

## A continuum theory of diatomic solids: viewed as directed media

H. DEMIRAY

*Marmara Research Institute Division of Applied Mathematics P.K. 141, Kadıköy, İstanbul, Turkey*

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### SUMMARY

A generalized continuum model for diatomic solids is presented in this study. Considering the relative displacement of a particle in a cell as a single director, the field and the constitutive equations of diatomic solids are obtained through the use of Toupin's [3] variational principle. Propagation of a longitudinal wave in such a medium is also reported, and the result found here is compared with those of lattice dynamics.

### 1. Introduction

It is a well known fact that most of the elastic materials are made of complex atoms rather than simple atoms. It is therefore apparent that, from the point of view of lattice dynamics, the internal structure of such solids is multi-atomic. The classical continuum theory of solids is based upon the assumption that each lattice cell behaves like a single material point particle and ignores the relative motions of constituent atoms in the cell. In another words, the internal structure of such a complex cell is not taken into account. As a result of this oversimplification, the field equations of classical continuum theories for nonpolar elastic materials give non-dispersive wave solutions. However, the results of phonon dispersion experiments (c.f. Brockhouse et al. [5], Harrison [6], and Wallis [7]) show that the phase velocity changes with wave number. These facts have forced researchers to build up generalized continuum theories that may take the internal structure of lattice cells into account. In these theories the idea of classical rigid point particles is replaced by a generalized particle which may have local motions as well. Among such studies it may be worthy to mention the director theory of Toupin [3], the micromorphic theory of Eringen and Şuhubi [8], and the multipolar theory of Green and Rivlin [9]. These theories which are mathematically complete, however, have found little applications in physical problems concerning the elastic solids.

Starting from difference equations of diatomic lattices of infinite extent, Mindlin [10] has obtained the field equations for linear diatomic solids. Since the concepts of stress tensors and associated surface tractions are not introduced in [10], one is not able to solve any physical problem for which the boundary conditions are expressed in terms of surface tractions. The continuum theory of diatomic solids of finite extent is first given by Demiray [1, 2], in which the concept of partial stress is also introduced. In that work we have assumed that, from a mathematical point of view, a diatomic solid may be considered to consist of two simple elastic media, providing the appropriate interactions between the constituents. After introduction of such a mathematical model and partial stress tensors, it has principally become possible to solve any boundary value problem concerning diatomic elastic solids.

In this study, a generalized single continuum model (directed continuum) for diatomic solids is introduced. In building up such a model, each cell of the diatomic lattice is considered to be a generalized particle which may have local motions as well as the gross motion. Characterizing this local motion by a single director ( $\mathbf{d}$ ), the field, nonlinear and linear constitutive equations of such a generalized continuum are obtained by use of Toupin's [3] variational principle developed for directed media. A comparison between present model and the one presented in [1] is made and some special cases are discussed. Finally, using the field equations of present study, the propagation of longitudinal waves is studied and the values of material constants are obtained in terms of lattice characteristics.

## 2. Kinematics and basic laws

We consider an elastic body  $\mathcal{B}_0$  composed of diatomic molecules. In our previous works [1, 2] we have assumed that, from the mathematical view point, such an elastic medium may be considered to consist of two initially overlapping simple elastic media, providing the appropriate interactions between the constituent particles. In other words, we implicitly assumed that initially both particles in a lattice cell occupy the same space point and ignored the orientation of one particle relative to the other in the same cell. Generally speaking, in order to locate a cell in a three dimensional  $E$ -space, we need six numbers or two vectors. If these two vectors are measured with respect to the same origin, one obtains the model introduced in [1, 2]. However, if the location of one of these particles in a cell is described relative to the other in the same cell, the mechanical model so introduced will be conceptually different from the previous one. In the latter case, the vector connecting two atoms in one cell may be considered as a single director. As might easily be realized, the first model corresponds two interacting elastic solid continua, while the second one is built upon the assumptions of a single elastic continuum with a deformable director. In the present study we will be concerned with second model and formulate the problem accordingly.

Now we consider an elastic body  $\mathcal{B}_0$  that is the collection of the same type of material particles to each of which a director is attached. Let the initial coordinate of a material particle be denoted by  $\mathbf{X}$  and the associated director by  $\mathbf{D}(\mathbf{X})^*$ . Upon deformation of the body, the new position of the same material point at time  $t$  will be denoted by  $\mathbf{x}$  and the corresponding director by  $\mathbf{d}$ , Figure 1.

Thus the motion of such a generalized elastic continuum is described by

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t), \quad \forall \mathbf{X} \in \mathcal{B}_0, \quad t \in I = [t_1, t_2] \quad (2.1)$$

$$\mathbf{d} = \mathbf{d}(\mathbf{X}, t), \quad (2.2)$$

such that  $\mathbf{x} \rightarrow \mathbf{X}$  and  $\mathbf{d} \rightarrow \mathbf{D}$  as  $t \rightarrow t_1$ , where  $t_1$  is the reference time parameter.

Equation (2.1) is *one-to-one onto*, so that it has a unique inverse, given by

$$\mathbf{X} = \mathbf{X}(\mathbf{x}, t) \quad (2.3)$$

\* In fact, the magnitude of this vector  $\mathbf{D}$  corresponds to initial distance between two neighboring particles in a cell.

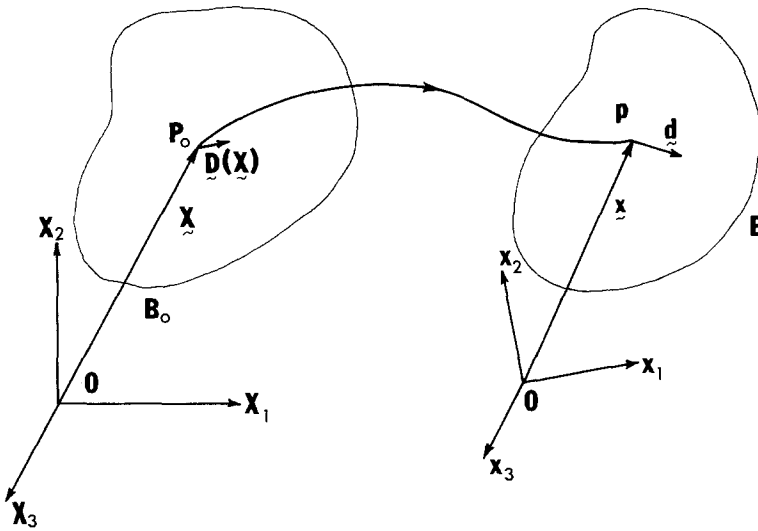


Figure 1. The motion of generalized body.

