

On the theory of the elasticity of crystals

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1. Introduction

The branch of mathematical physics known as the theory of the elasticity of solids is based on certain notions regarding elastic stresses and strains which have been accepted doctrine for many years. It is therefore rather surprising to find that those notions are not sustainable and that the theory based on them has to be laid aside in favour of a stricter formulation. The need for such revision was broadly indicated in a recent publication in these *Proceedings* by the present authors (1955); but in view of the importance of the matter, the present paper is prefaced by a clearer and more precise exposition of the necessity for a revision of the classical theory.

Our recent paper dealt with the case of isotropic solids in a formal manner, considering them as homogeneous substances exhibiting the highest possible symmetry in their elastic properties. Usually, however, the so-called isotropic solids are merely polycrystalline aggregates, and a discussion of their elastic behaviour should therefore properly be based on a consideration of the nature and properties of such aggregates. This is a task which we hope to be able to address ourselves in the not-too-distant future. In the present paper we shall consider the case of truly homogeneous but anisotropic solids, in other words, crystals. The subject will be dealt with from the phenomenological standpoint since this proves to be entirely adequate. We may remark, however, that the conclusions reached are in complete accord with the results of the atomistic approach to the theory of elasticity as developed both from the static and dynamic standpoints in a paper by one of us (Viswanathan, 1954) and illustrated by a detailed discussion of a particular case of great interest, viz., diamond.

2. The physical characters of elastic stress and strains

A solid body may be defined as a material in which the volume elements retain their relative positions and orientations alike when the solid is at rest and when it is in a state of movement, translatory or rotatory, as the case may be. Elastic

stresses and strains arise when the situation thus described is departed from to ever so small an extent. Hence, it is evident that the theory of elasticity is concerned with changes in the relative orientations of the volume elements of the solid, in other words, with linear displacements and/or angular movements of the volume elements with respect to their neighbours. This is illustrated by the familiar examples of a straight bar which is stretched or bent or twisted by the application of appropriate external stresses. From the general considerations indicated above as well as from the particular examples mentioned, it is clear that only in very special cases would elastic strains be such that a straight line drawn through the solid in any direction in the unstrained condition remains straight in the strained state, suffering only elongations or contractions. In the general case, and inevitably so when the strains involve differential rotations, a straight line in the unstrained condition would be curved in the strained state, and such curvature cannot possibly be ignored in the theory. Hence, it is clear that we have, in general, to consider strains and stresses which are heterogeneous, in other words, strains and stresses whose specifications vary from point to point within the solid. These variations necessarily enter into the equations of equilibrium in the static state and into the equations of motion in dynamic behaviour.

3. Analytical specification of stresses and strains

The mathematical theory of elasticity proceeds on the basis that the strains and stresses in the interior of the solid can be expressed in terms of the movements of the smallest possible elements of volume into which it can be imagined to be subdivided and of the forces acting on them. If the volume elements be small enough, their movements can be described completely in terms of the three positional co-ordinates of each element and their variations. Likewise, when the elements of volume are small enough, the interactions between each element and its neighbours can be expressed in terms of tractive forces alone, it being then clearly unnecessary to introduce anything in the nature of couples or torques. On the basis of these ideas, the state of strain in the solid at any given point can be expressed by resolving the displacement of the elementary volume originally located at such point along three mutually perpendicular directions and differentiating these three components of displacement again along each of the three axes in turn. We thus obtain the nine components of the strain tensor. Likewise, for specifying the state of stress to which the volume element is subject, we consider the tractive forces acting on an infinitesimal area drawn respectively normal to the three co-ordinate planes in turn at the position of the element and then again resolve these tractive forces along each of the three co-ordinate axes. We thus obtain the nine components of the stress tensor.

It is evident that this method of representation of the stresses and strains

uniquely defines the state of the solid at any point and also enables us to determine whether the element of volume would or would not remain in equilibrium. If the components of stress do not vary along any of the three axes, the element would necessarily remain at rest. If, on the other hand, the stress components vary, their differential coefficients along the normals to the planes on which they act gives us a measure of the forces on the volume element in their respective directions. Adding up the three forces along each axis thus evaluated and putting their sums separately equal to zero, we obtain the conditions of equilibrium.

The well known and familiar treatments given in the standard treatises proceed on the basis that the components of the strain and stress tensors are both reducible in number from nine to six. The arguments on which the reduction in number from nine to six of the components of strain is based may be summarised by the statement that the elastic strains can be separated into what are called "pure strains" and "rotations," and that the latter can be ignored. That this argument is unsustainable will be evident at once from the remarks made in the foregoing section regarding the physical nature of elastic strains. We have, in general, to take account of both differential displacements and differential rotations and it is therefore not permissible to eliminate the rotational parts of the strain, these being physically quite as real as the irrotational parts.

The arguments justifying the reduction in the number of the independent components of stress from nine to six are based upon the idea that equilibrium would be possible only if the angular momenta of the tractions taken about each of the three co-ordinate axes in turn cancel each other out. That this idea is misconceived will be evident from the remarks already made earlier regarding the conditions necessary for equilibrium. In the case of homogeneous strains, the tractive forces acting on each volume element necessarily balance each other. In the case of heterogeneous strains, the conditions of equilibrium can be expressed in terms of the differential coefficients of the stress components along the normals to the planes on which they act, as already explained. In either case, if the equilibrium conditions for each volume element of the solid are satisfied, then the solid as a whole necessarily remains in equilibrium; vice versa, if the external stresses acting on the solid are such that it remains as a whole in equilibrium, the elastic stresses would everywhere necessarily be such as to ensure equilibrium of the individual volume elements. It follows that no general relations connecting the magnitude of the tensor components and enabling their number to be reduced from nine to six can be derived from considerations based on the conditions for equilibrium.

We may summarise our conclusions by stating that neither the reduction of the strain components nor the reduction of the stress components in number from nine to six has any theoretical justification; a correct and complete theory of elasticity has necessarily to take all the nine components of the stress and strain tensors into consideration.

