

view, material points in each of these configurations (in the same order) will be specified by position vectors  $\mathbf{R}$ ,  $\boldsymbol{\pi}$  and  $\mathbf{r}$ , with coordinates  $(X_\alpha)$ ,  $(\xi_k)$  and  $(x_k)$  respectively.

The deformations which take  $K_0 \rightarrow \tilde{K}$  and  $\tilde{K} \rightarrow K(t)$  are specified by the one to one mappings

$$\xi_k = \xi_k(X_\alpha), \quad X_\alpha = X_\alpha(\xi_k) \quad \alpha, k = 1, 2, 3,$$

$$\tilde{J} = \det|\partial \xi_k / \partial X_\alpha| \neq 0 \tag{3}$$

and

$$x_k = x_k(\xi_1, t), \quad \xi_k = \xi_k(x_1, t) \quad k, l = 1, 2, 3$$

$$t > 0$$

$$J' = \det|\partial x_k / \partial \xi_1| \neq 0. \tag{4}$$

The deformations specified by eqns. (3) and (4) are equivalent to passage from the natural to the current configurations such that

$$x_k = x_k(X_\alpha, t), \quad X_\alpha = X_\alpha(x_k, t)$$

$$J = \det|\partial x_k / \partial X_\alpha| \neq 0. \tag{5}$$

Mass densities  $\rho_0, \tilde{\rho}$  and  $\rho$  associated with configurations  $K_0, \tilde{K}$  and  $K(t)$  are related to the above Jacobians by

$$\tilde{J} = \rho_0 / \tilde{\rho}, \quad J' = \tilde{\rho} / \rho, \quad J = \rho_0 / \rho. \tag{6}$$

If  $\mathbf{u}(\boldsymbol{\pi}, t)$  represents the displacement vector of a material point currently occupying position  $\mathbf{r}(t)$ , which at time  $t=0$  had the initial position  $\boldsymbol{\pi}$ , then

$$u_k(\xi_1, t) = x_k(\xi_1, t) - \xi_k. \tag{7}$$

While  $K_0 \rightarrow \tilde{K}$  may be arbitrary, the superimposed time dependent deformations  $\tilde{K} \rightarrow K(t)$  are restricted to infinitesimal magnitudes, i.e.,  $\partial u_k / \partial \xi_1 \ll 1$  for all  $t > 0$ .

Relative to the initial configuration  $\tilde{K}$ , appropriate constitutive relations for a general theory of elasticity are given by<sup>13</sup>

$$\tilde{t}_{k1} = \tilde{J}^{-1} \left[ 2 \frac{\partial \Sigma}{\partial \tilde{C}_{\alpha\beta}} \right] \xi_{k,\alpha} \xi_{1,\beta} = \tilde{t}_{1k} \tag{8}$$

$$\tilde{T}_{\alpha\beta} = \tilde{J} \frac{\partial X_\alpha}{\partial \xi_k} \frac{\partial X_\beta}{\partial \xi_1} \tilde{t}_{k1} = 2 \frac{\partial \Sigma}{\partial \tilde{C}_{\alpha\beta}} = \tilde{T}_{\beta\alpha} \tag{9}$$

which are the Cauchy and Kirchhoff–Piola stress tensors respectively, where

$$\tilde{C}_{\alpha\beta} = \xi_{k,\alpha} \xi_{1,\beta} \delta_{k1} = \tilde{C}_{\beta\alpha}, \quad \xi_{k,\alpha} = \frac{\partial \xi_k}{\partial X_\alpha} \tag{10}$$

are the components of the Green–Cauchy deformation tensor. Constitutive relations of this kind

presume the existence of a strain energy density  $\Sigma$  which is a continuous and continuously differentiable function of the  $C_{\alpha\beta}$ . A mixed Kirchhoff–Piola stress tensor is also defined by the relations

$$\tilde{T}_{\alpha k} = \tilde{J} \frac{\partial X_\alpha}{\partial \xi_1} \tilde{t}_{k1} = \tilde{T}_{\alpha\beta} \xi_{k,\beta} = \frac{\partial \Sigma}{\partial \xi_{k,\alpha}} \tag{11}$$

which in the absence of body force are solutions of the equilibrium equations

$$\tilde{T}_{\alpha k,\alpha} = 0 \tag{12}$$

in the initial configuration  $\tilde{K}$ . In the current configuration  $K(t)$  these same stress components satisfy the equations of motion

$$T_{\alpha k,\alpha} = \rho_0 \frac{\partial^2 u_k}{\partial t^2}. \tag{13}$$

Expanding  $T_{\alpha k}$  in the displacement gradients about  $\tilde{K}$

$$T_{\alpha k} = \tilde{T}_{\alpha k} + [x_{1,\beta} - \xi_{1,\beta}] \left( \frac{\partial \tilde{T}_{\alpha k}}{\partial x_{1,\beta}} \right)_{\mathbf{r}=\boldsymbol{\pi}} + \dots$$