The gross translational velocity of a generalized material particle<sup>1</sup> and its local (or micro) velocity are defined by

$$v \equiv \frac{\partial x}{\partial t} \Big|_x, \quad \dot{v} \equiv \frac{\partial d}{\partial t} \Big|_x. \tag{2.4.a, b}$$

Similarly, the gross and local accelerations of a material particle are

$$a \equiv \frac{\partial^2 x}{\partial t^2} \Big|_x, \quad \dot{b} \equiv \frac{\partial^2 d}{\partial t^2} \Big|_x. \tag{2.5a, b}$$

Following Toupin's [3] director theory we introduce a function

$$L(X, t) \equiv L(X, x, d, \dot{x}, \dot{d}, F, G, t) \tag{2.6}$$

called the action density. Here  $F = \nabla x$ ,  $G = \nabla d$ ,  $\nabla \equiv \partial/\partial X$ ,  $t$  is the time derivative. The equations of motion and the boundary conditions for such materials are obtained from Hamilton's principle in the form of the variational equation

$$\delta \int_I \int_V L(X, t) dV dt + \int_I \int_V (Z \cdot \delta x + W \cdot \delta d) dV dt + \int_I \int_S (T^0 \cdot \delta x + H^0 \cdot \delta d) dS dt - \int_V (P \cdot \delta x + Q \cdot \delta d) dV \Big|_{t_1}^{t_2} = 0, \tag{2.7}$$

where  $V$  is the volume of undeformed body  $B_0$ ,  $S$  is the material surface enclosing the body,  $Z$  and  $W$  are certain generalized body forces,  $T^0$  and  $H^0$  denote certain generalized surface

<sup>1</sup> Here, by a generalized material particle we mean the reference particle whose mass is the sum of masses of all particles in a cell considered.

tractions,  $\mathbf{P}$  and  $\mathbf{Q}$  are certain generalized moments, and  $I \equiv [t_1, t_2]$  is the time interval in which the motion of the body is evolved. The variations  $\delta \mathbf{x}$  and  $\delta \mathbf{d}$  should vanish at  $t_1$  and  $t_2$ .

Noticing equation (2.6), if one performs the variation (2.7) and makes use of the of the generalized Green–Gauss theorem one obtains

$$\int_I \int_V [(T_{kl,k} - \dot{P}_l + Z_l - g_l)\delta x_l + (H_{kl,k} - \dot{Q}_l + W_l - R_l)\delta d_l] dV dt + \int_I \int_S [(T_l^0 - T_{kl}N_k)\delta x_l + (H_l^0 - H_{kl}N_k)\delta d_l] dS dt = 0, \quad (2.8)$$

where  $N$  is the exterior unit normal vector and other quantities are defined by

$$T_{kl} = -\frac{\partial L}{\partial F_{lK}}, \quad P_l = \frac{\partial L}{\partial \dot{x}_l}, \quad g_l = -\frac{\partial L}{\partial x_l}, \quad (2.9a)$$

$$H_{kl} = -\frac{\partial L}{\partial G_{lK}}, \quad Q_l = \frac{\partial L}{\partial \dot{d}_l}, \quad R_l = -\frac{\partial L}{\partial d_l}. \quad (2.9b)$$

Equation (2.8) is satisfied for all independent variations of  $\delta x_l$  and  $\delta d_l$  if and only if

$$T_{kl,k} + Z_l = \dot{P}_l + g_l, \quad H_{kl,k} + W_l = \dot{Q}_l + R_l, \quad \text{in } V, \quad (2.10, 11)$$

$$T_{kl}N_k = T_l^0, \quad H_{kl}N_k = H_l^0, \quad \text{on } S. \quad (2.12, 13)$$

So far we have not said anything about the invariance requirements of the action density  $L$ . To make further progress in the problem, we will study the invariance requirements of the action density in the sequel.

### 3. Invariance and conservation

We shall say that two motions of a given medium differ by a *Euclidean displacement* if

$$x_i^*(X, t^*) = R_{ij}x_j(X, t) + c_i, \quad d_i^*(X, t^*) = R_{ij}d_j(X, t), \quad t^* = t + a, \quad (3.1)$$

where the starred quantities define one of the motions and the unstarred quantities the other. All quantities are referred to a common rectangular Cartesian inertial frame of reference,  $R_{ij}$  is a constant proper matrix, and  $c_i$  and  $a$  are also constant.

It is postulated that the *action density*  $L$  is *invariant* under the transformation (3.1). The restrictions imposed by this requirement are given by

$$\frac{\partial L}{\partial x_i} = 0, \quad \frac{\partial L}{\partial t} = 0, \quad K_{[ij]} = 0, \quad (3.2)$$

where

$$K_{ij} = d_i \frac{\partial L}{\partial d_j} + F_{iK} \frac{\partial L}{\partial F_{jK}} + G_{iK} \frac{\partial L}{\partial G_{jK}} + \dot{x}_i \frac{\partial L}{\partial \dot{x}_j} + \dot{d}_i \frac{\partial L}{\partial \dot{d}_j}. \quad (3.3)$$