4. The stress-strain relationships

Writing the nine components of the strain tensor as

$$\begin{array}{cccccccccc} u_{xx} & u_{yy} & u_{zz} & u_{yz} & u_{zy} & u_{zx} & u_{xz} & u_{xy} & u_{yx} \\ u_1 & u_2 & u_3 & u_4 & u_5 & u_6 & u_7 & u_8 & u_9 \end{array}$$

and likewise the nine components of the stress tensor as

$$\begin{array}{cccccccccc} T_{xx} & T_{yy} & T_{zz} & T_{yz} & T_{zy} & T_{zx} & T_{xz} & T_{xy} & T_{yx} \\ T_1 & T_2 & T_3 & T_4 & T_5 & T_6 & T_7 & T_8 & T_9 \end{array}$$

the stress-strain relations can be expressed in the general form

$$T_m = \sum_{n=1}^9 d_{mn} u_n \quad (m = 1, 2, \dots, 9) \quad (1)$$

and involve 81 constants. Here the constant d_{mn} relates the stress T_m to the strain u_n and is the ratio of the two for a deformation in which all components other than u_n vanish.

The 81 constants figuring in (1) are not all independent, but reduce in the first instance to forty-five for all solids in view of the relations

$$d_{mn} = d_{nm} \quad (m, n = 1, 2, \dots, 9). \quad (2)$$

The above relations follow from the well known theorem of reciprocity relating forces and the corresponding displacements of dynamical systems. The reciprocity relations further enable us to write down the expression for the deformation energy per unit volume in the neighbourhood of any point and this is given by

$$U = \frac{1}{2} \sum_{m=1}^9 T_m u_m$$

or

$$2U = \sum_m \sum_n d_{mn} u_m u_n. \quad (3)$$

Thus in the general case of a completely anisotropic solid, we have forty-five elastic constants instead of the 21 contemplated by the classical theory.

The number of independent elastic constants which is forty-five for a completely anisotropic solid diminishes in the case of solids possessing the various elements of symmetry characteristic of the different crystal classes, coming down to four for crystals of the classes T_d , O and O_h . The number of surviving constants in each symmetry class can be computed in an elegant fashion by adopting the group-theoretical method developed by Bhagavantam (1949). One is concerned in the present case with a linear relationship between nine stress components and nine strain components, the constants of proportionality being the elastic constants (matrix d_{mn}). Further, the elements of the "elastic constants 9

by 9 matrix" satisfy the relation $d_{mn} = d_{nm}$. With these restrictions, the transformation matrix for the elastic constants can be written out and the corresponding character can be deduced. This comes out as

$$\chi_j(R) = 16c^4 \pm 16c^3 + 8c^2 \pm 4c + 1 \quad (4)$$

where $c = \cos \phi$, R is a symmetry operation and ϕ , the rotation. The *plus* sign is used for proper rotations, and *minus* for an improper one. The corresponding character for the 21-constant theory is

$$\chi_j(R) = 16c^4 \pm 8c^3 - 4c^2 + 1 \quad (5)$$

Table 1 gives the number of independent constants according to the two formulae for each symmetry class, while the constants that survive and those that vanish

Table 1

Crystal system	Point group	No. of elastic constants	
		I	II
Triclinic	All	21	45
Monoclinic	All	13	25
Orthorhombic	All	9	15
Tetragonal	$C_4(4)$	7	13
	$S_4(\bar{4})$		
	$C_{4h}(4/m)$		
	$D_4(422)$		
	$S_{4v} = D_{2d}(42m)$	6	9
	$D_{4h}(4/m2/m2/m)$		
Trigonal	$C_3(3)$	7	15
	$S_6(\bar{3})$		
	$D_3(32)$	6	10
	$C_{3v}(3m)$		
	$D_{3d}(\bar{3}2/m)$		
Hexagonal	$C_6(6)$	5	11
	$C_{3h}(\bar{6})$		
	$C_{6h}(6/m)$		
	$D_6(622)$		
	$C_{6v}(6mm)$	5	8
	$D_{3h}(\bar{6}m2)$		
	$D_{6h}(6/m2/m2/m)$		
Cubic	$T(23)$	3	5
	$T_h(2/m\bar{3})$		
	$O(432)$	3	4
	$T_d(43m)$		
	$O_h(4/m\bar{3}2/m)$		

are exhibited in detail for the various cases in tables 2 to 12. A comparison of these tables amongst themselves will enable the reader to realise how the existence of common symmetry elements results in the appearance of common features in the tables of elastic constants. For example, all the twenty constants that vanish for

Table 2

Triclinic (C_1, C_i)								
d_{11}	d_{12}	d_{13}	d_{14}	d_{15}	d_{16}	d_{17}	d_{18}	d_{19}
	d_{22}	d_{23}	d_{24}	d_{25}	d_{26}	d_{27}	d_{28}	d_{29}
		d_{33}	d_{34}	d_{35}	d_{36}	d_{37}	d_{38}	d_{39}
			d_{44}	d_{45}	d_{46}	d_{47}	d_{48}	d_{49}
				d_{55}	d_{56}	d_{57}	d_{58}	d_{59}
					d_{66}	d_{67}	d_{68}	d_{69}
						d_{77}	d_{78}	d_{79}
							d_{88}	d_{89}
								d_{99}

45 constants

Table 3

Monoclinic (C_2, C_2, C_{2h})—diad axis $\parallel z$, plane of reflection \perp to z									
d_{11}	d_{12}	d_{13}	0	0	0	0	d_{18}	d_{19}	
	d_{22}	d_{23}	0	0	0	0	d_{28}	d_{29}	
		d_{33}	0	0	0	0	d_{38}	d_{39}	
			d_{44}	d_{45}	d_{46}	d_{47}	0	0	
				d_{55}	d_{56}	d_{57}	0	0	
					d_{66}	d_{67}	0	0	
						d_{77}	0	0	
							d_{88}	d_{89}	
								d_{99}	