Since the displacement gradients  $u_{1,\beta} = (\partial u_1 / \partial \xi_m) \cdot \xi_{m,\beta}$ , with  $\partial u_1 / \partial \xi_m \ll 1$ ,

$$T_{\alpha k} = \tilde{T}_{\alpha k} + \tilde{A}_{k\alpha 1\beta} u_{1,\beta} \tag{14}$$

where in view of relations (10) and (11)

$$\tilde{A}_{k\alpha 1\beta} = \frac{\partial \tilde{T}_{\alpha k}}{\partial \xi_{1,\beta}} = \frac{\partial^2 \Sigma}{\partial \xi_{k,\alpha} \partial \xi_{1,\beta}}$$

$$= 4 \frac{\partial^2 \Sigma}{\partial \tilde{C}_{\alpha\gamma} \partial \tilde{C}_{\beta\delta}} \xi_{k,\gamma} \xi_{1,\delta} + 2 \frac{\partial \Sigma}{\partial \tilde{C}_{\alpha\beta}} \delta_{k1}. \tag{15}$$

Linearized equations of motion about the initial configuration in the form

$$[\tilde{A}_{k\alpha 1\beta} u_{1,\beta}]_{,\alpha} = \rho_0 \frac{\partial^2 u_k}{\partial t^2} \tag{16}$$

follow from eqns. (13) and (14), with due account taken of eqn. (12). Relative to the coordinates  $(\xi_k)$  of the initial state these equations transform to

$$\frac{\partial}{\partial \xi_p} \left[ \tilde{J}^{-1} \tilde{A}_{k\alpha 1\beta} \xi_{p,\alpha} \xi_{q,\beta} \frac{\partial u_1}{\partial \xi_q} \right] = \tilde{\rho} \frac{\partial^2 u_k}{\partial t^2} \tag{17}$$

after use of the identity  $(\partial / \partial \xi_p) [\tilde{J}^{-1} \xi_{p,\alpha}] = 0$ .

For initial deformations  $K_0 \rightarrow \tilde{K}$  which are homogeneous, corresponding deformation gradients  $\xi_{k,\alpha}$  as well as the strain energy derivatives in eqns. (15) have constant values throughout  $\tilde{K}$ . Equation (17) accordingly reduces to

$$\mathcal{J}^{-1} \tilde{A}_{k\alpha\lambda\beta} \xi_{p,\alpha} \xi_{q,\beta} \frac{\partial^2 u_1}{\partial \xi_p \partial \xi_q} = \tilde{\rho} \frac{\partial^2 u_k}{\partial t^2}. \quad (18)$$

If the displacements superimposed on the homogeneously deformed initial state are small amplitude plane waves

$$\mathbf{u} = \text{Re} [A e^{i(\bar{k}\mathbf{v} \cdot \mathbf{r} - \omega t)}] \quad (19)$$

where  $\bar{k}$  is the wave number,  $\mathbf{v}$  the propagation direction and  $\omega$  the frequency, then eqn. (19) will be solutions of the equations of motion (18) if

$$\tilde{A}_{k\alpha\lambda\beta} \xi_{p,\alpha} \xi_{q,\beta} v_p v_q A_1 = \left( \rho_0 \frac{\omega^2}{\bar{k}^2} \right) A_k = \rho_0 U^2 A_k \quad (20)$$

which is a wave propagation condition, with  $\omega^2/\bar{k}^2 = U^2$  the wave speeds. The second-order quantities

$$\begin{aligned} \tilde{Q}_{kl}(\mathbf{v}) &= \tilde{A}_{k\alpha\lambda\beta} \xi_{p,\alpha} \xi_{q,\beta} v_p v_q \\ &= \left\{ 4 \frac{\partial^2 \Sigma}{\partial \bar{C}_{\alpha\gamma} \partial \bar{C}_{\beta\delta}} \xi_{p,\alpha} \xi_{q,\beta} \xi_{k,\gamma} \xi_{l,\delta} \right. \\ &\quad \left. + 2 \frac{\partial \Sigma}{\partial \bar{C}_{\alpha\beta}} \xi_{p,\alpha} \xi_{q,\beta} \delta_{kl} \right\} v_p v_q \end{aligned} \quad (21)$$

