ANALYSIS OF ELASTIC STRAINS

10 nm

We consider the elastic properties of a crystal viewed as a homogeneous continuous medium rather than as a periodic array of atoms. The continuum approximation is usually valid for elastic waves of wavelengths λ longer than 10^{-6} cm, which means for frequencies below 10^{11} or 10^{12} Hz. Some of the material below looks complicated because of the unavoidable multiplicity of subscripts on the symbols. The basic physical ideas are simple: we use Hooke's law and Newton's second law. **Hooke's law** states that in an elastic solid the strain is directly proportional to the stress. The law applies to small strains only. We say that we are in the **nonlinear region** when the strains are so large that Hooke's law is no longer satisfied.

In linear region

We specify the strain in terms of the components e_{xx}, e_{yy}, e_{zz}, e_{xy}, e_{yz}, e_{zx} which are defined below. We treat infinitesimal strains only. We shall not distinguish in our notation between isothermal (constant temperature) and adiabatic (constant entropy) deformations. The small differences between the isothermal and adiabatic elastic constants are not often of importance at room temperature and below.

We imagine that three orthogonal vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ of unit length are embedded securely in the unstrained solid, as shown in Fig. 14. After a small uniform deformation of the solid has taken place, the axes are distorted in orientation and in length. In a uniform deformation each primitive cell of the crystal is deformed in the same way. The new axes $\mathbf{x}'$, $\mathbf{y}'$, $\mathbf{z}'$ may be written in terms of the old axes:

Define Deformation:

$$\begin{aligned}
\mathbf{x}' &= (1+\epsilon_{xx})\hat{\mathbf{x}} + \epsilon_{xy}\hat{\mathbf{y}} + \epsilon_{xz}\hat{\mathbf{z}} \ ; \\
\mathbf{y}' &= \epsilon_{yx}\hat{\mathbf{x}} + (1+\epsilon_{yy})\hat{\mathbf{y}} + \epsilon_{yz}\hat{\mathbf{z}} \ ; \\
\mathbf{z}' &= \epsilon_{zx}\hat{\mathbf{x}} + \epsilon_{zy}\hat{\mathbf{y}} + (1+\epsilon_{zz})\hat{\mathbf{z}} \ .
\end{aligned} \tag{26}$$

The coefficients $\epsilon_{\alpha\beta}$ define the deformation; they are dimensionless and have values $\ll 1$ if the strain is small. The original axes were of unit length, but the new axes will not necessarily be of unit length. For example,

$$\mathbf{x}' \cdot \mathbf{x}' = 1 + 2\epsilon_{xx} + \epsilon_{xx}^2 + \epsilon_{xy}^2 + \epsilon_{xz}^2 \ ,$$

whence $x' \cong 1 + \epsilon_{xx} + \cdots$. The fractional changes of length of the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ axes are ϵ_{xx}, ϵ_{yy}, ϵ_{zz}, respectively, to the first order.

What is the effect of the deformation (26) on an atom originally at $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$? The origin is taken at some other atom. If the deformation is uniform, then after deformation the point will be at the position $\mathbf{r}' = x\mathbf{x}' + y\mathbf{y}' + z\mathbf{z}'$. This is obviously correct if we choose the $\hat{\mathbf{x}}$ axis such that $\mathbf{r} = x\hat{\mathbf{x}}$; then $\mathbf{r}' = x\mathbf{x}'$ by definition of $\mathbf{x}'$. The displacement $\mathbf{R}$ of the deformation is defined by

$$\mathbf{R} \equiv \mathbf{r}' - \mathbf{r} = x(\mathbf{x}' - \hat{\mathbf{x}}) + y(\mathbf{y}' - \hat{\mathbf{y}}) + z(\mathbf{z}' - \hat{\mathbf{z}}) \ , \tag{27}$$

or, from (26),

$$\mathbf{R}(\mathbf{r}) \equiv (x\epsilon_{xx} + y\epsilon_{yx} + z\epsilon_{zx})\hat{\mathbf{x}} + (x\epsilon_{xy} + y\epsilon_{yy} + z\epsilon_{zy})\hat{\mathbf{y}} + (x\epsilon_{xx} + y\epsilon_{yz} + z\epsilon_{zz})\hat{\mathbf{z}} \ . \tag{28}$$