With the conditions (3.2) and (3.3) in mind, consider now the variational equation (2.7) which summarizes the equations of motion, boundary conditions, and initial and final data. Equation (2.7) must hold for all admissible variations of  $\delta x_i$  and  $\delta d_i$  that are geometrically consistent. In particular it must be valid for

$$\begin{aligned} (1) \quad & \delta x_i = c_i, & \delta d_i &= 0, \\ (2) \quad & \delta x_i = \Omega_{ij} x_j, & \delta d_i &= \Omega_{ij} d_j, \\ (3) \quad & \delta x_i = \dot{x}_i, & \delta d_i &= \dot{d}_i, \end{aligned} \tag{3.4}$$

where  $\Omega_{ij} = -\Omega_{ji}$  is the constant and infinitesimal rotation tensor. The necessary and sufficient conditions that (2.7) hold for these special types of variations are:

$$\int_V P_i dV \Big|_{t_1}^{t_2} - \int_I \int_S T_i^0 dS dt - \int_I \int_V Z_i dV dt = 0, \tag{3.5}$$

$$\begin{aligned} \int_V L_{ij} dV \Big|_{t_1}^{t_2} - \int_I \int_S (x_{[i} T_{j]}^0 + d_{[i} H_{j]}^0) dS dt - \\ - \int_I \int_V (x_{[i} Z_{j]} + d_{[i} W_{j]}) dV dt = \int_I \int_V K_{[ij]} dV dt = 0, \end{aligned} \tag{3.6}$$

$$\int_V E dV \Big|_{t_1}^{t_2} - \int_I \int_S (T_i^0 \dot{x}_i + H_i^0 \dot{d}_i) dS dt - \int_I \int_V (Z_i \dot{x}_i + W_i \dot{d}_i) dV dt = 0, \tag{3.7}$$

where, in (3.7), we have set

$$E = P_i \dot{x}_i + Q_i \dot{d}_i - L, \tag{3.8}$$

which we call the *energy density*, and in (3.6) we have set

$$L_{ij} = -L_{ji} = x_{[i} P_{j]} + d_{[i} Q_{j]}, \tag{3.9}$$

which we call the *density of angular momentum*. Inspection of (3.5), (3.6), and (3.7) shows that the difference between the values of total linear momentum, angular momentum, and energy of a body at times  $t_1$  and  $t_2$  is equal, respectively to the resultant linear impulse, the resultant of angular impulse, and the work done by the generalized forces  $T_i^0, H_i^0, Z_i$ , and  $W_i$  during the time interval  $I$ .

From the definition (3.9) of the density of angular momentum one sees that, in general, the angular momentum of a macroelement is not equal to the moment of the linear momentum. Also, from (3.5) and (3.6), one sees that the torque exerted on a body is not, in general, equal to the moment of the body forces  $Z_i$  and the surface traction  $T_i^0$ .

We now specialize the problem and consider a directed medium for which the generalized momenta are assumed to be given by

$$P_i = \rho^0 \dot{x}_i + \rho_2^0 \dot{d}_i, \quad Q_i = \rho_2^0 (\dot{x}_i + \dot{d}_i), \tag{3.10, 11}$$

where  $\rho_0$  is the total undeformed mass density of the medium, and  $\rho_2^0$  is the initial mass density of particles associated with directors.

Substitution of (3.10) and (3.11) into (2.9a, b)<sub>2</sub> yields the following differential equations

$$P_i = \frac{\partial L}{\partial \dot{x}_i} = \rho^0 \dot{x}_i + \rho_2^0 \dot{d}_i, \quad Q_i = \frac{\partial L}{\partial \dot{d}_i} = \rho_2^0 (\dot{x}_i + \dot{d}_i). \quad (3.12, 13)$$

Solving these two simultaneous partial differential equations for  $L$ , one obtains

$$L = \rho^0 \frac{1}{2} \dot{x}^2 + \rho_2^0 \mathbf{d} \cdot \dot{\mathbf{x}} + \rho_2^0 \frac{1}{2} \dot{\mathbf{d}}^2 - \Sigma(\mathbf{F}, \mathbf{d}, \mathbf{G}, \mathbf{X}). \quad (3.14)$$

Introducing (3.10), (3.11) and (3.14) into equation (3.8) the energy density is found to be

$$E = \rho^0 \frac{1}{2} \dot{x}^2 + \rho_2^0 \mathbf{d} \cdot \dot{\mathbf{x}} + \rho_2^0 \frac{1}{2} \dot{\mathbf{d}}^2 + \Sigma(\mathbf{F}, \mathbf{d}, \mathbf{G}, \mathbf{X}). \quad (3.15)$$

Here the function  $\Sigma$  will be called as the strain energy density function of the generalized continuum. By inspection of equation (3.15) one sees that the total kinetic energy density of the medium is given by

$$T = \rho^0 \frac{1}{2} \dot{x}^2 + \rho_2^0 \frac{1}{2} \dot{\mathbf{d}}^2 + \rho_2^0 \mathbf{d} \cdot \dot{\mathbf{x}} = T_c + T_d + \rho_2^0 \mathbf{d} \cdot \dot{\mathbf{x}}. \quad (3.16)$$

As might be seen from equation (3.16), the total kinetic energy of the medium is not separable, i.e., the total kinetic energy is not the sum of the classical kinetic energy and directorial kinetic energy. These two types of kinetic energies are correlated through the last term of equation (3.16). The total kinetic energy is separable if and only if the classical particle velocity is perpendicular to the director velocity.

Inserting (3.16) into equations (2.9a, b), the generalized stresses, momenta and other interacting forces may be given by

$$T_{Kl} = \frac{\partial \Sigma}{\partial F_{lK}}, \quad P_k = \rho^0 \dot{x}_k + \rho_2^0 \dot{d}_k, \quad g_k = 0, \quad (3.17)$$

$$H_{Kl} = \frac{\partial \Sigma}{\partial G_{lK}}, \quad Q_k = \rho_2^0 (\dot{x}_k + \dot{d}_k), \quad R_k = \frac{\partial \Sigma}{\partial d_k}. \quad (3.18)$$

Thus, the field equations and boundary conditions can be re-expressed as follows

$$T_{Kl,K} + \rho^0 f_l = \rho_0 \ddot{x}_l + \rho_2^0 \ddot{d}_l, \quad \text{in } V, \quad (3.19)$$

$$T_{Kl} N_K = T_l^0, \quad \text{on } S, \quad (3.20)$$

$$H_{Kl,K} + \rho_2^0 g_l - R_l = \rho_2^0 (\ddot{x}_l + \ddot{d}_l), \quad \text{in } V, \quad (3.21)$$

$$H_{Kl} N_K = H_l^0, \quad \text{on } S, \quad (3.22)$$

where  $Z_l = \rho^0 f_l$  and  $W_l = \rho_2^0 g_l$  are respectively the total and directorial body forces per unit volume.

