ELASTIC BEHAVIOUR OF MATTER UNDER VERY HIGH PRESSURES

Simple Shear

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Abstract

This paper deals with the study of the elastic behaviour of substances which are initially subjected to a finite simple shear. Following the earlier work of Bhagavantam and Chelam on the formulation of an effective elastic energy to deal with such cases, expressions have been derived for the effective elastic constants in the case of a substance of cubic symmetry.

Introduction

In previous papers (Bhagavantam and Chelam 1960) a convenient approach to the problem of elastic behaviour of matter under high pressures was indicated. The case of a finite simple shear was excluded from those papers, as the general theory would have become very complicated if it were to cover this case as well. This is because a simple shear has to be specified by an unsymmetrical Jacobian Matrix. In all other cases so far considered, this matrix is symmetric. The case of a simple shear acting on a substance of cubic symmetry is now considered separately and expressions derived for the 'effective elastic constants'. The results can be easily simplified so as to be applicable to an isotropic substance, by using the appropriate additional symmetry relations

Strain Matrix for Finite Shear

For details of the notation employed here, reference may be made to the papers cited earlier and also to Murnaghan (1951). We take the undeformed state of the body (State I) and consider its finite deformation by a simple shear to State II, the displacement being specified by

$$x_0 = a + \theta b \; ; \quad y_0 = b \; ; \quad z_0 = c \qquad [1]$$

Here a, b, c are the initial coordinates of a typical particle and x_0, y_0, z_0 the coordinates of the same particle after the prescribed deformation, referred to a convenient set of axes. This deformation is thus given by the unsymmetrical matrix

$$J_0 = \begin{vmatrix} 1 & \theta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \qquad [2]$$

The strain matrix appropriate to such deformation is given by the Murnaghan formula $\eta_0 = \frac{1}{2}(J_0^* J_0 - E_3)$ where J_0^* is the transpose of J_0 and E_3 the unit matrix of dimension 3. Hence the strain matrix for State II is given by

$$\eta_0 = \begin{vmatrix} 0 & \frac{1}{2}\theta & 0 \\ \frac{1}{2}\theta & \frac{1}{2}\theta^2 & 0 \\ 0 & 0 & 0 \end{vmatrix} \qquad [3]$$

We now impose an infinitesimal deformation specified by the displacement [4] on State II, so as to study the elastic behaviour of the substance for such deformations from State II.

$$\begin{aligned} x &= (1+\delta_1)\, x_0 + \delta_6\, y_0 + \delta_5\, z_0 \\ y &= \delta_6\, x_0 + (1+\delta_2)\, y_0 + \delta_4\, z_0 \\ z &= \delta_5\, x_0 + \delta_4\, y_0 + (1+\delta_3) z_0 \end{aligned} \qquad [4]$$

Thus x, y, z are the final positions of the particle and the Jacobian J_δ specifying displacement from State II to final State III is

$$J_\delta = \begin{vmatrix} 1+\delta_1 & \delta_6 & \delta_5 \\ \delta_6 & 1+\delta_2 & \delta_4 \\ \delta_5 & \delta_4 & 1+\delta_3 \end{vmatrix} \qquad [5]$$

From [1] and [4], it is easy to see that the Jacobian corresponding to the total deformation from State I to State III is given by

$$J = J_\delta J_0 \qquad [6]$$

Hence the corresponding strain matrix is given by

$$\eta = \tfrac{1}{2}[(J_\delta J_0)^* J_\delta J_0 - E_3] = [\tfrac{1}{2} J_0^* J_\delta^* J_\delta J_0 - \tfrac{1}{2} E_3] = J_0^* (\delta\eta + \tfrac{1}{2} E_3) J_0 - \tfrac{1}{2} E_3 \qquad [7]$$

where $\delta\eta$ is the symmetric matrix $\frac{1}{2}[J_\delta^* J_\delta - E_3]$ with elements given by

$$\begin{aligned} \delta\eta_1 &= \delta_1 + \tfrac{1}{2}(\delta_1^2 + \delta_6^2 + \delta_5^2) & \delta\eta_4 &= \delta_4 + \tfrac{1}{2}(\delta_2\delta_4 + \delta_3\delta_4 + \delta_5\delta_6) \\ \delta\eta_2 &= \delta_2 + \tfrac{1}{2}(\delta_2^2 + \delta_4^2 + \delta_6^2) & \delta\eta_5 &= \delta_5 + \tfrac{1}{2}(\delta_1\delta_5 + \delta_3\delta_5 + \delta_4\delta_6) \\ \delta\eta_3 &= \delta_3 + \tfrac{1}{2}(\delta_3^2 + \delta_4^2 + \delta_5^2) & \delta\eta_6 &= \delta_6 + \tfrac{1}{2}(\delta_1\delta_6 + \delta_2\delta_6 + \delta_4\delta_5) \end{aligned} \qquad [8]$$