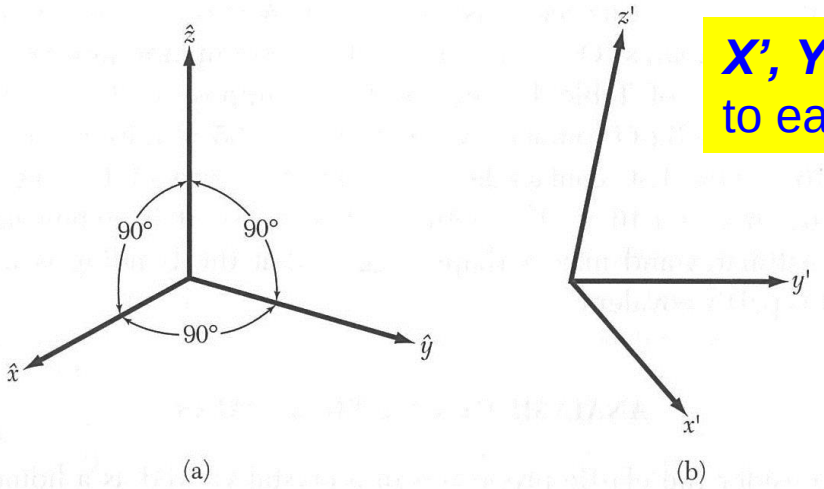
ϵ_{xz}

This may be written in a more general form by introducing u, v, w such that the displacement is given by

$$\mathbf{R}(\mathbf{r}) = u(\mathbf{r})\hat{\mathbf{x}} + v(\mathbf{r})\hat{\mathbf{y}} + w(\mathbf{r})\hat{\mathbf{z}} \ . \tag{29}$$

If the deformation is nonuniform we must relate u, v, w to the local strains. We take the origin of $\mathbf{r}$ close to the region of interest; then comparison of (28) and (29) gives, by Taylor series expansion of $\mathbf{R}$ using $\mathbf{R}(0) = 0$,

$$x\epsilon_{xx} \cong x\frac{\partial u}{\partial x} \ ; \qquad y\epsilon_{yx} = y\frac{\partial u}{\partial y} \ ; \qquad \text{etc.} \tag{30}$$



X', Y', Z' are not orthogonal to each other !

Figure 14 Coordinate axes for the description of the state of strain; the orthogonal unit axes in the unstrained state (a) are deformed in the strained state (b).

It is usual to work with coefficients $e_{\alpha\beta}$ rather than $\epsilon_{\alpha\beta}$. We define the strain components e_{xx}, e_{yy}, e_{zz} by the relations

Define 6 strain components

$$e_{xx} \equiv \epsilon_{xx} = \frac{\partial u}{\partial x} \; ; \qquad e_{yy} \equiv \epsilon_{yy} = \frac{\partial v}{\partial y} \; ; \qquad e_{zz} \equiv \epsilon_{zz} = \frac{\partial w}{\partial z} \; , \tag{31}$$

using (30). The other strain components e_{xy}, e_{yz}, e_{zx} are defined in terms of the changes in angle between the axes: using (26) we may define

$$e_{xy} \equiv \mathbf{x}' \cdot \mathbf{y}' \cong \epsilon_{yx} + \epsilon_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \; ;$$

$$e_{yz} \equiv \mathbf{y}' \cdot \mathbf{z}' \cong \epsilon_{zy} + \epsilon_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \; ;$$

$$e_{zx} \equiv \mathbf{z}' \cdot \mathbf{x}' \cong \epsilon_{zx} + \epsilon_{xz} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \; . \tag{32}$$

Note X', Y', Z' are not orthogonal to each other !

Keep only the 1st order terms

We may replace the $\cong$ signs by $=$ signs if we neglect terms of order ϵ^2. The six dimensionless coefficients $e_{\alpha\beta}(=e_{\beta\alpha})$ completely define the strain.

