

The elasticity of crystals*

The materials used in engineering construction are mostly polycrystalline solids and their elastic behaviour is of the utmost practical importance. It follows that the subject of the elasticity of crystals is of more than merely academic interest. Of recent years the importance of its study has greatly been enhanced by several circumstances. The experimenter today can in many cases work with synthetically prepared crystals of large size and good quality. He has at his disposal several new techniques enabling him to determine their elastic behaviour and obtain precise results. These techniques are mostly based upon the production of waves or standing oscillations in the crystal with the aid of piezoelectric oscillators. These latter oscillators are themselves of importance in technical acoustics and communication engineering. The subject also stands in the closest relation to the structure of crystals as revealed by X-ray diffraction and spectroscopic studies. It is thus an integral part of the rapidly developing physics of the solid state.

2. The notions of stress and strain

The science of elasticity is based on the fundamental notions of stress and strain and—subject to a restriction on their magnitude—on the proportionality between them known as Hooke's law. The precise definition of stress and strain is thus a matter of fundamental importance. Such definitions have necessarily to be comprehensive. They have to cover cases where their magnitudes vary from point to point within the crystal and also cases in which the stresses and strains vary with time as in the theory of wave-propagation. It is essential, further, that they take account of the elastic anisotropy which all crystals exhibit, in other words, the fact that the effect of an impressed force depends on the direction in which it is applied.

An important remark which should be made here is that it is unnecessary to introduce atomistic considerations in defining stress or strain. This is obvious since the phenomena with which we are concerned are open to macroscopic

*1. "On the theory of the elasticity of crystals," by Sir C V Raman and Dr K S Viswanathan.

2. "Evaluation of the four elastic constants of some cubic crystals," by Sir C V Raman and D Krishnamurti. Memoir Nos. 73 and 76 of the Raman Research Institute, Bangalore, *Proc. Indian Acad. Sci.* 42, 51 and 111 (1955).

observation. To take account of the variability of stress and strain with the location we define these quantities in relation to a particular point within the solid. The legitimacy of this procedure rests upon the fact that it is possible to imagine the volume of the substance to be divided into elements of such small dimensions that each element can be regarded as a mass particle and yet is large enough to justify its physical properties being assumed to be the same as those of the material in bulk. We are thereby enabled to specify the position of any volume element by its three co-ordinates in space and its state of equilibrium or of motion in terms of simple forces or tractions acting on the volume element.

3. The elastic constants

The foregoing remarks are preliminary to a specification of stress and strain which is logically consistent with the approach made to the subject. We define stress in terms of the tractive force assumed to act on an infinitesimal area drawn through a given point within the solid. Since this area can be set normal to each of the three co-ordinate axes in turn and for each such setting the acting force can be resolved into three components parallel to these axes respectively, we have nine components of stress. Likewise, strain is expressed in terms of the difference in displacements of two neighbouring points within the solid. Since the line joining these two points can be set parallel to each of the three co-ordinate axes in turn and the difference of their displacements in each case can itself be resolved along each of these axes in turn, we have nine components to deal with. The stress-strain relationships of proportionality would in the general case thus involve 9×9 or 81 elastic constants. The well known law of reciprocity which enables us to

Table 1

Crystal system	Point group (Schoenflies notation)	No. of elastic constants		
		General	Dynamic	Classical
Triclinic	All	45	36	21
Monoclinic	All	25	20	13
Orthorhombic	All	15	12	9
Tetragonal	C_4, S_4, C_{4h}	13	10	7
	$D_4, C_{4v}, D_{2d}, D_{4h}$	9	7	6
Trigonal	C_3, S_6	15	12	7
	D_3, C_{3v}, D_{3d}	10	8	6
Hexagonal	C_6, C_{3h}, C_{6h}	11	8	5
	$D_6, C_{6v}, D_{3h}, D_{6h}$	8	6	5
Cubic	T, T_h	5	4	3
	O, T_d, O_h	4	3	3