Hence if $\Delta\eta$ is the matrix denoting the increase in the strain elements from State II (*i e*) putting $\eta = \eta_0 + \Delta\eta$, we get from [7] and [3]

$$\triangle\eta = J_0^* \,\delta\eta\, J_0 \qquad [9]$$

$$= \begin{vmatrix} 1 & 0 & 0 \\ \theta & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \begin{vmatrix} \delta\eta_1 & \delta\eta_6 & \delta\eta_5 \\ \delta\eta_6 & \delta\eta_2 & \delta\eta_4 \\ \delta\eta_5 & \delta\eta_4 & \delta\eta_3 \end{vmatrix} \begin{vmatrix} 1 & \theta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \qquad [10]$$

It will be observed that where as $\delta\eta$ is an increase of strain elements measured with reference to conditions of State II, $\triangle\eta$ gives the values of such increases when referred to State I. From [10] we get

$$\begin{aligned} \triangle\eta_1 &= \delta\eta_1 & \triangle\eta_4 &= \theta\delta\eta_5 + \delta\eta_4 \\ \triangle\eta_2 &= \theta^2\,\delta\eta_1 + 2\theta\delta\eta_6 + \delta\eta_2 & \triangle\eta_5 &= \delta\eta_5 \\ \triangle\eta_3 &= \delta\eta_3 & \triangle\eta_6 &= \theta\delta\eta_1 + \delta\eta_6 \end{aligned} \qquad [11]$$

STRAIN ENERGY AND ITS INCREASE DUE TO ADDITIONAL DEFORMATION

The strain energy ϕ per unit volume of State I developed upto cubic powers of the strain components is given, for a substance of cubic symmetry, by [Ref. 1]

$$\begin{aligned} \phi = {} & \tfrac{1}{2}\, c_{11}\left(\eta_1^2+\eta_2^2+\eta_3^2\right) + c_{12}\left(\eta_1\eta_2+\eta_2\eta_3+\eta_3\eta_1\right) + 2c_{44}\left(\eta_4^2+\eta_5^2+\eta_6^2\right) \\ & + C_{111}\left(\eta_1^3+\eta_2^3+\eta_3^3\right) + C_{112}\left\{\eta_1\eta_2\left(\eta_1+\eta_2\right)+\eta_2\eta_3\left(\eta_2+\eta_3\right)+\eta_3\eta_1\left(\eta_3+\eta_1\right)\right\} \\ & + C_{123}\,\eta_1\eta_2\eta_3 + C_{456}\,\eta_4\eta_5\eta_6 + C_{144}\left(\eta_1\eta_4^2+\eta_2\eta_5^2+\eta_3\eta_6^2\right) \\ & + C_{155}\left\{\eta_1\left(\eta_5^2+\eta_6^2\right)+\eta_2\left(\eta_4^2+\eta_6^2\right)+\eta_3\left(\eta_4^2+\eta_5^2\right)\right\} \end{aligned} \qquad [12]$$

Here, all the η's are measured from State I When the substance attains State II, the η's attain values given by $\eta_1=\eta_3=\eta_4=\eta_5=0$, $\eta_2=\frac{1}{2}\theta^2$, $\eta_6=\frac{1}{2}\theta$, and substitution of these values in [12] gives the strain energy of State II. When each of these strain components increases further by $\triangle\eta_1$, $\triangle\eta_2 \ldots \triangle\eta_6$, the resulting increase in strain energy can be easily obtained from the Taylor expansion

$$\phi\left(\eta+\triangle\eta\right)-\phi\left(\eta\right) = \sum\frac{\partial\phi}{\partial\eta_r}\triangle\eta_r + \tfrac{1}{2}\sum\frac{\partial^2\phi}{\partial\eta_r\,\partial\eta_s}\triangle\eta_r\,\triangle\eta_s \qquad [13]$$

on neglecting higher powers of $\triangle\eta$. Here the derivatives of ϕ are to be computed at State II, (*i e.*) after obtaining the derivatives from [12] we set $\eta_2=\frac{1}{2}\theta^2$, $\eta_6=\frac{1}{2}\theta$ and all other η_r as zero. We thus get