Dilation

The fractional *increase* of volume associated with a deformation is called the dilation. The dilation is negative for hydrostatic pressure. The unit cube of edges $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ has a volume after deformation of

$$V' = \mathbf{x}' \cdot \mathbf{y}' \times \mathbf{z}' \ , \tag{33}$$

by virtue of a well-known result for the volume of a parallelepiped having edges $\mathbf{x}'$, $\mathbf{y}'$, $\mathbf{z}'$. From (26) we have

Keep only the 1st order terms

$$\mathbf{x}' \cdot \mathbf{y}' \times \mathbf{z}' = \begin{vmatrix} 1+\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & 1+\epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & 1+\epsilon_{zz} \end{vmatrix} \cong 1 + e_{xx} + e_{yy} + e_{zz} \ . \tag{34}$$

Products of two strain components have been neglected. The dilation δ is then given by

Dilation

$$\delta \equiv \frac{V' - V}{V} \cong e_{xx} + e_{yy} + e_{zz} \ . \tag{35}$$

Stress Components

The force acting on a unit area in the solid is defined as the stress. There are nine stress components: $X_x, X_y, X_z, Y_x, Y_y, Y_z, Z_x, Z_y, Z_z$. The capital letter indicates the direction of the force, and the subscript indicates the normal to the plane to which the force is applied. In Fig. 15 the stress component X_x represents a force applied in the x direction to a unit area of a plane whose normal lies in the x direction; the stress component X_y represents a force applied in the x direction to a unit area of a plane whose normal lies in the y direction. The number of independent stress components is reduced from nine to six by applying to an elementary cube (as in Fig. 16) the condition that the angular acceleration vanish, and hence that the total torque must be zero. It follows that

Reduce from 9 to 6 stress components

$$Y_z = Z_y \ ; \qquad Z_x = X_z \ ; \qquad X_y = Y_x \ . \tag{36}$$

The six independent stress components may be taken as $X_x, Y_y, Z_z, Y_z, Z_x, X_y$.

Stress components have the dimensions of force per unit area or energy per unit volume. The strain components are ratios of lengths and are dimensionless.

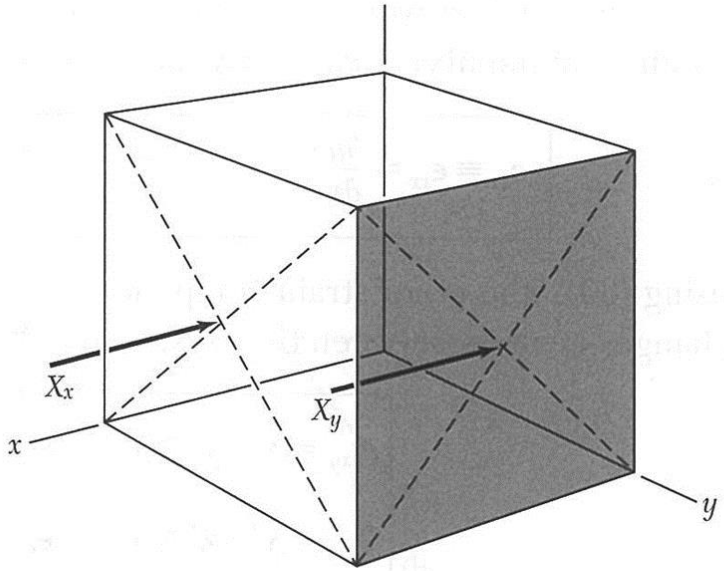


Figure 15 Stress component X_x is a force applied in the x direction to a unit area of a plane whose normal lies in the x direction; X_y is applied in the x direction to a unit area of a plane whose normal lies in the y direction.

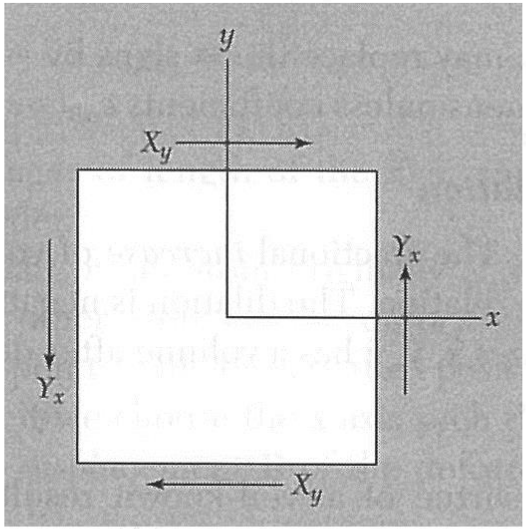


Figure 16 Demonstration that for a body in static equilibrium $Y_x = X_y$. The sum of the forces in the x direction is zero. The sum of the forces in the y direction is also zero. The total force vanishes. The total torque about the origin is also zero if $Y_x = X_y$.

