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EFFECTIVE ELASTIC MODULI UNDER HYDROSTATIC STRESS—I. QUASI-HARMONIC THEORY*

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Abstract—Fourth-order finite strain expressions for the effective elastic moduli of a solid under hydrostatic stress are derived from a general expression for effective elastic moduli. Expressions in terms of the strain tensors **E** and $\boldsymbol{\eta}$ are given. The expressions are then written in terms of the moduli and their pressure derivatives evaluated at an arbitrary reference state. The temperature dependence of these expressions is derived from the fourth-order quasi-harmonic expression for the lattice vibrational energy. Some general thermodynamic relations are derived between the parameters which specify the thermal effects and the pressure and temperature derivatives of the elastic moduli at the reference state. General relations between isothermal and isentropic elastic moduli and their pressure and temperature derivatives are also given. Much of the development is valid for materials of arbitrary symmetry, but the complete development is given only for materials of cubic symmetry.

1. INTRODUCTION

In a previous paper[1], henceforth referred to as Paper I, finite strain equations were derived giving pressure in solids as a function of volume and temperature, the thermal contribution being evaluated in the quasi-harmonic approximation, which results from the fourth-order anharmonic theory of lattice dynamics[2]. Paper I was a reconsideration of the theory given by Thomsen[3]. As Thomsen[4] generalized his theory, so this paper generalizes Paper I to give the effective elastic moduli of a solid as functions of volume and temperature.

A number of points which were made in Paper I carry directly over to the present treatment, and so these points will not be discussed in detail here. In particular, it may be noted that general finite strain relations may be written in an implicitly frame-indifferent form in terms of a whole class of frame-indifferent strain tensors, and not just in terms of the "Lagrangian" strain tensor, $\boldsymbol{\eta}$ (defined later)[5]. Also, that the finite strain expansion of quasi-harmonic thermal contributions may be terminated two orders earlier than the expansion of the static lattice contributions, and that the reference state will again be left arbitrary. The equations will again be developed in terms of the particular strain tensors $\boldsymbol{\eta}$ and **E**. It should again be emphasized that the frame-indifferent analogue, **E**, of the "Eulerian" strain tensor, $\boldsymbol{\epsilon}$, should be used rather than $\boldsymbol{\epsilon}$, in general. Equations in terms of the displacement gradient, **e** (defined later), will not be developed here. They were useful to the discussion in Paper I, but are not essential to the development.

The equations developed in Paper I can be generalized in two ways—by including the effects of non-hydrostatic stress, and by considering anisotropic materials. A number of authors have discussed the various ways in which second- and higher-order elastic constants (which arise when arbitrary large stresses are considered) may be defined, and their relationship with the "effective" elastic moduli (which arise when infinitesimal stresses are added to prevailing large stresses) [e.g. 3, 6–13]. In general, materials cannot sustain very large non-hydrostatic stresses, and, especially in geophysics, the case of most interest is that of an infinitesimal non-hydrostatic stress superimposed on an arbitrarily large hydrostatic stress. Accordingly, equations will be developed directly for this special case, without reference to the more general treatments. Although much of this paper is valid for materials of arbitrary symmetry, parts of the treatment are greatly simplified by considering only isotropic materials or materials of cubic symmetry, for which the response to a hydrostatic stress is an isotropic

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strain, which can be specified with a single scalar strain parameter.

The treatment separates into three parts. First, the appropriate finite strain expressions for the effective elastic moduli are derived and written in terms of the moduli and their pressure derivatives at zero pressure. Second, the temperature dependence of these moduli is derived from lattice dynamics. Third, some general thermodynamic relations are derived between the equation of state parameters and the elastic moduli and their pressure and temperature derivatives, and between isothermal and isentropic elastic moduli and their pressure and temperature derivatives.

2. EFFECTIVE ELASTIC MODULI UNDER HYDROSTATIC STRESS

In this section, exact general expressions for effective elastic moduli under arbitrary prestress [e.g. 7, 10] are specialized to the case of hydrostatic prestress and, further, to the case of a material of cubic symmetry. The general expressions can be derived by considering either the response of a prestressed material to a further infinitesimal stress, or the equations governing small amplitude waves. The expressions, after specialization, will also be written explicitly in terms of the particular finite strain measures to be used here, and the parameters in these expressions will be related to the pressure derivatives of the effective moduli.