Equations (3.17)–(3.22) are the material description of the constitutive relations and the field equations for the generalized continuum under consideration. In some cases it might be useful to express these quantities in terms of the values measured on deformed configuration. Let the Jacobian of the motion be denoted by  $J = \det \mathbf{F}$ . Multiplying the both sides of equations (3.19) and (3.21) by  $1/J$ , and of (3.20) and (3.22) by  $dA/da$ , where  $dA$  and  $da$  are the undeformed and deformed elementary areas, we obtain the following equations.

$$t_{kl,k} + \rho f_l = \rho \ddot{x}_l + \rho_2 \dot{d}_l, \quad \text{in } v, \tag{3.23}$$

$$t_{kl}n_k = t_l, \quad \text{on } s, \tag{3.24}$$

$$h_{kl,k} + \rho_2 g_l - \hat{R}_l = \rho_2 (\ddot{x}_l + \dot{d}_l), \quad \text{in } v, \tag{3.25}$$

$$h_{kl}n_k = h_l, \quad \text{on } s, \tag{3.26}$$

where

$$t_{kl} \equiv \frac{1}{J} T_{kl} F_{kK}, \quad h_{kl} \equiv \frac{1}{J} H_{kl} F_{kK}, \quad \hat{R}_l = \frac{1}{J} R_l, \quad t_l \equiv T_l^0 dA/da, \\ h_l \equiv H_l^0 dA/da, \quad \rho \equiv \rho^0/J, \quad \rho_2 \equiv \rho_2^0/J, \quad n_k = J dA/da F_{kK}^{-1} N_K. \tag{3.27}$$

Here  $t_{kl}, h_{kl}, t_l,$  and  $h_l$  are the generalized Eulerian stress tensors and associated surface tractions,  $\rho$  and  $\rho_2$  are respectively the deformed total mass density of the generalized material particles, and associated directors, and  $n_k$  is the exterior unit normal of the material surface in the deformed configuration.

Using the relations (3.17)<sub>2</sub>, (3.18)<sub>2</sub>, and (3.27) in equations (3.2) and (3.3), the condition that is to be satisfied by the generalized stresses and forces is given by

$$\varepsilon_{ijk}(d_i \hat{R}_j + t_{ij} + d_{i,l} h_{lj}) = 0. \tag{3.28}$$

So far we have worked with the vector  $d$  and its gradient  $G = \nabla d$ . Since, in our case,  $D$  is a constant vector, it may be convenient to express the strain energy function  $\Sigma$  in terms of  $w \equiv d - D$  and  $S \equiv \nabla w$ ; where  $w$  corresponds to the relative displacement vector. In this case, the generalized stresses and reaction force  $R_l$  take the following form:

$$T_{kl} = \frac{\partial \Sigma}{\partial F_{lK}}, \quad H_{kl} = \frac{\partial \Sigma}{\partial S_{lK}}, \quad R_l = \frac{\partial \Sigma}{\partial w_l}. \tag{3.29}$$

Since  $\Sigma$  is a state variable, it must be form-invariant under the local rotation of the spatial frame of reference. We will, therefore, next study the implication of this requirement. Let  $M$  be a group of orthogonal transformations of the spatial frame of reference  $x(MM^T = M^T M = I)$  and  $\bar{w}, \bar{F},$  and  $\bar{S}$  be the transformed values of  $w, F,$  and  $S$ . Then the following relations are valid.

$$(\bar{w}, \bar{F}, \bar{S}) = M(w, F, S). \tag{3.30}$$

The strain energy function  $\Sigma$  should be form-invariant under the transformation (3.30), i.e.,

$$\Sigma(X, w, F, S) = \Sigma(X, \bar{w}, \bar{F}, \bar{S}). \tag{3.31}$$

Such a requirement implies that the strain energy function should be a function of the following form (c.f. Spencer [4])

$$\Sigma = \Sigma(X, C, \Gamma, B), \tag{3.32}$$

where

$$C = F^T F, \quad \Gamma = F^T S, \quad B = F^T w. \tag{3.33}$$

Here the superscript (T) denotes the transpose of the corresponding tensorial quantity.

Introducing (3.32) into (3.29) and noting the relations (2.21), the generalized stresses and the reaction force become

$$T_{KI} = 2 \frac{\partial \Sigma}{\partial C_{KL}} F_{iL} + \frac{\partial \Sigma}{\partial \Gamma_{KL}} S_{iL} + \frac{\partial \Sigma}{\partial B_K} w_i \tag{3.34}$$

$$H_{KI} = \frac{\partial \Sigma}{\partial \Gamma_{LK}} F_{iL}, \quad R_i = \frac{\partial \Sigma}{\partial B_K} F_{iK} \tag{3.35, 36}$$

By this form of constitutive equations, the condition (3.18) is identically satisfied.

In some cases it is convenient to express the generalized stresses and reactive forces in terms of Lagrangian strain tensor  $E_{KL} \equiv \frac{1}{2}(C_{KL} - \delta_{KL})$ ; where  $\delta_{KL}$  is Kronecker delta. If this is the case, the equation (3.34) takes the following form

$$T_{KI} = \frac{\partial \Sigma}{\partial E_{KL}} F_{iL} + \frac{\partial \Sigma}{\partial \Gamma_{KL}} S_{iL} + \frac{\partial \Sigma}{\partial B_K} w_i, \tag{3.37}$$

while (3.35) and (3.36) formally remain the same.

The set of equations (3.34)–(3.36) gives the most general form of constitutive equations for the directed medium considered. Various other nonlinear constitutive equations may be deduced from this general formulation. In what follows we shall study the linear constitutive equations only.