In static equilibrium, total torque about the origin is zero.

⇒ $Y_x = X_y$

ELASTIC COMPLIANCE AND STIFFNESS CONSTANTS

Hooke's law states that for sufficiently small deformations the strain is directly proportional to the stress, so that the strain components are linear functions of the stress components:

$$
\begin{aligned}
e_{xx} &= S_{11}X_x + S_{12}Y_y + S_{13}Z_z + S_{14}Y_z + S_{15}Z_x + S_{16}X_y \ ; \\
e_{yy} &= S_{21}X_x + S_{22}Y_y + S_{23}Z_z + S_{24}Y_z + S_{25}Z_x + S_{26}X_y \ ; \\
e_{zz} &= S_{31}X_x + S_{32}Y_y + S_{33}Z_z + S_{34}Y_z + S_{35}Z_x + S_{36}X_y \ ; \\
e_{yz} &= S_{41}X_x + S_{42}Y_y + S_{43}Z_z + S_{44}Y_z + S_{45}Z_x + S_{46}X_y \ ; \\
e_{zx} &= S_{51}X_x + S_{52}Y_y + S_{53}Z_z + S_{54}Y_z + S_{55}Z_x + S_{56}X_y \ ; \\
e_{xy} &= S_{61}X_x + S_{62}Y_y + S_{63}Z_z + S_{64}Y_z + S_{65}Z_x + S_{66}X_y \ .
\end{aligned}
$$

For six strain components

(37)

$$
\begin{aligned}
X_x &= C_{11}e_{xx} + C_{12}e_{yy} + C_{13}e_{zz} + C_{14}e_{yz} + C_{15}e_{zx} + C_{16}e_{xy} \ ; \\
Y_y &= C_{21}e_{xx} + C_{22}e_{yy} + C_{23}e_{zz} + C_{24}e_{yz} + C_{25}e_{zx} + C_{26}e_{xy} \ ; \\
Z_z &= C_{31}e_{xx} + C_{32}e_{yy} + C_{33}e_{zz} + C_{34}e_{yz} + C_{35}e_{zx} + C_{36}e_{xy} \ ; \\
Y_z &= C_{41}e_{xx} + C_{42}e_{yy} + C_{43}e_{zz} + C_{44}e_{yz} + C_{45}e_{zx} + C_{46}e_{xy} \ ; \\
Z_x &= C_{51}e_{xx} + C_{52}e_{yy} + C_{53}e_{zz} + C_{54}e_{yz} + C_{55}e_{zx} + C_{56}e_{xy} \ ; \\
X_y &= C_{61}e_{xx} + C_{62}e_{yy} + C_{63}e_{zz} + C_{64}e_{yz} + C_{65}e_{zx} + C_{66}e_{xy} \ .
\end{aligned}
$$

For six stress components

(38)

The quantities S_{11}, S_{12} . . . are called **elastic compliance constants** or elastic constants; the quantities C_{11}, C_{12}, . . . are called the **elastic stiffness constants** or moduli of elasticity. The S's have the dimensions of [area]/[force] or [volume]/[energy]. The C's have the dimensions of [force]/[area] or [energy]/[volume].

Elastic Energy Density

The 36 constants in (37) or in (38) may be reduced in number by several considerations. The elastic energy density U is a quadratic function of the strains, in the approximation of Hooke's law (recall the expression for the energy of a stretched spring). Thus we may write

The C's are the elastic stiffness constants

$$U = \frac{1}{2} \sum_{\lambda=1}^{6} \sum_{\mu=1}^{6} \tilde{C}_{\lambda\mu} e_\lambda e_\mu \ , \tag{39}$$

where the indices 1 through 6 are defined as:

$$1 \equiv xx \ ; \quad 2 \equiv yy \ ; \quad 3 \equiv zz \ ; \quad 4 \equiv yz \ ; \quad 5 \equiv zx \ ; \quad 6 \equiv xy \ . \tag{40}$$

The $\tilde{C}$'s are related to the C's of (38), as in (42) below.