interchange the directions of force and displacement without change in the constant of proportionality between them results in the number 81 being reduced to $(9 + 36) = 45$ constants in all. Thus, it requires 45 elastic constants to describe the elastic behaviour of a triclinic crystal. For crystals of other classes, the number of independent constants is diminished by reason of their symmetry properties, the more so the higher the symmetry of the crystal. The number of independent elastic constants in each case can be readily worked out using the formulae based on group theory given by Bhagavantam. Table 1 exhibits the situation thus disclosed. The first column shows the symmetry class in the usual language of crystallography, while column 2 shows the subdivisions of those classes grouped together according to their elastic behaviour. The third column shows the number of independent elastic constants for these sub-classes.

4. Wave-propagation in crystals

Writing down the equations of motion of the volume of elements of the medium in terms of the space variations of the stress components acting upon them, one can investigate the propagation of waves through the material. It emerges that in any given direction within the solid, three types of waves can be propagated, their velocities being different in each case and also varying with the direction. The wave velocity for each of the three types and for any particular direction of propagation is expressible as a function of the direction and of certain linear combinations of the elastic constants. The number of these combinations is less than the number of general elastic constants in each case. The number can be calculated from formulae based on group theory and is shown in the fourth column of table 1.

5. Remarks on the classical theories

Cauchy, the celebrated French mathematician of the 19th century, in his memoir presented to the Academy of Sciences at Paris in the year 1822 proposed a reduction of the number of components of stress and strain from 9 to 6 in each case. His arguments will be found reproduced in numerous text-books and indeed they form the basis of the mathematical theory of elasticity as hitherto developed. A critical examination shows however that those arguments are not sustainable. In the case of the strain components, the reduction was sought to be justified by eliminating movements which were thought to be rigid body rotations. Actually the quantities eliminated are differential rotations of the same nature as those which appear in the deformation of solids by torsion or flexure and which are quite as much a part of the elastic deformations as extensions and contractions. Hence their elimination is not justified. The argument on which the reduction of

the number of stress components from 9 to 6 was based was that the angular momenta of the tractions acting on a volume element taken about each of the coordinate axes in turn and summed up should vanish. But since by definition the stresses are assumed to be in the nature of tractive forces acting on volume elements small enough to be regarded as single mass particles, no consideration of angular momenta is called for. Indeed, once we accept the definition of stress and strain, it becomes logically imperative to take account of all the nine components of each.

On the basis Cauchy's assumptions the stress-strain relations of proportionality are $6 \times 6 = 36$ in number and these by application of the reciprocity relationship reduce to $6 + 15 = 21$ in all for a triclinic crystal. Their number is smaller for the crystals of higher symmetry classes and is shown in column 5 of table 1 against each of them. The reduction in number of the stress and strain components from 9 to 6 is in effect equivalent to assuming that differential rotations within the solid play no part in the theory of elasticity and to imposing a corresponding restriction on the nature of the acting stresses. As already remarked, differential rotations play a fundamental role both in static deformations, especially in torsion, as also generally in wave-propagation. In other words, the classical theory is of restricted validity confined to certain types of static deformation and to particular cases of wave propagation. Since however it has been employed to interpret experimental data in other cases as well, it is useful to express the 21 constants in terms of the more general 45 constants, thereby enabling the latter to be evaluated from the existing data of experiments.

6. The data of experiment

As will be seen from table 1 the simplest cases of all are crystals belonging to the *Td* and the *Oh* classes of the cubic system. The general theory gives four elastic constants which may be designated as respectively d_{11} , d_{12} , d_{44} and d_{45} while in the classical theory we have only three constants which have been designated as C_{11} , C_{12} and C_{44} . The linear combinations of the elastic constants which determine the velocities of wave propagation are in the former theory d_{11} , d_{44} and $(d_{12} + d_{45})$ while in the classical theory they are C_{11} , C_{44} and $(C_{12} + C_{44})$. Likewise, the expressions for the bulk modulus in the new and the old theory are respectively $(d_{11} + 2d_{12})/3$ and $(C_{11} + 2C_{12})/3$. Since the number of elastic constants of these classes is four, while the number of linear combinations that can be determined by dynamic measurements is three, it follows that at least one additional determination by static methods is necessary to enable all the four constants to be evaluated. The most appropriate of such determinations appears to be the bulk-modulus of which very precise measurements have been made by Bridgman and his collaborators at Harvard. It is necessary of course to correct the isothermal static value of the constant to obtain the adiabatic bulk modulus.