$$\begin{aligned} \phi\left(\eta+\triangle\eta\right)-\phi\left(\eta\right) = {} & \theta^2\left(\tfrac{1}{2}c_{12}+\tfrac{1}{4}C_{155}\right)\triangle\eta_1 \\ & + \theta^2\left(\tfrac{1}{2}c_{11}+\tfrac{1}{4}C_{155}\right)\triangle\eta_2 + \theta^2\left(\tfrac{1}{2}c_{12}+\tfrac{1}{4}C_{144}\right)\triangle\eta_3 \end{aligned}$$

$$+ 2c_{44}\,\theta\,\Delta\eta_6 + \left(\tfrac{1}{2}\,c_{11} + \tfrac{1}{2}\,C_{112}\,\theta^2\right)\Delta\eta_1^2 + \left(\tfrac{1}{2}\,c_{11} + \tfrac{3}{2}\,C_{111}\,\theta^2\right)\Delta\eta_2^2$$
$$+ \left(\tfrac{1}{2}\,c_{11} + \tfrac{1}{2}\,C_{112}\,\theta^2\right)\Delta\eta_3^2 + \left(2c_{44} + \tfrac{1}{2}\,C_{155}\,\theta^2\right)\Delta\eta_4^2 + \left(2c_{44} + \tfrac{1}{2}C_{144}\,\theta^2\right)\Delta\eta_5^2$$
$$+ \left(2c_{44} + \tfrac{1}{2}C_{155}\,\theta^2\right)\Delta\eta_6^2 + \left(c_{12} + C_{112}\,\theta^2\right)\Delta\eta_1\Delta\eta_2 + \left(c_{12} + C_{112}\,\theta^2\right)\Delta\eta_2\Delta\eta_3$$
$$+ \left(c_{12} + \tfrac{1}{2}\,C_{123}\,\theta^2\right)\Delta\eta_3\Delta\eta_1 + \tfrac{1}{2}\,C_{456}\,\theta\,\Delta\eta_4\Delta\eta_5 + C_{144}\,\theta\,\Delta\eta_3\Delta\eta_6$$
$$+ C_{155}\,\theta\left(\Delta\eta_1\Delta\eta_6 + \Delta\eta_2\Delta\eta_6\right) \qquad [14]$$

In a simple shear, there is no change in volume involved from State I to state II. This is clear also by inspection of the determinant of J_0 which is 1. Hence $\phi(\eta + \Delta\eta) - \phi(\eta)$ may be eqated to ϕ', which gives the strain energy of the additional deformation per unit volume of State II. By using relations [11] we can express ϕ' in terms of $\delta\eta$ rather than $\Delta\eta$ and this gives us

$$\phi' = c_1'\,\delta\eta_1 + c_2'\,\delta\eta_2 + c_3'\,\delta\eta_3 + 2c_6'\,\delta\eta_6 + \tfrac{1}{2}\left(b_{11}\,\delta\eta_1^2 + b_{22}\,\delta\eta_2^2 + b_{33}\,\delta\eta_3^2\right)$$
$$+ 2\left(b_{44}\,\delta\eta_4^2 + b_{55}\delta\eta_5^2 + b_{66}\,\delta\eta_6^2\right) + b_{12}\,\delta\eta_1\,\delta\eta_2 + b_{23}\,\delta\eta_2\,\delta\eta_3 + b_{13}\,\delta\eta_1\,\delta\eta_3$$
$$+ 2\left(b_{45}\,\delta\eta_4\,\delta\eta_5 + b_{16}\,\delta\eta_1\,\delta\eta_6 + b_{26}\,\delta\eta_2\,\delta\eta_6 + b_{36}\,\delta\eta_3\,\delta\eta_6\right) \qquad [15]$$

where the values of the various coefficients are as under, retaining up to the squares only of the θ.