I. 1st consideration

The stress components are found from the derivative of U with respect to the associated strain component. This result follows from the definition of potential energy. Consider the stress X_x applied to one face of a unit cube, the opposite face being held at rest:

From Eq. 38

$$X_x = \frac{\partial U}{\partial e_{xx}} \equiv \frac{\partial U}{\partial e_1} = \tilde{C}_{11} e_1 + \frac{1}{2} \sum_{\beta=2}^{6} (\tilde{C}_{1\beta} + \tilde{C}_{\beta 1}) e_\beta \quad . \qquad (41)$$

Note that only the combination $\frac{1}{2}(\tilde{C}_{\alpha\beta} + \tilde{C}_{\beta\alpha})$ enters the stress-strain relations. It follows that the elastic stiffness constants are symmetrical:

$$C_{\alpha\beta} = \tfrac{1}{2}(\tilde{C}_{\alpha\beta} + \tilde{C}_{\beta\alpha}) = C_{\beta\alpha} \quad . \qquad (42)$$

Thus the thirty-six elastic stiffness constants are reduced to twenty-one.

Reduce 36 down to 21 !

II. 2nd Consideration

Elastic Stiffness Constants of Cubic Crystals

The number of independent elastic stiffness constants is reduced further if the crystal possesses symmetry elements. We now show that in cubic crystals there are only three independent stiffness constants. C_{11}, C_{12}, C_{44}

We assert that the elastic energy density of a cubic crystal is

$$U = \tfrac{1}{2}C_{11}(e_{xx}^2 + e_{yy}^2 + e_{zz}^2) + \tfrac{1}{2}C_{44}(e_{yz}^2 + e_{zx}^2 + e_{xy}^2) + C_{12}(e_{yy}e_{zz} + e_{zz}e_{xx} + e_{xx}e_{yy}) \quad (43)$$

and that no other quadratic terms occur; that is, For cubic crystals only

$$(e_{xx}e_{xy} + \cdots) \; ; \qquad (e_{yz}e_{zx} + \cdots) \; ; \qquad (e_{xx}e_{yz} + \cdots) \quad (44)$$

do not occur.

The minimum symmetry requirement for a cubic structure is the existence of four three-fold rotation axes. The axes are in the [111] and equivalent directions (Fig. 17). The effect of a rotation of $2\pi/3$ about these four axes is to interchange the x, y, z axes according to the schemes

$$\begin{aligned} &x \to y \to z \to x \ ; \qquad -x \to z \to y \to -x \ ; \\ &x \to z \to -y \to x \ ; \qquad -x \to y \to z \to -x \ , \end{aligned} \tag{45}$$

according to the axis chosen. Under the first of these schemes, for example,

$$e_{xx}^2 + e_{yy}^2 + e_{zz}^2 \to e_{yy}^2 + e_{zz}^2 + e_{xx}^2 \ ,$$

and similarly for the other terms in parentheses in (43). Thus (43) is invariant under the operations considered. But each of the terms exhibited in (44) is odd in one or more indices. A rotation in the set (45) can be found which will change the sign of the term, because $e_{xy} = -e_{x(-y)}$, for example. Thus the terms (44) are not invariant under the required operations.