The treatment requires measures of the finite strain induced by the large prestress and of the additional superposed infinitesimal strain. Consider a point in the material which, in the "natural", i.e. unstressed, state has position vector (referred to Cartesian axes) $\mathbf{a} = (a_1, a_2, a_3)$. Denote its position vector after the material is subjected to the prestress as $\mathbf{X}$, and its position vector after the additional infinitesimal stress as $\mathbf{x}$. Then the displacement gradients $\mathbf{e}$, $\mathbf{f}$ and $\mathbf{u}$ may be defined by

$$x_i - a_i = e_{ij}a_j = f_{ij}x_j, \tag{1}$$

$$x_i - X_i = u_{ij}X_j, \tag{2}$$

where u_{ij} is infinitesimal, all quantities are referred to the same Cartesian axes, and the summation convention for repeated indices is assumed.

The Cauchy stress tensor, $\mathbf{T}$, is related, in general, to the Helmholtz free energy, A, and the density, ρ, of a material by [14, Section 82]

$$T_{ij} = \rho\left(\frac{\partial A}{\partial u_{ij}}\right)_T, \tag{3}$$

and the effective elastic moduli are [7]

$$C_{ijkl} = \frac{\partial T_{ij}}{\partial u_{kl}} \tag{4a}$$

$$= \rho\frac{\partial^2 A}{\partial u_{ij}\partial u_{kl}} - T_{ij}\delta_{kl}. \tag{4b}$$

In deriving (4b), the following relation [4] was used:

$$\frac{\partial \rho}{\partial u_{kl}} = -\rho\delta_{kl}. \tag{5}$$

The moduli defined by (4a) are isothermal or isentropic according to whether the derivative is taken isothermally or isentropically.

Thurston [7] showed that in the special case of hydrostatic prestress the effective moduli are identically given by either $\mathbf{C}$ or $\mathbf{c}$:

$$c_{ijkl} \equiv \frac{\partial T_{ij}}{\partial s_{kl}} = C_{ijkl} \tag{6}$$

where $\mathbf{s}$ is the symmetric component of $\mathbf{u}$:

$$s_{ij} = \frac{1}{2}(u_{ij} + u_{ji}),\quad \omega_{ij} = \frac{1}{2}(u_{ij} - u_{ji}), \tag{7}$$

and $\boldsymbol{\omega}$ is the antisymmetric component. Rewriting $\mathbf{u}$ as

$$u_{ij} = s_{ij} + \omega_{ij}$$
$$= \frac{1}{2}(s_{ij} + s_{ji} + \omega_{ij} - \omega_{ji}), \tag{8}$$

and differentiating, one obtains that

$$\frac{\partial}{\partial s_{kl}} = \frac{1}{2}\left(\frac{\partial}{\partial u_{kl}} + \frac{\partial}{\partial u_{lk}}\right). \tag{9}$$

Thus, in the special case of hydrostatic prestress, $T_{ij} = -P\delta_{ij}$, the effective elastic moduli can be written

$$c_{ijkl} = \frac{1}{2}\left(\frac{\partial T_{ij}}{\partial u_{kl}} + \frac{\partial T_{ij}}{\partial u_{lk}}\right) \tag{10a}$$

$$= \frac{1}{2}\rho\left(\frac{\partial^2 A}{\partial u_{ij}\partial u_{kl}} + \frac{\partial^2 A}{\partial u_{ij}\partial u_{lk}}\right) + P\delta_{ij}\delta_{kl}. \tag{10b}$$

Note that the form (10b) is symmetric under the interchange of subscript pairs (ij)–(kl), as well as under the interchange of k and l. This guarantees symmetry under the interchange of i and j. Thus the form (10) has the full Voigt symmetry of moduli associated with infinitesimal deformations.

The expressions (3) and (10) are referred, through $\mathbf{u}$, to the prestressed state described through the coordinates $\mathbf{X}$. They can be referred to the natural state, described by $\mathbf{a}$, through $\mathbf{e}$ or $\mathbf{f}$, defined by (1). The tensors $\mathbf{e}$ and $\mathbf{f}$ are not themselves frame-indifferent [5, 14], and so will not lead to constitu-