$$c_1' = \theta^2\left(\tfrac{1}{2}\,c_{12} + 2c_{44} + \tfrac{1}{4}\,C_{155}\right); \quad c_2' = \theta^2\left(\tfrac{1}{2}\,c_{11} + \tfrac{1}{4}\,C_{155}\right); \quad c_3' = \theta^2\left(\tfrac{1}{2}\,c_{12} + \tfrac{1}{4}\,C_{144}\right)$$
$$c_4' = 0; \qquad c_5' = 0; \qquad c_6' = \theta c_{44}$$
$$b_{11} = c_{11} + \theta^2\left(2c_{12} + 4c_{44} + C_{112} + 2C_{155}\right) \qquad b_{12} = c_{12} + \theta^2\left(c_{11} + C_{112} + C_{155}\right)$$
$$b_{22} = c_{11} + \theta^2\,3C_{111} \qquad b_{23} = c_{12} + \theta^2 C_{112}$$
$$b_{33} = c_{11} + \theta^2\,C_{112} \qquad b_{13} = c_{12} + \theta^2\left(c_{12} + \tfrac{1}{2}\,C_{123} + C_{144}\right)$$
$$b_{44} = c_{44} + \theta^2\,C_{155/4} \qquad b_{16} = \theta\left(c_{12} + 2c_{44} + \tfrac{1}{2}\,C_{155}\right)$$
$$b_{55} = c_{44} + \theta^2\left(c_{44} + \tfrac{1}{4}\,C_{144} + \tfrac{1}{4}\,C_{456}\right) \qquad b_{26} = \theta\left(c_{11} + \tfrac{1}{2}\,C_{155}\right)$$
$$b_{66} = c_{44} + \theta^2\left(c_{11} + \tfrac{5}{4}\,C_{155}\right) \qquad b_{36} = \theta\left(c_{12} + \tfrac{1}{2}\,C_{144}\right)$$
$$b_{45} = \theta\left(2c_{44} + \tfrac{1}{4}\,C_{456}\right)$$

There are thus 4 first order and 13 second order nonvanishing coefficients in [15]. When the substance is isotropic, we can obtain appropriate values in [16] by using the additional relations

$$c_{44} = \tfrac{1}{2}\left(c_{11} - c_{12}\right); \qquad C_{144} = 2C_{112} - C_{123}; \qquad C_{155} = 3C_{111} - C_{112};$$
$$C_{456} = 6\,C_{111} - 6\,C_{112} + 2\,C_{123}$$

Effective Elastic Constants and Effective Elastic Energy

On expressing each $\delta\eta$ in terms of $\delta_1, \delta_2 \ldots \delta_6$, by means of relations [8], we can write ϕ' as

$$\phi' = \Delta W + \phi_e$$

where
$$\Delta W = c_1' \delta_1 + c_2' \delta_2 + c_3' \delta_3 + 2c_4' \delta_4 + 2c_5' \delta_5 + 2c_6' \delta_6$$

and
$$\phi_e = \tfrac{1}{2}\left(c_{11}' \delta_1^2 + c_{22}'\delta_2^2 + c_{33}' \delta_3^2\right) + 2\left(c_{44}' \delta_4^2 + c_{55}' \delta_5^2 + c_{66}' \delta_6^2\right)$$
$$+ \left(c_{12}' \delta_1\delta_2 + c_{23}'\delta_2\delta_3 + c_{13}' \delta_1\delta_3\right) + 2\left(c_{45}'\delta_4\delta_5 + c_{16}'\delta_1\delta_6 + c_{26}' \delta_2\delta_6 + c_{36}' \delta_3\delta_6\right) \qquad [17]$$

Here the new constants c_{rs}' are connected with b_{rs} by the relations

$$c_{11}' = b_{11} + c_1' ; \qquad c_{22}' = b_{22} + c_2' ; \qquad c_{33}' = b_{33} + c_3'$$
$$c_{44}' = b_{44} + \tfrac{1}{4}\left(c_2' + c_3'\right), \qquad c_{55}' = b_{55} + \tfrac{1}{4}\left(c_1' + c_3'\right), \qquad c_{66}' = b_{66} + \tfrac{1}{4}\left(c_1' + c_2'\right)$$
$$c_{12}' = b_{12} ; \qquad c_{23}' = b_{23} ; \qquad c_{13}' = b_{13}$$
$$c_{45}' = b_{45} + \tfrac{1}{2} c_6' ; \qquad c_{16}' = b_{16} + \tfrac{1}{2} c_6' ; \qquad c_{26}' = b_{26} + \tfrac{1}{2} c_6' ,$$
$$c_{36}' = b_{36} \qquad [18]$$

In the earlier papers, it has been pointed out that the first orders constants $c_1', c_2' \ldots c_6'$ represent the six components of the initial stress $T_1, T_2 \ldots T_6$, associated with the deformation of State II and that ΔW is thus the work done by them during the small displacement under consideration. Hence $\phi_e = \phi' - \Delta W$ represented the total potential energy associated with the 'δ' deformation, and this was also called the effective elastic energy, the coefficients in the same being the effective elastic constants. Accordingly, we can now give expressions for the initial stresses $T_1, T_2 \ldots T_6$, and also for the effective elastic constants c_{rs}' from [18].