#### 4. Linear constitutive equations

In order to be able to see some simple but obvious applications of the theory developed here, the linear constitutive relations play a central role. For a theory that is geometrically linear, the constitutive independent variables take the following form

$$\tilde{E}_{KL} \equiv \frac{1}{2}(U_{K,L} + U_{L,K}), \quad \tilde{\Gamma}_{KL} \equiv W_{K,L}, \quad \tilde{B}_K \equiv W_K \tag{4.1}$$

where  $U_K$  and  $W_K$  are respectively the Cartesian components of the classical displacement vector  $\mathbf{u}$  and directional displacement vector  $\mathbf{w}$  with respect to material coordinate  $\mathbf{X}$ .

For this purpose, it is convenient to expand the strain energy function  $\Sigma$  into a power series of  $\tilde{E}, \tilde{\Gamma}$ , and  $\tilde{B}$  as follows:

$$\begin{aligned} \Sigma = & \Sigma_0 + \Sigma_{1K} \tilde{B}_K + \Sigma_{2KL} \tilde{E}_{KL} + \Sigma_{3KL} \tilde{\Gamma}_{KL} + \Sigma_{4KLM} \tilde{E}_{KL} \tilde{B}_M + \Sigma_{5KL} \tilde{B}_K \tilde{B}_L \\ & + \Sigma_{5KL} \tilde{B}_K \tilde{B}_L + \Sigma_{6KLM} \tilde{\Gamma}_{KL} \tilde{B}_M + \Sigma_{7KLMN} \tilde{E}_{KL} \tilde{E}_{MN} + \Sigma_{8KLMN} \tilde{\Gamma}_{KL} \tilde{\Gamma}_{MN} \\ & + \Sigma_{9KLMN} \tilde{E}_{KL} \tilde{\Gamma}_{MN} \end{aligned} \tag{4.2}$$

where  $\Sigma_0, \Sigma_{1K}, \dots, \Sigma_{9KLMN}$  are, in general, functions of  $\mathbf{X}$ . Throughout this work, we will assume that the body under consideration is homogeneous, so that these coefficients are constant. Here, we also note that some of these coefficients have the following symmetry relations.

$$\begin{aligned} \Sigma_{2KL} = \Sigma_{2LK}, \quad \Sigma_{4KLM} = \Sigma_{4LKM}, \quad \Sigma_{5KL} = \Sigma_{5LK}, \\ \Sigma_{7KLMN} = \Sigma_{7LKMN} = \Sigma_{7MNKL}, \quad \Sigma_{8KLMN} = \Sigma_{8MNKL}, \quad \Sigma_{9KLMN} = \Sigma_{9LKMN}. \end{aligned} \tag{4.3}$$



The use of (4.2) in (3.35)–(3.37) gives the most general and linear constitutive relations for anisotropic materials; but we will not list them here. In this work we are rather interested in isotropic materials. For this particular case, the nonvanishing elastic moduli are:

$$\begin{aligned} \Sigma_{2KL} &= \alpha_0 \delta_{KL}, & \Sigma_{3KL} &= \beta_0 \delta_{KL}, & \Sigma_{3KL} &= \frac{1}{2} \nu \delta_{KL}, \\ \Sigma_{7KLMN} &= \frac{1}{2} \lambda \delta_{KL} \delta_{MN} + \frac{1}{2} \mu (\delta_{KM} \delta_{LN} + \delta_{KM} \delta_{LM}), \\ \Sigma_{8KLMN} &= \frac{1}{2} \alpha_1 \delta_{KL} \delta_{MN} + \frac{1}{2} \alpha_2 \delta_{KM} \delta_{LN} + \frac{1}{2} \alpha_3 \delta_{KN} \delta_{LM}, \\ \Sigma_{9KLMN} &= \beta_1 \delta_{KL} \delta_{MN} + \beta_2 (\delta_{KM} \delta_{LN} + \delta_{KN} \delta_{LM}). \end{aligned} \tag{4.4}$$

Hence the strain energy function takes the following form

$$\begin{aligned} \Sigma &= \Sigma_0 + \alpha_0 \tilde{E}_{RR} + \beta_0 \tilde{I}_{RR} + \frac{1}{2} \nu \tilde{B}_K \tilde{B}_K + \frac{1}{2} \lambda (\tilde{E}_{RR})^2 + \mu \tilde{E}_{KL} \tilde{E}_{KL} + \frac{1}{2} \alpha_1 (\tilde{I}_{RR})^2 \\ &+ \frac{1}{2} \alpha_2 \tilde{I}_{KL} \tilde{I}_{LK} + \frac{1}{2} \alpha_3 \tilde{I}_{LK} \tilde{I}_{LK} + \beta_1 \tilde{E}_{RR} \tilde{I}_{PP} + \beta_2 (\tilde{E}_{KM} \tilde{I}_{MK} + \tilde{E}_{KM} \tilde{I}_{MK}). \end{aligned} \tag{4.5}$$

Introducing (4.5) into (3.35)–(3.37) and neglecting the powers of  $U_{K,L}$ ,  $W_{K,L}$  and  $W_K$  higher than one, the following linear constitutive equations are obtained

$$T_{Kl} = \delta_{iL} [\lambda \tilde{E}_{RR} \delta_{KL} + 2\mu \tilde{E}_{KL} + \beta_1 \tilde{I}_{RR} \delta_{KL} + \beta_2 (\tilde{I}_{KL} + \tilde{I}_{LK})], \tag{4.6}$$

$$H_{Kl} = \delta_{iL} [\alpha_1 \tilde{I}_{RR} \delta_{KL} + \alpha_2 \tilde{I}_{KL} + \alpha_3 \tilde{I}_{LK} + \beta_1 \tilde{E}_{RR} \delta_{KL} + 2\beta_2 \tilde{E}_{KL}], \tag{4.7}$$

$$R_l = \delta_{iK} (\nu B_K), \tag{4.8}$$

where  $\delta_{iK}$  is the coordinate shifter. In arriving this result we have assumed that the medium is initially stress free (in general sense), i.e.,  $T_{Kl} \rightarrow H_{Kl} \rightarrow 0$  as  $\tilde{E} \rightarrow \tilde{I} \rightarrow w \rightarrow 0$ . In this case the coefficients  $\alpha_0$  and  $\beta_0$  must vanish.