25 constants

Table 4

Orthorhombic (C_{2v}, D_2, D_{2h})									
d_{11}	d_{12}	d_{13}	0	0	0	0	0	0	0
	d_{22}	d_{23}	0	0	0	0	0	0	0
		d_{33}	0	0	0	0	0	0	0
			d_{44}	d_{45}	0	0	0	0	0
				d_{55}	0	0	0	0	0
					d_{66}	d_{67}	0	0	0
						d_{77}	0	0	0
							d_{88}	d_{89}	
								d_{99}	

15 constants

Table 5

Tetragonal (C_4, S_4, C_{4h})—tetrad axis $\parallel z$									
d_{11}	d_{12}	d_{13}	0	0	0	0	d_{18}	d_{19}	
	d_{11}	d_{13}	0	0	0	0	$-d_{19}$	$-d_{18}$	
		d_{33}	0	0	0	0	d_{38}	$-d_{38}$	
			d_{44}	d_{45}	d_{46}	0	0	0	
				d_{55}	0	$-d_{46}$	0	0	
					d_{55}	d_{45}	0	0	
						d_{44}	0	0	
							d_{88}	d_{89}	
								d_{88}	

13 constants

Table 6

Tetragonal ($C_{4v}, S_{4v}, D_4, D_{4h}$)—tetrad axis $\parallel z$									
d_{11}	d_{12}	d_{13}	0	0	0	0	0	0	0
	d_{11}	d_{13}	0	0	0	0	0	0	0
		d_{33}	0	0	0	0	0	0	0
			d_{44}	d_{45}	0	0	0	0	0
				d_{55}	0	0	0	0	0
					d_{55}	d_{45}	0	0	0
						d_{44}	0	0	0
							d_{88}	d_{89}	
								d_{88}	

9 constants

Table 7

Trigonal (C_3, S_6)—triad axis $\parallel z$									
d_{11}	d_{12}	d_{13}	d_{14}	d_{15}	d_{16}	d_{17}	d_{18}	$-d_{18}$	
	d_{11}	d_{13}	$-d_{14}$	$-d_{15}$	$-d_{16}$	$-d_{17}$	d_{18}	$-d_{18}$	
		d_{33}	0	0	0	0	d_{38}	$-d_{38}$	
			d_{44}	d_{45}	d_{46}	0	d_{17}	$-d_{17}$	
				d_{55}	0	$-d_{46}$	$-d_{16}$	$-d_{16}$	
					d_{44}	d_{45}	d_{15}	d_{15}	
						d_{55}	d_{14}	d_{14}	
							d_{88}	d_{89}	
								d_{88}	

$$d_{88} = d_{11} - d_{12} - d_{89}$$

15 constants

monoclinic crystals also disappear in the orthorhombic, tetragonal and cubic systems. Likewise, all the thirty constants that vanish for orthorhombic crystals vanish also for those tetragonal crystals which possess three mutually perpendicular diad axes and for all cubic crystals. A noteworthy feature is that the

Table 8

Trigonal (D_3, D_{3d}, C_{3v})—triad axis $\parallel z$								
d_{11}	d_{12}	d_{13}	d_{14}	d_{15}	0	0	0	0
	d_{11}	d_{13}	$-d_{14}$	$-d_{15}$	0	0	0	0
		d_{33}	0	0	0	0	0	0
			d_{44}	d_{45}	0	0	0	0
				d_{55}	0	0	0	0
					d_{44}	d_{45}	d_{15}	d_{15}
						d_{55}	d_{14}	d_{14}
							d_{88}	d_{89}
								d_{88}

$d_{88} = d_{11} - d_{12} - d_{89}$

10 constants

Table 9

Hexagonal (C_{3h}, C_6, C_{6h})—hexad axis $\parallel z$								
d_{11}	d_{12}	d_{13}	0	0	0	0	d_{18}	$-d_{18}$
	d_{11}	d_{13}	0	0	0	0	d_{18}	$-d_{18}$
		d_{33}	0	0	0	0	d_{38}	$-d_{38}$
			d_{44}	d_{45}	d_{46}	0	0	0
				d_{55}	0	$-d_{46}$	0	0
					d_{44}	d_{45}	0	0
						d_{55}	0	0
							d_{88}	d_{89}
								d_{88}

$d_{88} = d_{11} - d_{12} - d_{89}$

11 constants

Table 10

Hexagonal ($D_{3h}, C_{6v}, D_6, D_{6h}$)—hexad axis $\parallel z$								
d_{11}	d_{12}	d_{13}	0	0	0	0	0	0
	d_{11}	d_{13}	0	0	0	0	0	0
		d_{33}	0	0	0	0	0	0
			d_{44}	d_{45}	0	0	0	0
				d_{55}	0	0	0	0
					d_{44}	d_{45}	0	0
						d_{55}	0	0
							d_{88}	d_{89}
								d_{88}

$d_{88} = d_{11} - d_{12} - d_{89}$

8 constants

Table 11

Cubic (T, T _h)								
d_{11}	d_{12}	d_{12}	0	0	0	0	0	0
	d_{11}	d_{12}	0	0	0	0	0	0
		d_{11}	0	0	0	0	0	0
			d_{44}	d_{45}	0	0	0	0
				d_{55}	0	0	0	0
					d_{44}	d_{45}	0	0
						d_{55}	0	0
							d_{44}	d_{45}
								d_{55}

5 constants

Table 12

Cubic (T _d , O, O _h)								
d_{11}	d_{12}	d_{12}	0	0	0	0	0	0
	d_{11}	d_{12}	0	0	0	0	0	0
		d_{11}	0	0	0	0	0	0
			d_{14}	d_{45}	0	0	0	0
				d_{44}	0	0	0	0
					d_{44}	d_{45}	0	0
						d_{44}	0	0
							d_{44}	d_{45}
								d_{44}

4 constants

cubic crystals which exhibit a four-fold axis of symmetry have only four different elastic constants, whereas those cubic crystals that do not exhibit this feature have five constants different from each other.