define components of the acoustical tensor, which reduces the wave propagation condition to the familiar characteristic or eigenvalue equation

$$[\tilde{Q}_{kl}(\mathbf{v}) - (\rho_0 U^2) \delta_{kl}] A_1 = 0 \quad (22)$$

with  $\rho_0 U_{(i)}^2$ ,  $i=1, 2, 3$ , the eigenvalues and  $A_{(i)1}$  the corresponding eigenvectors (displacement amplitudes) which define the acoustical axes for a given propagation direction  $\mathbf{v}$ .

The character of the wave propagation depends on the nature of the matrix  $Q = (\tilde{Q}_{kl}(\mathbf{v}))$ . The eigenvalues and eigenvectors will be real valued if the components  $\tilde{Q}_{kl}(\mathbf{v})$  are real and symmetric. When the eigenvalues are real and distinct the associated eigenvectors define three real mutually orthogonal acoustic axes. If  $Q$  is furthermore a positive-definite matrix, *i.e.*, satisfies for every propagation direction  $\mathbf{v}$  the so-called strongly elliptic condition

$$\tilde{Q}_{kl}(\mathbf{v}) h_k h_l > 0 \quad (23)$$

for arbitrary non-zero vector  $\mathbf{h}$ , then the squared wave speeds will be positive, thereby admitting only real propagation speeds<sup>11,14</sup>.

Solids which respond elastically are characterized as hyperelastic if they possess a strain energy function which is continuous and continuously differentiable in some measure of the deformation. The

development given above makes this presumption, from which follows, as examination of eqns. (15) and (21) will show, symmetry of the acoustical tensor. Thus for hyperelastic solids the square of the wave speeds and the corresponding acoustical axes are real, and for each direction of propagation there exists at least one mutually orthogonal set of acoustic axes. The wave speeds will not necessarily be real however, unless condition (23) is additionally satisfied.

The strain energy function for the alkali metals at zero temperature, given explicitly by eqn. (1), is of course not presumed but derived. Being continuous and continuously differentiable in the deformation tensor  $C_{\alpha\beta}$ , it thereby characterizes these metals as hyperelastic and furthermore assures symmetry of the acoustic tensor and real values for the squared wave speeds. The necessary and sufficient conditions which guarantee positive squared wave speeds  $U_{(i)}^2$ , and thus real wave speeds  $U_{(i)}$ , for arbitrary initial homogeneous deformation can be obtained from condition (23), where eqn. (1) is used in conjunction with eqn. (21). This calculation however involves several dozens of terms and is much too complicated to permit any interpretation. In the next section theoretical wave speeds for several propagation directions superimposed on different states of initial compression are calculated. The values obtained are all real and positive indicating positive-definite character of the acoustic matrix  $Q$ .

As  $\bar{K} \rightarrow K_0$ ,  $(\xi_k) \rightarrow (X_k)$  and  $\xi_{k,\alpha} \rightarrow \delta_{k\alpha}$ . Using the strain energy density eqn. (1) with zero temperature lattice spacing values as given in Table 1,

$$2 \frac{\partial \Sigma}{\partial \bar{C}_{\alpha\beta}} = \bar{T}_{\alpha\beta} \rightarrow T_{\alpha\beta} = 0$$

in the natural state. The quantities (15) correspondingly reduce to

$$\tilde{A}_{k\alpha\lambda\beta} \rightarrow A_{\kappa\alpha\lambda\beta} = \left[ 4 \frac{\partial^2 \Sigma}{\partial C_{\kappa\alpha} \partial C_{\lambda\beta}} \right]_{C=I} = C_{\kappa\alpha\lambda\beta}$$

which are the second-order elastic coefficients.  $C$  is the matrix  $(C_{\alpha\beta})$  and  $I$  the identity matrix. Theoretical calculation of the  $C_{\kappa\alpha\lambda\beta}$  using eqn. (1) compare quite well with experimental values, particularly for potassium, rubidium, and cesium<sup>1,2</sup>. The equations of motion (16) likewise become the equations of motion of classical linear elasticity for small deformation about the natural configuration  $K_0$

$$A_{\kappa\alpha\lambda\beta} u_{\lambda,\beta\alpha} = \rho_0 \frac{\partial^2 u_\kappa}{\partial t^2}.$$