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A general procedure to derive magic strain tensors

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Abstract. A general procedure is described which enables the calculation of so-called 'magic' strain tensors, *i.e.* symmetric tensors which transform a specified space lattice into itself. Numerical examples for cubic lattices are given.

Introduction. The lattice constants of a space lattice may be changed by the application of a homogeneous strain, conveniently described by a symmetric strain tensor. This tensor could be such that the strained lattice is indistinguishable from the unstrained lattice, apart from a rotation. Following Boyer (1989), we will call such a tensor 'magic', and present a method to find such tensors by straightforward calculation.

Method of calculation. Consider the space lattices $\mathbf{a}_{hkl}=h\mathbf{a}_1+k\mathbf{a}_2+l\mathbf{a}_3$ and $\mathbf{b}_{hkl}=h\mathbf{b}_1+k\mathbf{b}_2+k\mathbf{b}_3$, with h,k,l integers, and the unit-cell vectors $\mathbf{a}_1,\ldots,\mathbf{b}_3$ defined by their components $a_{1x},\ldots,b_{3z}$ in some Cartesian frame of reference XYZ. A 3×3 tensor $\mathbf{T}$ transforms the a lattice into the b lattice if $TA=B$, or $\mathbf{T}=BA^{-1}$, where $A_{ij}=a_{ji}$ and $B_{ij}=b_{ji}$ ($i,j=1,2,3$; x,y,z replaced by 1,2,3, respectively).

In general, $\mathbf{T}$ will be not symmetric, but, according to the polar-decomposition theorem (*e.g.* Leigh,1968), $\mathbf{T}$ can be written as the product of an orthogonal tensor $\mathbf{Q}$ and a positive-definite tensor $\mathbf{U}$, *i.e.* $\mathbf{T}=\mathbf{QU}$. We can then write

$$\mathbf{U}A=\mathbf{R}B \tag{1}$$

with $\mathbf{R}=\mathbf{Q}^{-1}$, expressing that a symmetric tensor $\mathbf{U}$ can be found that transforms the a lattice into the b lattice, provided b is rotated into the proper orientation with respect to a. $\mathbf{U}$ and $\mathbf{R}$ can be found from

$$\mathbf{U}=(\tilde{\mathbf{T}}\mathbf{T})^{1/2} \tag{2}$$

$$\mathbf{R}=\mathbf{U}\mathbf{T}^{-1}. \tag{3}$$

If the matrices A and B are constructed from different (primitive) unit cells of the *same* lattice, $\mathbf{U}$ will be a magic tensor for that lattice.

The treatment can be extended to more than three dimensions, as can the notion of magic tensors.

Practical execution. In order to obtain $\mathbf{P}^{1/2}$ from $\mathbf{P}=\tilde{\mathbf{T}}\mathbf{T}$, $\mathbf{P}$ must be diagonalized,

$$\mathbf{P}'=S^{-1}\mathbf{P}S, \tag{4}$$

involving the calculation of the diagonal elements p_i of $\mathbf{P}'$, which are the (positive) roots of a cubic equation (see, *e.g.*, *International Tables for X-ray Crystallography*, 1959). $\mathbf{P}^{1/2}$ follows from

$$\mathbf{P}^{1/2}=S(\mathbf{P}')^{1/2}S^{-1}, \tag{5}$$

where $(\mathbf{P}')^{1/2}$ is obtained from $\mathbf{P}'$ by replacing p_i by $(p_i)^{1/2}$.

The significance of $\mathbf{U}$ becomes apparent by diagonalization: the strain may be viewed as equivalent to different expansions in three mutually perpendicular directions. These principal directions are given by the eigenvectors (which are the column vectors of S), the expansions by the eigenvalues $u_i(=p_i{}^{1/2})$ of $\mathbf{U}$. Obviously, $u_1u_2u_3=1$. The orthogonal tensor $\mathbf{R}$ describes a

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rotation through an angle γ about an axis with direction cosines l_i, which can be calculated from

$$\cos\gamma = \tfrac{1}{2}|\mathrm{Tr}(\mathbf{R}) - 1| \quad (6)$$

$$l_i = (-\mathbf{R}_{jk} + \mathbf{R}_{kj})/2\sin\gamma \quad (7)$$

with i,j,k being a cyclic permutation of 1,2,3. If $\gamma = 180°$ the l_i must be calculated from

$$l_i = \pm[\tfrac{1}{2}(1 + \mathbf{R}_{ii})]^{1/2} \quad (7')$$

where the sign should be chosen to comply with $\mathbf{R}_{ij} = 2l_il_j$, $i \neq j$.