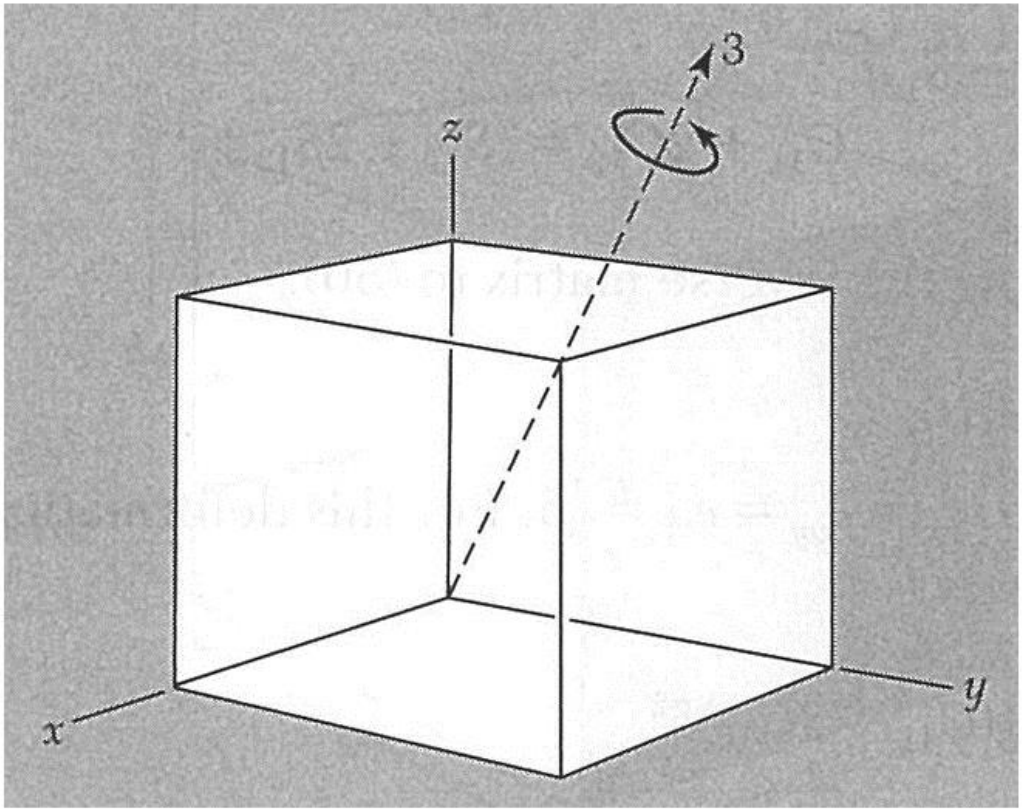


Figure 17 Rotation by $2\pi/3$ about the axis marked 3 changes $x \to y$; $y \to z$; and $z \to x$.

It remains to verify that the numerical factors in (43) are correct. By (41),

$$\partial U/\partial e_{xx} = X_x = C_{11}e_{xx} + C_{12}(e_{yy} + e_{zz}) \ . \tag{46}$$

The appearance of $C_{11}e_{xx}$ agrees with (38). On further comparison, we see that

$$\text{(1)}\ C_{12} = C_{13} \ ; \quad \text{(2)}\ C_{14} = C_{15} = C_{16} = 0 \ . \tag{47}$$

(1) Because *y* is equivalent to z for a cubic crystal
(2) This is due to the basic definitions of C_{14}, C_{15}, C_{16}

Further, from (43),

$$\partial U/\partial e_{xy} = X_y = C_{44}e_{xy} \ ; \tag{48}$$

on comparison with (38) we have

$$C_{61} = C_{62} = C_{63} = C_{64} = C_{65} = 0 \ ; \qquad C_{66} = C_{44} \ . \tag{49}$$

Thus from (43) we find that the array of values of the elastic stiffness constants is reduced for a cubic crystal to the matrix

	e_{xx}	e_{yy}	e_{zz}	e_{yz}	e_{zx}	e_{xy}
X_x	C_{11}	C_{12}	C_{12}	0	0	0
Y_y	C_{12}	C_{11}	C_{12}	0	0	0
Z_z	C_{12}	C_{12}	C_{11}	0	0	0
Y_z	0	0	0	C_{44}	0	0
Z_x	0	0	0	0	C_{44}	0
X_y	0	0	0	0	0	C_{44}

(50)

Thus we have only C_{11}, C_{12}, C_{44}

For cubic crystals the stiffness and compliance constants are related by

$C_{44} = 1/S_{44}$; $C_{11} - C_{12} = (S_{11} - S_{12})^{-1}$;

$$C_{11} + 2C_{12} = (S_{11} + 2S_{12})^{-1} . \qquad (51)$$

These relations follow on evaluating the inverse matrix to (50).

Bulk Modulus and Compressibility

Consider the uniform dilation $e_{xx} = e_{yy} = e_{zz} = \frac{1}{3}\delta$. For this deformation the energy density (43) of a cubic crystal is

$$U = \tfrac{1}{6}(C_{11} + 2C_{12})\delta^2 \ . \tag{52}$$

We may define the **bulk modulus** B by the relation

$$U = \tfrac{1}{2}B\delta^2 \ , \tag{53}$$

which is equivalent to the definition $-V\,dp/dV$. For a cubic crystal,

$$B = \tfrac{1}{3}(C_{11} + 2C_{12}) \ . \tag{54}$$

The **compressibility** K is defined as $K = 1/B$. Values of B and K are given in Table 3.