In small deformation theory the difference between the material and the spatial coordinate systems may be disregarded. Hence the spatial description of the constitutive relations may be given by

$$t_{kl} = \lambda \tilde{e}_{rr} \delta_{kl} + 2\mu \tilde{e}_{kl} + \beta_1 \tilde{\gamma}_{rr} \delta_{kl} + \beta_2 (\tilde{\gamma}_{kl} + \tilde{\gamma}_{lk}), \tag{4.9}$$

$$h_{kl} = \alpha_1 \tilde{\gamma}_{rr} \delta_{kl} + \alpha_2 \tilde{\gamma}_{kl} + \alpha_3 \tilde{\gamma}_{lk} + \beta_1 \tilde{e}_{rr} \delta_{kl} + 2\beta_2 \tilde{e}_{kl}, \tag{4.10}$$

$$R_k = \nu w_k,$$

where  $\delta_{kl}$  is the Kronecker delta and the other quantities are defined by

$$\tilde{e}_{kl} \equiv \frac{1}{2}(u_{k,l} + u_{l,k}), \quad \tilde{\gamma}_{kl} \equiv w_{k,l}, \quad w_k \equiv W_K \delta_{kK}. \tag{4.12}$$

For real elastic materials, in order to have a stable motion (or deformation), the strain energy density function must be positive for all admissible values of the generalized displacements. This requirement puts certain restrictions on the material constants,  $\lambda$ ,  $\mu$ ,  $\nu$ ,  $\alpha_i$ , and  $\beta_i$ . To this end, we decompose the tensors  $\tilde{e}_{kl}$  and  $\tilde{\gamma}_{kl}$  into equivoluminal and deviatoric parts as follows:

$$\tilde{e}_{kl} = \frac{1}{3} \tilde{e}_{rr} \delta_{kl} + \tilde{e}'_{kl}, \quad \tilde{\gamma}_{kl} = \frac{1}{3} \tilde{\gamma}_{rr} \delta_{kl} + \tilde{\varphi}'_{kl} + \tilde{\omega}_{kl} \tag{4.13}$$

where  $\tilde{e}'_{rr} = 0$ ,  $\tilde{\varphi}'_{rr} = 0$ ,  $\tilde{\omega}_{rr} = 0$ , and

$$\tilde{\varphi}'_{kl} \equiv \frac{1}{2}(w_{k,l} + w_{l,k}) - \frac{1}{3} \tilde{\gamma}_{rr} \delta_{kl}, \quad \tilde{\omega}_{kl} \equiv \frac{1}{2}(w_{k,l} - w_{l,k}). \tag{4.14}$$

Inserting (4.13) into equation (4.5) and noting the relations (4.14), the strain energy function becomes

$$\begin{aligned}\Sigma = & \Sigma_0 + \frac{1}{2}v w^2 + \frac{1}{2}(\alpha_2 - \alpha_3)\tilde{\omega}_{kl}\tilde{\omega}_{kl} + (\lambda/2 + \mu/3)(\tilde{\epsilon}_{rr})^2 \\ & + \frac{1}{6}(3\alpha_1 + \alpha_2 + \alpha_3)(\tilde{\gamma}_{rr})^2 + (\alpha_1 + 2\beta_2/3)\tilde{\epsilon}_{rr}\tilde{\gamma}_{qq} + \mu\tilde{\epsilon}'_{kl}\tilde{\epsilon}'_{kl} \\ & + \frac{1}{2}(\alpha_2 + \alpha_3)\tilde{\varphi}'_{kl}\tilde{\varphi}'_{kl} + 2\beta_2\tilde{\epsilon}_{kl}\tilde{\varphi}'_{kl}.\end{aligned}\quad (4.15)$$

In order that the strain energy function  $\Sigma$  be positive for all arbitrary variations of independent constitutive variables, the following inequalities must hold

$$\begin{aligned}v \geq 0, \quad \alpha_2 - \alpha_3 \geq 0, \quad 3\lambda + 2\mu \geq 0, \quad 3\alpha_1 + \alpha_2 + \alpha_3 \geq 0, \quad \mu \geq 0, \quad \alpha_2 + \alpha_3 \geq 0, \\ (3\lambda + 2\mu)(3\alpha_1 + \alpha_2 + \alpha_3) - (3\alpha_1 + 2\beta_2)^2 \geq 0, \quad \mu(\alpha_2 + \alpha_3) - 2\beta_2^2 \geq 0.\end{aligned}\quad (4.16)$$

Introducing (4.9)–(4.11) into equations (3.23)–(3.26), the field equations and the boundary conditions are obtained to be

$$(\lambda + \mu)\nabla(\nabla \cdot \mathbf{u}) + \mu\nabla^2 \mathbf{u} + (\beta_1 + \beta_2)\nabla(\nabla \cdot \mathbf{w}) + \beta_2\nabla^2 \mathbf{w} + \rho \mathbf{f} = \rho \ddot{\mathbf{u}} + \rho_2 \ddot{\mathbf{w}}, \quad (4.17)$$

$$(\beta_1 + \beta_2)\nabla(\nabla \cdot \mathbf{u}) + \beta_2\nabla^2 \mathbf{u} + (\alpha_1 + \alpha_2)\nabla(\nabla \cdot \mathbf{w}) + \alpha_3\nabla^2 \mathbf{w} - v\mathbf{w} + \rho_2 \mathbf{g} = \rho_2(\ddot{\mathbf{u}} + \ddot{\mathbf{w}}), \quad (4.18)$$

$$t_{kl}n_k = t_l, \quad h_{kl}n_k = h_l. \quad (4.19)$$

These field equations and the boundary conditions may be used to determine the mechanical field completely. Before we give the solution of an illustrative example, it might be interesting to see the connection between the field equations and the constitutive relations of diatomic solids and directed (or oriented) continuum described herein. This is done in the remaining part of this section.

