S}\mathbf{O}, \quad (7)$$

since substituting (3) in (7) and taking into account $\mathbf{O}^T \mathbf{g}\mathbf{O} = \mathbf{I}$, we validate independently formula (4). Furthermore, we can obtain from above the well known definitions for the symmetric Cartesian tensors of linear and finite deformations.

Let us denote for this purpose the strain tensors \mathbf{D} and \mathbf{d} in the Cartesian reference frame by η and ϵ :

$$\eta = \mathbf{O}^T \mathbf{D}\mathbf{O}$$

$$\epsilon = \mathbf{O}^T \mathbf{d}\mathbf{O}.$$

If \mathbf{D} and \mathbf{d} are expressed by (5) and (6) it follows that

$$\epsilon = \frac{1}{2}(\mathbf{O}^T \mathbf{g}\mathbf{S}\mathbf{O} + \mathbf{O}^T \mathbf{S}^T \mathbf{g}\mathbf{O}) \quad (8)$$

$$\eta = \frac{1}{2}(\mathbf{O}^T \mathbf{g}\mathbf{S}\mathbf{O} + \mathbf{O}^T \mathbf{S}^T \mathbf{g}\mathbf{O} + \mathbf{O}^T \mathbf{S}^T \mathbf{g}\mathbf{S}\mathbf{O}). \quad (9)$$

From (7) it is seen that (8) and (9) can be written in the conventional form (Murnaghan, 1951; Nye, 1957):

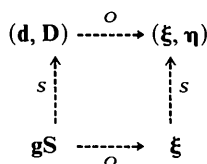
$$\begin{aligned}\boldsymbol{\varepsilon} &= \frac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\xi}^T) \\ \boldsymbol{\eta} &= \frac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\xi}^T + \boldsymbol{\xi}^T \boldsymbol{\xi}).\end{aligned}$$

Finally, expressing $\boldsymbol{\xi}$ in these equations by (4), it can be shown that (Schlenker, Gibbs & Boisen, 1978; Catti, 1985)

$$\begin{aligned}\boldsymbol{\varepsilon} &= \frac{1}{2}(\mathbf{O}'^{-1} \mathbf{O} + \mathbf{O}^T \mathbf{O}'^{-1T}) - \mathbf{I} \\ \boldsymbol{\eta} &= \frac{1}{2}(\mathbf{O}^T \mathbf{O}'^{-1T} \mathbf{O}'^{-1} \mathbf{O} - \mathbf{I}).\end{aligned}$$

Concluding remarks

We can express all these matrix relations in the following tensor diagram which illustrates the one-to-one correspondence between the tensors \mathbf{gS} , \mathbf{D} and \mathbf{d} in the crystallographic reference frame and the tensors $\boldsymbol{\xi}$, $\boldsymbol{\eta}$ and $\boldsymbol{\varepsilon}$ in the Cartesian reference frame:



where O and S denote orthogonalization and symmetrization operations.

Therefore, mathematically we can visualize the homogeneous lattice deformation as a transformation of the basis vectors in the crystallographic reference frame or as a transformation of the atomic coordinates in the Cartesian reference frame.

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Calculation of the point-by-point error in protein crystallographic electron-density functions. By EATON EDWARD LATTMAN, *Department of Biophysics, Johns Hopkins University, School of Medicine, Baltimore, MD 21205-2185, USA*

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Abstract

In protein crystallographic studies, the mean-square error at each point in the electron-density function is given, in space group $P1$, by

$$\begin{aligned}\sigma^2(\mathbf{x}) &= (1/V^2) \sum_{\text{all } \mathbf{h}} F_o^2 [1 - m(\mathbf{h})^2] \\ &+ (1/V^2) \sum_{\text{all } \mathbf{h}} F_o^2 \{m_2(\mathbf{h}) \exp [i\alpha_2(\mathbf{h})] \\ &- m(\mathbf{h})^2 \exp [2i\alpha_B(\mathbf{h})]\} \exp (-4\pi i \mathbf{h} \cdot \mathbf{x}).\end{aligned}$$

Here, F_o is the observed structure-factor amplitude; $m(\mathbf{h}) \exp [i\alpha_B(\mathbf{h})] = \int P[\alpha(\mathbf{h})] \exp (i\alpha) d\alpha$ is the weighted phase factor in the 'best' Fourier coefficient of Blow & Crick; $m_2(\mathbf{h}) \exp (i\alpha_2) = \int P[\alpha(\mathbf{h})] \exp (2i\alpha) d\alpha$ is similar to a traditional second moment. $P[\alpha(\mathbf{h})] d\alpha$ is the probability that the phase angle for a given reflection has value between α and $\alpha + d\alpha$.

Introduction

It is common practice in protein crystallography to make estimates of the error in each structure factor $F(\mathbf{h})$. The most commonly used error models lead to an estimate of $P[\alpha(\mathbf{h})]$, the probability density function for the phase $\alpha(\mathbf{h})$ (Blow & Crick, 1959; Hendrickson & Lattman, 1970). Errors in the structure-factor amplitudes are generally ignored. $P(\alpha)$ is of great importance in developing correct weights for the structure factors in Fourier syntheses. For example, the commonly used 'best' Fourier coefficient of Blow & Crick (1959) uses the centroid-weighted phase factor given in (7).

Little attention has been paid to the corresponding errors in the electron-density function $\rho(\mathbf{x})$. Yet there are many operations, such as solvent flattening and molecular averaging, in which appropriate weighting could be very important. An objective measure of the local quality of the electron-density map might help to distinguish structural