5. Wave-propagation in crystals

The general equations of motion of an elastic solid are given by

$$\begin{aligned}
 \rho \frac{\partial^2 u_x}{\partial t^2} &= \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{\partial T_{xz}}{\partial z} \\
 \rho \frac{\partial^2 u_y}{\partial t^2} &= \frac{\partial T_{yx}}{\partial x} + \frac{\partial T_{yy}}{\partial y} + \frac{\partial T_{yz}}{\partial z} \\
 \rho \frac{\partial^2 u_z}{\partial t^2} &= \frac{\partial T_{zx}}{\partial x} + \frac{\partial T_{zy}}{\partial y} + \frac{\partial T_{zz}}{\partial z}
 \end{aligned}
 \tag{6}$$

where ρ is the density of the medium and T_{xx}, \dots are the stress components. If the solid is in equilibrium, the quantities on the left-hand side of these equations, representing the acceleration of a unit volume element, will vanish and we get the conditions of equilibrium of the solid.

To evaluate the velocity of propagation of waves in the solid in any given direction, we first seek solutions of the above equations which are in the form of plane waves of the type

$$\mathbf{u} = \mathbf{A} \exp i \frac{2\pi}{\lambda} (vt - \mathbf{e} \cdot \mathbf{r}). \quad (7)$$

Denoting the components of \mathbf{A} in the directions of the co-ordinate axes by A^x, A^y, A^z and using once again the four-suffixed symbols for the elastic constants, we now get on substitution of (7) in (6) that

$$\rho v^2 A^x = \sum_{\bar{x}\bar{y}} \sum_{\bar{x}\bar{y}} d_{\bar{x}\bar{x}\bar{y}\bar{y}} e_{\bar{x}} e_{\bar{y}} A^y \quad (8)$$

and two similar equations for the y and z components.

For a wave progressing in the direction (lmn) equation (8) can alternatively be written as

$$\begin{aligned} (\lambda_{xx} - \rho v^2) A^x + \lambda_{xy} A^y + \lambda_{xz} A^z &= 0 \\ \lambda_{xy} A^x + (\lambda_{yy} - \rho v^2) A^y + \lambda_{yz} A^z &= 0 \\ \lambda_{xz} A^x + \lambda_{yz} A^y + (\lambda_{zz} - \rho v^2) A^z &= 0 \end{aligned} \quad (9)$$

where $\lambda_{xx}, \lambda_{xy}, \dots$ are given by the scheme

$$\begin{pmatrix} \lambda_{xx} \\ \lambda_{yy} \\ \lambda_{zz} \\ \lambda_{yz} \\ \lambda_{zx} \\ \lambda_{xy} \end{pmatrix} = \begin{pmatrix} d_{11} & d_{88} & d_{77} & 2d_{78} & 2d_{17} & 2d_{18} \\ d_{99} & d_{22} & d_{44} & 2d_{24} & 2d_{49} & 2d_{29} \\ d_{66} & d_{55} & d_{33} & 2d_{35} & 2d_{36} & 2d_{56} \\ d_{69} & d_{25} & d_{34} & (d_{23} + d_{45}) & (d_{39} + d_{46}) & (d_{59} + d_{26}) \\ d_{16} & d_{58} & d_{37} & (d_{57} + d_{38}) & (d_{67} + d_{13}) & (d_{15} + d_{68}) \\ d_{19} & d_{28} & d_{47} & (d_{27} + d_{48}) & (d_{14} + d_{79}) & (d_{12} + d_{89}) \end{pmatrix} \begin{pmatrix} l^2 \\ m^2 \\ n^2 \\ mn \\ nl \\ lm \end{pmatrix}$$

Equations (9) determine the velocities of propagation of the three types of waves in any direction for crystals of the triclinic system which possess no symmetry of structure at all. The number of constants figuring in the wave equations will diminish rapidly as we pass on to crystals of higher symmetry, and become only three for crystals of the T_h , O and O_h classes. We tabulate below the wave equations for the different classes of crystals taking into account of their symmetry.

I. Monoclinic system (C_2, C_2, C_{2h})—diad axis parallel to the z-axis

$$(d_{11}l^2 + d_{88}m^2 + d_{77}n^2 + 2d_{18}lm - \rho v^2)A^x + \{d_{19}l^2 + d_{28}m^2 + d_{47}n^2 + (d_{12} + d_{89})lm\}A^y + \{(d_{38} + d_{57})mn + (d_{13} + d_{67})nl\}A^z = 0.$$

$$\{d_{19}l^2 + d_{28}m^2 + d_{47}n^2 + (d_{12} + d_{89})lm\}A^x + (d_{99}l^2 + d_{22}m^2 + d_{44}n^2 + 2d_{29}lm - \rho v^2)A^y + \{(d_{23} + d_{45})mn + (d_{39} + d_{46})nl\}A^z = 0.$$

$$\{(d_{38} + d_{57})mn + (d_{13} + d_{67})nl\}A^x + \{(d_{23} + d_{45})mn + (d_{39} + d_{46})nl\}A^y + (d_{66}l^2 + d_{55}m^2 + d_{33}n^2 + 2d_{56}lm - \rho v^2)A^z = 0.$$

The wave equations contain *twenty* independent constants.

II. Orthorhombic system (C_{2v}, D_2, D_{2h})

$$(d_{11}l^2 + d_{88}m^2 + d_{77}n^2 - \rho v^2)A^x + (d_{12} + d_{89})lmA^y + (d_{13} + d_{67})nlA^z = 0,$$

$$(d_{12} + d_{89})lmA^x + (d_{99}l^2 + d_{22}m^2 + d_{44}n^2 - \rho v^2)A^y + (d_{23} + d_{45})mnA^z = 0.$$

$$(d_{13} + d_{67})nlA^x + (d_{23} + d_{45})mnA^y + (d_{66}l^2 + d_{55}m^2 + d_{33}n^2 - \rho v^2)A^z = 0.$$

The wave-equations involve *twelve* distinct constants.