#### *Classical equations of diatomic solids:*

Following Demiray [1, 2] the motion of a diatomic solid viewed as the collection of two simple but interacting continua may be characterized by

$$\mathbf{x}^{(\alpha)} = \mathbf{x}^{(\alpha)}(\mathbf{X}, t), \quad \alpha = 1, 2. \quad (4.20)$$

Selecting the coordinates of one of the particles in the continuum, say  $\alpha = 1$ , as the location of the generalized particle, the following identification holds true:

$$\begin{aligned}x_k^{(1)}(\mathbf{X}, t) & \equiv x_k(\mathbf{X}, t), \quad x_k^{(2)}(\mathbf{X}, t) \equiv x_k(\mathbf{X}, t) + d_k(\mathbf{X}, t), \\ F_{kK}^{(1)} & \equiv F_{kK}, \quad F_{kK}^{(2)} \equiv F_{kK} + G_{kK}.\end{aligned}\quad (4.21)$$

Employing (4.21) in equations (3.17) and (3.18) and performing the necessary differentiation we obtain

$$T_{Kl} = \frac{\partial \Sigma}{\partial F_{lK}^{(1)}} + \frac{\partial \Sigma}{\partial F_{kK}^{(2)}}, \quad P_k = \rho_1 \dot{x}_k^{(1)} + \rho_2 \dot{x}_k^{(2)}, \quad (4.22)$$

$$H_{Kl} = \frac{\partial \Sigma}{\partial F_{lK}^{(2)}}, \quad Q_k = \rho_2 \dot{x}_k^{(2)}, \quad R_k = \frac{\partial \Sigma}{\partial w_k}, \quad (4.23)$$

where  $\rho_1^0$  is the initial mass density of the species (1), i.e.,  $\rho_1^0 = \rho^0 - \rho_2^0$ . Comparing these constitutive equations with those of (3.6) and (3.7) of reference [1], we arrive at the following relations

$$T_{kl} = T_{kl}^{(1)} + T_{kl}^{(2)}, \quad H_{kl} = T_{kl}^{(2)}. \tag{4.24}$$

Similar comparisons can be made for the field equations. In this case, the equation (3.21) is equivalent to equation (2.9) of reference [1] while (3.19) is the sum of equations (2.8) and (2.9) of the same work.

In the case of linear constitutive theory it is also possible to obtain some relations between the material constants introduced by two different view points (or models). Comparing equations (4.9) and (4.10) of this study with those of corresponding equations in [1], we have

$$\begin{aligned} \lambda &= a_1 + a_2 + 2a_5, & \mu &= a_2 + a_4 + 2a_6, & \beta_1 &= a_3 + a_5, \\ \beta_2 &= a_4 + a_6, & \alpha_1 &= a_3, & \alpha_2 &= a_4 + a_7, & \alpha_3 &= a_4 - a_7, & \nu &= a_0 \end{aligned} \tag{4.25}$$

where  $a_0, a_1, \dots, a_7$  are the material constants introduced in [1].

As a result of these comparisons, one can see that there is one-to-one and unique correspondence between two models introduced for the mechanical description of diatomic solids.

### 5. Plane harmonic waves

To be an illustrative example, in this section we will study the propagation of plane harmonic waves in such a medium. For simplicity and easiness in comparing present result with those of lattice dynamics, we only investigate the longitudinal waves; the transverse waves may be studied in the same manner. Assuming that the wave is propagating in the  $x_1$  direction, in such a situation, the nonvanishing displacement components may be expressed by

$$u_1 = U_1 \exp[i(\omega t - kx_1)], \quad w_1 = W_1 \exp\{i(\omega t - kx_1)\}, \tag{5.1}$$

where  $\omega$  is the angular frequency,  $k$  is the wave number, and  $U_1$  and  $W_1$  are the complex amplitudes of the wave.

Introduction of (5.1) into (4.17) and (4.18), neglecting the body forces, yields the following homogeneous algebraic equations.

$$[\rho\omega^2 - (\lambda + 2\mu)k^2]U_1 + [\rho_2\omega^2 - (\beta_1 + 2\beta_2)k^2]W_1 = 0, \tag{5.2}$$

$$[\rho_2\omega^2 - (\beta_1 + 2\beta_2)k^2]U_1 + [\rho_2\omega^2 - (\alpha_1 + \alpha_2 + \alpha_3)k^2 - \nu]W_1 = 0. \tag{5.3}$$

In order to have a nonzero solution for  $U_1$  and  $W_1$ , the determinant of the coefficient matrix obtained from equations (5.2) and (5.3) must vanish. Thus,

$$\begin{aligned} \rho_2(\rho - \rho_2)\omega^4 - \{\rho[(\alpha_1 + \alpha_2 + \alpha_3)k^2 + \nu] + \rho_2[(\lambda + 2\mu) - 2(\beta_1 + 2\beta_2)]k^2\}\omega^2 \\ + \{[(\lambda + 2\mu)(\alpha_1 + \alpha_2 + \alpha_3) - (\beta_1 + 2\beta_2)^2]k^4 + (\lambda + 2\mu)\nu k^2\} = 0. \end{aligned} \tag{5.4}$$

By setting  $k = 0$  in equation (5.4), the cut-off frequencies are obtained to be

$$\omega_1 = \left[ \frac{\nu\rho}{\rho_2(\rho - \rho_2)} \right]^{\frac{1}{2}}, \quad \omega_2 = 0. \tag{5.5}$$

This result shows that one of these waves is acoustical, while the other is of optical character.