$$T_1 = c_1' = \theta^2\left(\tfrac{1}{2} c_{12} + \tfrac{1}{4} C_{155} + 2 c_{44}\right) \qquad T_4 = 0$$
$$T_2 = c_2' = \theta^2\left(\tfrac{1}{2} c_{11} + \tfrac{1}{4} C_{155}\right) \qquad T_5 = 0$$
$$T_3 = c_3' = \theta^2\left(\tfrac{1}{4} c_{12} + \tfrac{1}{4} C_{144}\right) \qquad T_6 = c_6' = \theta\, c_{44}$$
$$c_{11}' = b_{11} + T_1 = c_{11} + \theta^2\left(\tfrac{5}{2} c_{12} + 6 c_{44} + C_{112} + \tfrac{9}{4} C_{155}\right) \qquad [i]$$
$$c_{22}' = b_{22} + T_2 = c_{11} + \theta^2\left(c_{11}/2 + 3 C_{111} + \tfrac{1}{4} C_{155}\right) \qquad [ii]$$
$$c_{33}' = b_{33} + T_3 = c_{11} + \theta^2\left(\tfrac{3}{2} c_{12} + C_{112} + \tfrac{1}{4} C_{144}\right) \qquad [iii]$$
$$c_{44}' = b_{44} + \tfrac{1}{4}\left(T_2 + T_3\right) = c_{44} + \theta^2\left(\tfrac{1}{8} c_{11} + \tfrac{1}{8} c_{12} + \tfrac{1}{16} C_{144} + \tfrac{5}{16} C_{155}\right) \qquad [iv]$$
$$c_{55}' = b_{55} + \tfrac{1}{4}\left(T_3 + T_1\right) = c_{44} + \theta^2\left(\tfrac{1}{2} c_{12}' + \tfrac{3}{2} c_{44} + \tfrac{5}{16} C_{144} + \tfrac{1}{16} C_{155} + \tfrac{1}{4} C_{456}\right) \qquad [v]$$
$$c_{66}' = b_{66} + \tfrac{1}{4}\left(T_1 + T_2\right) = c_{44} + \theta^2\left(\tfrac{9}{8} c_{11} + \tfrac{3}{8} c_{12} + \tfrac{1}{2} c_{44} + \tfrac{11}{8} C_{155}\right) \qquad [vi]$$

$$c'_{12} = b_{12} = c_{12} + \theta^2 \left(c_{11} + C_{112} + C_{155}\right) \qquad [\text{vii}]$$

$$c'_{23} = b_{23} = c_{12} + \theta^2 C_{112} \qquad [\text{viii}]$$

$$c'_{13} = b_{13} = c_{12} + \theta^2 \left(c_{12} + \tfrac{1}{2} C_{123} + C_{144}\right) \qquad [\text{ix}]$$

$$c'_{45} = b_{45} + \tfrac{1}{2}\, T_6 = \theta \left(\tfrac{5}{2}\, c_{44} + \tfrac{1}{4}\, C_{456}\right) \qquad [\text{x}]$$

$$c'_{16} = b_{16} + \tfrac{1}{2}\, T_6 = \theta \left(c_{12} + \tfrac{5}{2}\, c_{44} + \tfrac{1}{2}\, C_{155}\right) \qquad [\text{xi}]$$

$$c'_{26} = b_{26} + \tfrac{1}{2}\, T_6 = \theta \left(c_{11} + \tfrac{1}{2}\, c_{44} + \tfrac{1}{2}\, C_{155}\right) \qquad [\text{xii}]$$

$$c'_{36} = b_{36} = \theta \left(c_{12} + \tfrac{1}{2}\, C_{144}\right) \qquad [\text{xiii}]$$

$$c'_{14} = c'_{15} = c'_{24} = c'_{25} = c'_{34} = c'_{35} = 0\,; \quad c'_{46} = c'_{56} = 0$$

The expressions for c'_{rs} given above, can be computed if the third order constants C_{111}, etc, are known. Sometimes, retention of the form of c'_{rs} in terms of the initial stresses (such as $c'_{11} = b_{11} + T_1$) would be useful, as this form reveals the dependence of the effective constants on the initial stress. It has already been mentioned that such meagre data as is available on third order constants seems to suggest that they are all negative and an order of magnitude larger than the second order ones. On this basis, it would seem that most of the effective elastic constants decrease with application of a finite shear. For a further discussion of this aspect, ϕ_e will have to be separated as sums of squares (normal coordinates) This question together with application to specific cases will be examined in a separate communication.

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