Results. Three examples are given to illustrate the method. Only cubic lattices (simple, as well as face-centered) are considered, in order to facilitate interpretation. The conventional lattice constant is taken as the unit of length. Unfortunately, the connection with integral numbers (*e.g.* $1.414214 = 2^{1/2}$) is obscured by machine calculations. Whenever figures in decimal notation could be identified as resulting from simple algebraic operations on integral numbers, they have been written so. Symbols r, s and t are short for $2^{1/2}$, $6^{1/2}$ and $41^{1/2}$, respectively.

Example 1

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad B = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

i.e. a simple cubic lattice. Since $\mathbf{T} = BA^{-1}$, $\mathbf{T} = B$, and the eigenvalues of $\mathbf{P}$ are the roots of the cubic equation

$$p^3 - 5p^2 + 6p - 1 = 0,$$

3.246980, 1.554958 and 0.198062, respectively.

From this, S, $\mathbf{U}$ and $\mathbf{R}$ may be calculated:

$$S = \begin{bmatrix} 0.328 & 0.737 & -0.591 \\ 0.737 & -0.591 & -0.328 \\ 0.591 & 0.328 & 0.737 \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} 0.871119 & 0.483435 & -0.086268 \\ 0.483435 & 1.268286 & 0.397167 \\ -0.086268 & 0.397167 & 1.354554 \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 0.871 & -0.388 & 0.301 \\ 0.483 & 0.785 & -0.388 \\ -0.086 & 0.483 & 0.871 \end{bmatrix}.$$

Since none of the eigenvalues of $\mathbf{U}$ (1.802, 1.247, 0.445) equals 1, and neither the rotation axis nor one of the eigenvectors of $\mathbf{U}$ is along a low-index direction, the significance of $\mathbf{U}$ is not immediately obvious. However, it is easily verified that $\mathbf{U}$ is a magic tensor of the simple cubic lattice.

Example 2

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

$$B = \mathbf{R}'\begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & -1 \end{bmatrix} = r^{-1}\begin{bmatrix} 1 & 0 & 1+r^{-1} \\ 1 & 0 & 1-r^{-1} \\ 0 & 2 & 1 \end{bmatrix}$$

i.e. a simple cubic lattice. $\mathbf{R}'$ is a 90° c.c.w. rotation about $[\bar{1}10]$. $\mathbf{U}$ is calculated to be

$$\mathbf{U} = \frac{1}{6}\begin{bmatrix} 2s+3 & -s & -2s+3 \\ -s & 2s & s \\ -2s+3 & s & 2s+3 \end{bmatrix}$$

with eigenvalues $\frac{1}{2}(s+r)$, $\frac{1}{2}(s-r)$, 1. The third eigenvector (corresponding to the unit eigenvalue) is in the [101] direction; the angle between the second eigenvector and the $[0\bar{1}0]$ direction is α, $\tan 2\alpha = r$. The effect of $\mathbf{U}$ is a rearrangement of lattice points in (101) planes, resulting in a c.w. rotation of the rectangular grid through an angle β, $\tan\beta = r$. This is apparent from $\mathbf{RR}'$ rather than from $\mathbf{R}$:

$$\mathbf{R} = \frac{1}{24}r\begin{bmatrix} 2s+3r+6 & 2s-3r+6 & -4s+6 \\ 2s-3rs & 2s+3rs & 2s \\ -2s+3r+6 & -2s-3r+6 & 4s+6 \end{bmatrix}.$$

Example 3

$$A = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \end{bmatrix} \quad B = \begin{bmatrix} 1/2 & 1 & 0 \\ 0 & 1/2 & 0 \\ 1/2 & 1/2 & 1 \end{bmatrix}$$

i.e. a f.c.c. lattice. $\mathbf{U}$ can be characterized by its eigenvalues,

$$u_{1,2} = \tfrac{1}{2}(7 \pm t)^{1/2}, \quad u_3 = r,$$

and its principal directions, which are in (for u_1 and u_2) and perpendicular (for u_3) to (011) planes. The u_2 direction is inclined to the $[0\bar{1}1]$ direction of close-packed rows by an angle α, $\tan\alpha = 1/8r(t - 3)$. As is apparent from the value of u_3, and the corresponding principal direction, (011) planes are transformed into (100) planes. The angle between the 'old' and 'new' directions of close-packed rows is β (or $90° - \beta$), $\cos\beta = (1 + u_1u_2)/(u_1 + u_2)$.

Concluding remarks. The examples chosen illustrate that the expansions u_i must deviate significantly from 1, in order to produce magic 'strains'. Accordingly, if the lattice points are oc-

cupied by atoms of one kind, large atomic shifts are involved, presumably incorporating high energy barriers. In favorable cases, however, the barrier height may be of the order of kT at the melting point, as has been demonstrated recently (Boyer, 1989). If so, the tensors could be of practical use for the description of atomic rearrangements in small clusters near melting.

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