III. Tetragonal (C_4, S_4, C_{4h})—tetrad axis parallel to the z-axis

$$\{d_{11}l^2 + d_{88}m^2 + d_{44}n^2 + 2d_{18}lm - \rho v^2\}A^x + \{d_{19}(l^2 - m^2) + (d_{12} + d_{89})lm\}A^y + \{(d_{38} - d_{46})mn + (d_{13} + d_{45})nl\}A^z = 0$$

$$\{d_{19}(l^2 - m^2) + (d_{12} + d_{89})lm\}A^x + \{d_{88}l^2 + d_{11}m^2 + d_{44}n^2 - 2d_{18}lm - \rho v^2\}A^y + \{(d_{13} + d_{45})mn + (d_{46} - d_{38})nl\}A^z = 0.$$

$$\{(d_{38} - d_{46})mn + (d_{13} + d_{45})nl\}A^x + \{(d_{13} + d_{45})mn + (d_{46} - d_{38})nl\}A^y + \{d_{55}(l^2 + m^2) + d_{33}n^2 - \rho v^2\}A^z = 0.$$

The number of independent constants contained in the wave equations is *ten*.

IV. Tetragonal ($C_{4v}, S_{4v}, D_4, D_{4h}$)—tetrad axis parallel to the z-axis

$$(d_{11}l^2 + d_{88}m^2 + d_{44}n^2 - \rho v^2)A^x + (d_{12} + d_{89})lmA^y + (d_{13} + d_{45})nlA^z = 0.$$

$$(d_{12} + d_{89})lmA^x + (d_{88}l^2 + d_{11}m^2 + d_{44}n^2 - \rho v^2)A^y + (d_{13} + d_{45})mnA^z = 0.$$

$$(d_{13} + d_{45})nlA^x + (d_{13} + d_{45})mnA^y + \{d_{55}(l^2 + m^2) + d_{33}n^2 - \rho v^2\}A^z = 0.$$

The number of independent constants contained in the wave-equations is *seven*.

V. *Trigonal system* (C_3, S_6)—*triad axis parallel to the z-axis*

$$\begin{aligned} &\{d_{11}l^2 + d_{88}m^2 + d_{55}n^2 + 2d_{14}mn + 2d_{17}nl + 2d_{18}lm - \rho v^2\}A^x \\ &+ \{d_{18}(m^2 - l^2) - 2d_{17}mn + 2d_{14}nl + (d_{12} + d_{89})lm\}A^y \\ &+ \{d_{16}l^2 - m^2\} + (d_{38} - d_{46})mn + (d_{13} + d_{45})nl + 2d_{15}lm\}A^z = 0. \end{aligned}$$

$$\begin{aligned} &\{d_{18}(m^2 - l^2) - 2d_{17}mn + 2d_{14}nl + (d_{12} + d_{89})lm\}A^x \\ &+ \{d_{88}l^2 + d_{11}m^2 + d_{44}n^2 - 2d_{14}mn - 2d_{17}nl - 2d_{18}lm - \rho v^2\}A^y \\ &+ \{d_{15}(l^2 - m^2) + (d_{13} + d_{45})mn + (d_{46} - d_{38})nl - 2d_{16}lm\}A^z = 0. \end{aligned}$$

$$\begin{aligned} &\{d_{16}(l^2 - m^2) + (d_{38} - d_{46})mn + (d_{13} + d_{45})nl + 2d_{15}lm\}A^x \\ &+ \{d_{15}(l^2 - m^2) + (d_{13} + d_{45})mn + (d_{46} - d_{38})nl - 2d_{16}lm\}A^y \\ &+ \{d_{44}l^2 + d_{55}m^2 + d_{33}n^2 - \rho v^2\}A^z = 0 \end{aligned}$$

where

$$d_{88} = (d_{11} - d_{12} - d_{89}).$$

The number of independent constants contained in the wave equations is *twelve*.

VI. *Trigonal* (D_3, D_{3d}, C_{3v})—*triad axis parallel to the z-axis*

$$\begin{aligned} &\{d_{11}l^2 + d_{88}m^2 + d_{55}n^2 + 2d_{14}mn - \rho v^2\}A^x + \{2d_{14}nl \\ &+ (d_{12} + d_{89})lm\}A^y + \{(d_{13} + d_{45})nl + 2d_{15}lm\}A^z = 0. \end{aligned}$$

$$\begin{aligned} &\{2d_{14}nl + (d_{12} + d_{89})lm\}A^x + \{d_{88}l^2 + d_{11}m^2 + d_{44}n^2 \\ &- 2d_{14}mn - \rho v^2\}A^y + \{d_{15}(l^2 - m^2) \\ &+ (d_{13} + d_{45})mn + d_{46}nl\}A^z = 0. \end{aligned}$$

$$\begin{aligned} &\{(d_{13} + d_{45})nl + 2d_{15}lm\}A^x + \{d_{15}(l^2 - m^2) \\ &+ (d_{13} + d_{45})mn + d_{46}nl\}A^y + \{d_{44}l^2 + d_{55}m^2 + d_{33}n^2 \\ &- \rho v^2\}A^z = 0. \end{aligned}$$

where

$$d_{88} = (d_{11} - d_{12} - d_{89}).$$

The number of independent constants contained in the wave equations is *eight*.

VII. Hexagonal (C_{3h}, C_6, C_{6h})—hexad axis parallel to the z-axis

$$\begin{aligned} & \{d_{11}l^2 + d_{88}m^2 + d_{55}n^2 + 2d_{18}lm - \rho v^2\}A^x + \{d_{18}(m^2 - l^2) \\ & \quad + (d_{12} + d_{89})lm\}A^y + \{(d_{38} - d_{46})mn + (d_{13} + d_{45})nl\}A^z = 0. \\ & \{d_{18}(m^2 - l^2) + (d_{12} + d_{89})lm\}A^x + \{d_{88}l^2 + d_{11}m^2 + d_{44}n^2 \\ & \quad - 2d_{18}lm - \rho v^2\}A^y + \{(d_{13} + d_{45})mn + (d_{46} - d_{38})nl\}A^z = 0. \\ & \{(d_{38} - d_{46})mn + (d_{13} + d_{45})nl\}A^x + \{(d_{13} + d_{45})mn \\ & \quad + (d_{46} - d_{38})nl\}A^y + \{d_{44}l^2 + d_{55}m^2 + d_{33}n^2 - \rho v^2\}A^z = 0. \end{aligned}$$

where

$$d_{88} = (d_{11} - d_{12} - d_{89}).$$

The number of independent constants contained in the wave equations is eight.