Table 2. Elastic constants in 10^{11} dynes/cm².

Substance	C_{11}	C_{12}	C_{44}	d_{11}	d_{12}	d_{44}	d_{45}
NaCl	4.877	1.232	1.269	4.877	1.34	1.269	1.16
KCl	4.038	0.663	0.628	4.038	0.779	0.628	0.512
KBr	3.455	0.56	0.507	3.455	0.655	0.507	0.412
NaBr	3.87	0.97	0.97	3.87	1.22	0.97	0.72
LiF	11.9	5.38	5.34	11.9	4.5	5.34	6.22
MgO	28.76	8.74	15.14	28.76	11.27	15.14	12.61
AgCl	6.05	3.64	0.624	6.05	3.482	0.624	0.782
Diamond	95	39	43	95	35.9	43	46.1
Ge	12.88	4.825	6.705	12.88	4.04	6.705	7.49
Si	16.56	6.386	7.953	16.56	6.56	7.953	7.78
ZnS	10.79	7.22	4.12	10.79	6.17	4.12	5.17
CaF ₂	16.6	4.87	3.58	16.6	4.29	3.58	4.16
Al	10.56	6.39	2.853	10.56	6.29	2.853	2.953
Cu	16.92	12.25	7.55	16.92	12.81	7.55	6.99
Ni	25.26	15.51	12.3	25.26	16.01	12.3	11.8
Ag	12.4	9.34	4.61	12.4	8.89	4.61	5.06

Many other points have to be borne in mind: the bulk modulus reduced to zero pressures should be used; both the static and dynamic determinations have to be reduced to the same temperature of observation and finally the nature of the material used in the two cases has to be comparable.

In table 2 are shown, for 16 different crystals of the Td and Oh classes, the values of the four elastic constants calculated in the manner explained. The three constants of the older theory are also shown in the table. The latter are those which appeared to be the most reliable values obtained by ultrasonic techniques, while the former were obtained by combining them with the value for the adiabatic bulk-modulus. The values of C_{11} and d_{11} are in each case identical; likewise those of C_{44} and d_{44} . But C_{12} and d_{12} are different and such difference is a measure of the failure of the three-constant theory to represent the actual elastic behaviour of the crystal. The difference between d_{44} and d_{45} also expresses the same situation in another way.

Certain general features emerge from the table. For all the four alkali halides which are soluble in water, C_{12} is less than d_{12} and likewise d_{45} is less than d_{44} . The regularity of behaviour taken in conjunction with the reliability of the data in these cases makes it clear that these differences are real and justify us in concluding that the elastic behaviour of cubic crystals cannot be expressed in terms of three constants, but needs four. Diamond, germanium, zinc blende and fluor spar also exhibit a parallel behaviour which is the reverse of that shown by the four water-soluble alkali-halides. In their cases, C_{12} is decidedly greater than

d_{12} , while *per contra* d_{44} is less than d_{45} and these differences are numerically more striking than in the case of the alkali-halides. Magnesium oxide for which the data are reliable exhibits a noteworthy behaviour; the differences between C_{12} and d_{12} and likewise between d_{44} and d_{45} are in the same sense as in the alkali halides but proportionately much larger. Differences of the same order of magnitude but in the opposite sense is shown by lithium fluoride. In the case of the metals crystallizing in the face-centred cubic system, we also find differences between C_{12} and d_{12} and between d_{44} and d_{45} , but they are not always in the same sense. This is a feature which need not surprise us in view of the very great differences exhibited by these metals in other respects.

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