VIII. Hexagonal ($D_{3h}, C_{6v}, D_6, D_{6h}$)—hexad axis parallel to the z-axis

$$\begin{aligned} & (d_{11}l^2 + d_{88}m^2 + d_{55}n^2 - \rho v^2)A^x + (d_{12} + d_{89})lmA^y \\ & \quad + (d_{13} + d_{45})nlA^z = 0. \\ & (d_{12} + d_{89})lmA^x + (d_{88}l^2 + d_{11}m^2 + d_{44}n^2 - \rho v^2)A^y \\ & \quad + (d_{13} + d_{45})mnA^z = 0. \\ & (d_{13} + d_{45})(nlA^x + mnA^y) + (d_{44}l^2 + d_{55}m^2 + d_{33}n^2 - \rho v^2)A^z = 0. \end{aligned}$$

Here again the relation

$$d_{88} = d_{11} - d_{12} - d_{89}$$

characteristic of crystals of the trigonal systems subsists, and number of independent constants appearing in the wave equations is six.

IX. Cubic (T and T_h)

$$\begin{aligned} & (d_{11}l^2 + d_{44}m^2 + d_{55}n^2 - \rho v^2)A^x + (d_{12} + d_{45})(lmA^y + nlA^z) = 0. \\ & (d_{12} + d_{45})lmA^x + (d_{11}m^2 + d_{44}n^2 + d_{55}l^2 - \rho v^2)A^y \\ & \quad + (d_{12} + d_{45})mnA^z = 0. \\ & (d_{12} + d_{45})(nlA^x + mnA^y) + (d_{11}n^2 + d_{44}l^2 + d_{55}m^2 - \rho v^2)A^z = 0. \end{aligned}$$

The number of independent elastic constants appearing in the wave equations is four.

X. Cubic (T_d, O and D_h)

$$\{d_{11}l^2 + d_{44}(m^2 + n^2) - \rho v^2\}A^x + (d_{12} + d_{45})\{(lmA^y + nlA^z)\} = 0.$$

$$(d_{12} + d_{45})l mA^x + \{d_{11}m^2 + d_{44}(l^2 + m^2) - \rho v^2\} A^y \\ + (d_{12} + d_{45})mn A^z = 0.$$

$$(d_{12} + d_{45})\{n l A^x + m n A^y\} + \{d_{11}l^2 + d_{44}(l^2 + m^2) - \rho v^2\} A^z = 0.$$

The number of independent constants appearing in the wave equations is *three*.

6. Static deformation problems

Equations (1) express the nine stress components in terms of the nine strain coefficients. One can work out the inverse transformation of (1) and express instead the strain coefficients as linear functions of the stress variables. The strain-stress relations can therefore alternatively be written also as

$$u_m = \sum_{n=1}^9 D_{mn} T_n \quad (m = 1, 2, \dots, 9) \quad (10)$$

If Δ_{mn} denotes the co-factor of the element d_{mn} in the determinant of the transformation (1) and $\Delta = \text{determinant } |d_{mn}|$, then $D_{mn} = (\Delta_{mn}/\Delta)$.

The strain-energy can be expressed purely as a function of the stress coefficients and we have another expression

$$2U = \sum_m \sum_n D_{mn} T_m T_n \quad (11)$$

for the deformation energy which is equivalent to (3).

In the classical theory the nine stress variables are reduced to six by means of the relations $T_{yz} = T_{zy}$; $T_{zx} = T_{xz}$; $T_{xy} = T_{yx}$. The deformation energy of the solid is thus a function of the six stress variables only. Adopting the usual convention of writing $T'_1, T'_2, T'_3, T'_4, T'_5, T'_6$ for $T_{xx}, T_{yy}, T_{zz}, T_{yz},$ or T_{zy}, T_{zx} or T_{xz}, T_{xy} or T_{yx} respectively, the classical expression (4) for the strain-energy becomes

$$2U_1 = \sum_m \sum_n^6 s_{mn} T'_m T'_n \quad (12)$$

The coefficients s_{mn} occurring in the above expression are the well known *elastic moduli* of the classical theory. One can obtain formulae for these moduli in terms of our constants D_{mn} by considering cases of homogeneous stresses for which the relations $T_{yz} = T_{zy}$; $T_{zx} = T_{xz}$; $T_{xy} = T_{yx}$ hold good. Making these substitutions in (11) and comparing the resulting expression with (2), we get $s_{mn} = D_{mn}$ when both m and n are 1, 2, or 3 and relations of the type

$$s_{14} = (D_{14} + D_{15}); \\ s_{44} = (D_{44} + 2D_{45} + D_{55}); \\ s_{45} = (D_{46} + D_{47} + D_{56} + D_{57}); \quad (13)$$

for the other coefficients.

We can now write down the expressions for the compressibility, Young's modulus, and the Poisson's ratio for any crystal in simple terms. In view of the fact that all these moduli are determinable from experiments dealing with purely homogeneous strains, the formulae for them are not essentially different from the corresponding ones of the classical theory. By following the same methods as those adopted in the latter³, we give below the formulae for these moduli in our present notation.

When the crystal is subjected to a uniform hydrostatic pressure P , we have from the first three of the equations (10)

$$\begin{aligned} u_1 &= (D_{11} + D_{12} + D_{13})P \\ &= (s_{11} + s_{12} + s_{13})P \quad \text{from (13)} \\ u_2 &= (s_{21} + s_{22} + s_{23})P \\ u_3 &= (s_{31} + s_{32} + s_{33})P. \end{aligned}$$

The linear compressibility modulus in the direction of the x -axis is therefore given by

$$k_x = (P/u_1) = 1/(s_{11} + s_{12} + s_{13}) \quad (14)$$

and the bulk modulus is expressed by the formula

$$k = P/(u_1 + u_2 + u_3) = 1/(s_{11} + s_{22} + s_{33} + 2s_{23} + 2s_{31} + 2s_{12}). \quad (15)$$

If the solid is subjected to a uniform tension T in the direction of the x -axis, obviously $T_1 = T$; $T_2 = T_3 = \dots T_9 = 0$. Hence it follows from (10) that the Young's modulus in the direction of the x -axis is given by

$$E = T/u_1 = (1/D_{11}) = (1/s_{11}). \quad (16)$$

Similarly the Poisson's ratio in the direction of the y -axis is given by

$$\sigma = -(s_{12}/s_{11}). \quad (17)$$

To write down the expressions for the Young's modulus and Poisson's ratio in any general direction (l, m, n), we require the law of transformation of the strain as well as the stress components when one passes over from one co-ordinate system to another. If the direction cosines of the axes Ox' , Oy' , Oz' of a new co-ordinate system referred to the original one are $(l_1 m_1 n_1)$, $(l_2 m_2 n_2)$ and $(l_3 m_3 n_3)$ respectively, we have

$$\begin{aligned} T_{x'x'} &= l_1^2 T_{xx} + m_1^2 T_{yy} + n_1^2 T_{zz} + m_1 n_1 (T_{yz} + T_{zy}) \\ &\quad + n_1 l_1 (T_{zx} + T_{xz}) + l_1 m_1 (T_{xy} + T_{yx}) \\ T_{x'y'} &= l_1 l_2 T_{xx} + m_1 m_2 T_{yy} + n_1 n_2 T_{zz} + (m_1 n_2 T_{yz} + m_2 n_1 T_{zy}) \\ &\quad + (n_1 l_2 T_{zx} + n_2 l_1 T_{xz}) + (l_1 m_2 T_{xy} + l_2 m_1 T_{yx}) \\ T_{y'x'} &= l_1 l_2 T_{xx} + m_1 m_2 T_{yy} + n_1 n_2 T_{zz} + (m_2 n_1 T_{yz} + m_1 n_2 T_{zy}) \\ &\quad + (n_2 l_1 T_{zx} + n_1 l_2 T_{xz}) + (l_2 m_1 T_{xy} + l_1 m_2 T_{yx}) \end{aligned} \quad (18)$$

$$u_{x'x'} = l_1^2 u_{xx} + m_1^2 u_{yy} + n_1^2 u_{zz} + m_1 n_1 (u_{yz} + u_{zy}) \\ + n_1 l_1 (u_{zx} + u_{xz}) + l_1 m_1 (u_{xy} + u_{yx}) \quad (19)$$

$$u_{x'y'} = l_1 l_2 u_{xx} + m_1 m_2 u_{yy} + n_1 n_2 u_{zz} + (m_1 n_2 u_{yz} + m_2 n_1 u_{zy}) \\ + (n_1 l_2 u_{zx} + n_2 l_1 u_{xz}) + (l_1 m_2 u_{xy} + l_2 m_1 u_{yx})$$

$$u_{y'x'} = l_1 l_2 u_{xx} + m_1 m_2 u_{yy} + n_1 n_2 u_{zz} + (m_2 n_1 u_{yz} + m_1 n_2 u_{zy}) \\ + (n_2 l_1 u_{zx} + n_1 l_2 u_{xz}) + (l_2 m_1 u_{xy} + l_1 m_2 u_{yx}).$$

Now, if the solid is subjected to a uniform tension T over the planes $x' = \text{const.}$ of which the normal has direction cosines (l_1, m_1, n_1) , we get from the transformation rules

$$T_{xx} = l_1^2 T; \quad T_{yy} = m_1^2 T; \quad T_{zz} = n_1^2 T; \quad T_{yz} = T_{zy} = m_1 n_1 T; \\ T_{zx} = T_{xz} = n_1 l_1 T; \quad T_{xy} = T_{yx} = l_1 m_1 T.$$

Further, $u_{x'x'}$ is given by (19). Hence denoting by \mathbf{q}_x the row vector $(l_1^2 m_1^2 n_1^2 m_1 n_1 n_1 l_1 l_1 m_1)$ with six components, we find the expression for the Young's modulus in the direction of the vector $(l_1 m_1 n_1)$ as

$$E_{x'} = 1/\mathbf{q}_x \cdot \mathbf{S} \tilde{\mathbf{q}}_x \quad (20)$$

where \mathbf{S} denotes the matrix (s_{mn}) . Similarly the Poisson's ratio in the direction of the y' -axis which has direction cosines (l_2, m_2, n_2) with respect to O_x, O_y and O_z is given by

$$\sigma_{y'} = -\frac{1}{2\phi} \left[l_2^2 \frac{\partial \phi}{\partial l_1^2} + m_2^2 \frac{\partial \phi}{\partial m_1^2} + n_2^2 \frac{\partial \phi}{\partial n_1^2} + m_2 n_2 \frac{\partial \phi}{\partial (m_1 n_1)} \right. \\ \left. + n_2 l_2 \frac{\partial \phi}{\partial (n_1 l_1)} + l_2 m_2 \frac{\partial \phi}{\partial (l_1 m_1)} \right] \quad (21)$$

where $\phi = \mathbf{q}_x \cdot \mathbf{S} \tilde{\mathbf{q}}_x$ and the differential coefficients are formed as if these arguments are independent.

It is interesting to note that only twenty-one of the forty-five constants figuring in (10) appear in the above formulae. As mentioned earlier, this is a consequence of the homogeneity of the strains applied to evaluate these static moduli.

The stresses and strains which appear when elastic materials are subject to torsion or flexure are essentially heterogeneous, and hence in dealing with them, our elastic moduli D_{mn} will appear in combinations other than those which figure in homogeneous deformations. The present theory is quite competent to handle such problems, but to deal with them in detail would carry us far beyond the scope of this paper.

7. Some concluding remarks

The main purpose of the present paper has been to establish the necessity for an amendment of the phenomenological theory of elasticity as universally accepted hitherto. Any theory to be acceptable should include in its scope elastic stresses and strains of the most general type and specify them in an analytical form from which the equations of equilibrium in static problems and the equations of motion in wave-propagation can be written down immediately. These requirements are not met by the present form of the theory but are completely satisfied if all the nine components of stress and strain in the usual tensor formulation are retained. When thus amended, the phenomenological theory is capable of handling all the problems of the subject, including those which arise in its practical applications. The more important of these are considered in detail in the course of the paper and the results are set out explicitly for the different crystal classes so that they could be readily made use of.

As already remarked in the introduction, the phenomenological theory as amended gives results in complete accord with those derived from the atomistic approach to the theory of elasticity of crystals based on the most general scheme of interatomic forces. To discuss the latter further or to give an account of the somewhat confused history of the subject would lie outside the scope of the present paper. A few remarks regarding these matters will however be found in the attached appendix.

Summary

The fundamental aspects of the phenomenological theory of elasticity are critically examined and it is shown that the tensor representation of the elastic strains and stresses in the general case should be in the unsymmetrical form. On this basis, the stress-strain relationships are deduced and tabulated for the different crystal classes. The equations determining the velocities of wave-propagation in different directions are also obtained and tabulated. Static deformation problems are then discussed and it is shown that in the particular case of homogeneous strains, the elastic constants group themselves in linear combinations which are equivalent to the elastic moduli of the theory in its familiar form. In wave-propagation, however, the strains and stresses are heterogeneous and hence all the elastic constants are involved and appear in linear combinations which are different and also larger in number than those which figure in the formulae for homogeneous deformations. These results are completely in accord with the consequences of the atomistic theory based on interatomic forces of the most general type.

Appendix

As is well known, the theory of the elasticity of solids in its present form was initiated by Cauchy who put forth the fundamental idea of expression elastic stresses and strains in the manner adopted in the phenomenological theory, and also developed the theory on an atomistic basis. Later theorists, notably Green, Stokes and Kelvin retained Cauchy's method of specifying elastic stresses and strains but adopted a purely phenomenological approach. The view advocated by them that a completely aelotropic body would have twenty-one elastic constants and not fifteen as derived by Cauchy received general acceptance.

In a paper published in these *Proceedings* some years ago by one of us (Raman, 1943), a theory of the dynamic behaviour of crystal lattices was developed based on the assumption of interatomic forces of the most general type. In subsequent years, the consequences of that theory was worked out in detail for the case of diamond and confirmed by a series of spectroscopic investigations on the scattering of light, the luminescence and infra-red absorption by that crystal. The high values of the interatomic force-constants disclosed by the spectroscopic behaviour of diamond were evidently related to its exceptional elastic behaviour. In the endeavour to place this relationship on a quantitative basis, a fresh approach was made by one of us (Viswanathan, 1954) to the atomistic theory of the elasticity of crystals, both from the static and dynamic points of view, and some surprising results emerged. Contrary to the assertion made in the papers of Max Born and his collaborators which also finds a place in their recent book (Born and Kun Huang, 1954), no difficulty was encountered in expressing the energy of static deformations in terms of interatomic forces of the most general type. It was found that this expression contained forty-five independent constants, but for homogeneous or irrotational strains they appeared in twenty-one distinct linear combinations. The dynamics of wave-propagation in crystals was also investigated and it was shown that the expressions for the wave-velocity contained the same forty-five constants but in different linear combinations. The work of Born and his school on the dynamic problem was critically examined and it was shown that the assumptions made by them in the attempt to reduce the forty-five constants which appeared in their theory to twenty-one had no theoretical justification.

The results of Born and his school were also contradicted by Laval in some recent publications (1951). More recently till, a series of papers have been published by Le Corre in which Laval's ideas have been further developed. On reading those papers, one obtains the impression that their author believes the results of the atomistic and phenomenological approaches to differ essentially. For example, in order to account for the non-symmetric character of the stress tensor, internal couples are postulated to balance the differences in the angular momenta. We may remark that there is no room for such a postulate, since the analytical specification of the stresses in terms of the tensor components should

itself suffice to describe the state of the solid completely. In the last paper of the series, a statement also appears that an atomistic approach is essential to solve such familiar problems in elasticity as torsion and flexure.

In conclusion, we have to thank Mr A K Ramdas for his help in the preparation of the tables appearing in the paper.

References

1. Raman C V and Viswanathan K S *Proc. Indian Acad. Sci.* **42** 1 (1955).
2. Bhagavantam S and Venkatrayudu T *Theory of Groups and Its Application to Physical Problems* (Chapter XVI).
3. Love A E H *The Mathematical Theory of Elasticity* (page 104).
4. Hearmon R F S *Rev. Mod. Phys.* **18** 409 (1946).
5. Raman Sir C V *Proc. Indian Acad. Sci.* **A18** 237 (1943).
6. Viswanathan K S *ibid.* **A35** 196 (1954).
7. Born M and Kun Huang *The Dynamical Theory of Crystal Lattices* 1954.
8. Laval J C.R. (Paris) **232** 1947 (1951).
9. Lava J *Etat solide (Rapports et Discussions), Congress Solvay Bruxelles, Stoops* 273.
10. Le Corre Y C.R. *Acad. Sci. (Paris)* **236** 1903 (1953).
11. Le Corre Y *Bull. Soc. Fr. Mineral* **76** 464 (1953).
12. Le Corre Y *ibid.* **77** 1363 and 1393 (1954).
13. Le Corre Y *ibid.* **78** 33 (1955).