In order to proceed further, one must know the values of material constants appearing in equations (5.4). Employing the lattice dynamic approach, the dispersion relation of a one-dimensional diatomic lattice is given in the Appendix. Comparing equations (5.2) and (5.3), with (A-8) and (A-9) the following relations are obtained

$$\begin{aligned} \lambda + 2\mu &= E_{11} + E_{22} + \frac{1}{2}E_{12}, & \beta_1 + 2\beta_2 &= E_{22} + \frac{1}{4}E_{12}, \\ \alpha_1 + \alpha_2 + \alpha_3 &= E_{22}, & \nu &= 2E_{12}/d^2, \end{aligned} \quad (5.6)$$

where  $d$  is the length of a cell in diatomic lattices, and  $E_{ij}$  are constants related to spring constants of the same lattice considered. These relations are not sufficient to determine all the material constants presented in this study. In addition, one should also consider the shear motions of a diatomic lattice.

Employing these relations in equation (5.4) the dispersion equation becomes

$$\begin{aligned} \rho_2(\rho - \rho_2)\omega^4 - \{[\rho E_{22} + \rho_2(E_{11} - E_{22})]k^2 + 2\rho E_{12}/d^2\}\omega^2 \\ + [(E_{11}E_{22} - \frac{1}{16}E_{12}^2)k^4 + 2E_{12}/d^2(E_{11} + E_{22} + \frac{1}{2}E_{12})k^2] = 0. \end{aligned} \quad (5.7)$$

The coefficients of this equation are known in terms of lattice characteristics.

For numerical calculations, it might be useful to introduce the following dimensionless quantities

$$\begin{aligned} \omega^2 &= \frac{2E_{12}\rho}{\rho_2(\rho - \rho_2)} \frac{\Omega^2}{d^2}, & \kappa_1 &= E_{11}/E_{12}, & \kappa_2 &= E_{22}/E_{12}, \\ \xi &= kd, & \gamma &= \rho_2/\rho. \end{aligned}$$

Introducing these quantities into equation (5.7), we get

$$\begin{aligned} \Omega^4 - \left\{ \frac{1}{2}[\kappa_2 + \gamma(\kappa_1 - \kappa_2)]\xi^2 + 1 \right\} \Omega^2 + \left[ \frac{\gamma(1 - \gamma)}{4} (\kappa_1\kappa_2 - \frac{1}{16})\xi^4 \right. \\ \left. + \frac{\gamma(1 - \gamma)}{2} (\kappa_1 + \kappa_2 + \frac{1}{2})\xi^2 \right] = 0. \end{aligned} \quad (5.8)$$

The roots of this algebraic equation can be expressed as

$$(\Omega_{ac}^{op})^2 = A(\xi) \pm A^{\frac{1}{2}}(\xi), \quad (5.9)$$

where  $A$  and  $A$  are defined by

$$\begin{aligned} A &\equiv \frac{1}{2} \left\{ \frac{1}{2} [\kappa_2 + \gamma(\kappa_1 - \kappa_2)] \xi^2 + 1 \right\}, \\ A &\equiv A^2 - \frac{\gamma(1 - \gamma)}{4} \left[ (\kappa_1\kappa_2 - \frac{1}{16})\xi^4 + 2(\kappa_1 + \kappa_2 + \frac{1}{2})\xi^2 \right]. \end{aligned} \quad (5.10)$$

Here the subscript ( $ac$ ) and superscript ( $op$ ) stand for the acoustical and optical branches, respectively.

From this general formulation, various limiting cases may be investigated. Some of them are given below:

(i) *Limit of low frequencies:* In this case, the terms comprising  $\Omega^4$  can be neglected as compared to  $\Omega^2$ . Equation (5.8) may, then, be simplified to

$$\begin{aligned}
 & - \left\{ \frac{1}{2}[\kappa_2 + \gamma(\kappa_1 - \kappa_2)]\xi^2 + 1 \right\} \Omega^2 + \\
 & + \gamma(1 - \gamma)/4 [(\kappa_1\kappa_2 - \frac{1}{16})\xi^4 + 2(\kappa_1 + \kappa_2 + \frac{1}{2})\xi^2] = 0.
 \end{aligned}
 \tag{5.11}$$

This equation gives only one root which is the frequency for acoustical waves. In addition, if the order of  $\Omega$  is the same with that of  $\xi$  (that is, the wave number is also small), the foregoing equation becomes

$$\Omega^2 = \frac{\gamma(1 - \gamma)}{2} (\kappa_1 + \kappa_2 + \frac{1}{2})\xi^2,
 \tag{5.12}$$

which gives a constant phase velocity as

$$v_p = \Omega/\xi = [\gamma(1 - \gamma)(\kappa_1 + \kappa_2 + \frac{1}{2})/2]^{\frac{1}{2}}.
 \tag{5.13}$$

This equation shows that for small wave numbers the wave with low frequency (acoustical wave) is not dispersive and the dispersion relation is given by (5.12) or (5.13). However, as is seen from equation (5.11), for larger values of the wave number, the wave turns out to be dispersive.

(ii) *Limit of high frequency:* In this special case the last two terms of equation (5.8) may be neglected (this is particularly true for small wave numbers). Hence the dispersion equation takes the form

$$\Omega^2 - [1 + \frac{1}{2}[\kappa_2 + \gamma(\kappa_1 - \kappa_2)]\xi^2] = 0.
 \tag{5.14}$$

This, indeed, gives the frequency of the wave associated with optical branch. Equation (5.14) shows that even for small wave numbers the wave characterizing the optical branch is dispersive.

Another point that we would like to discuss here is the behavior of function characterizing the optical branch around  $\xi = 0$ . In the first place, it can be shown that  $\xi = 0$  is an extremum point for the function  $\Omega_{op}$ . In order to see whether the group velocity  $v_g^{op} = d\Omega_{op}/d\xi$  is negative or positive around  $\xi = 0$ , one has to examine  $d^2\Omega_{op}/d\xi^2$  at  $\xi = 0$ . Thus, differentiating equation (5.8) twice with respect to  $\xi$  and noting that  $\Omega_{op}(\xi) = 1$  and  $d\Omega_{op}/d\xi = 0$  at  $\xi = 0$ , we get

$$\left. \frac{d^2\Omega}{d\xi^2} \right|_{\xi=0} = \frac{1}{2}[(1 - \gamma)^2\kappa_2 + \gamma^2\kappa_1 - \gamma(1 - \gamma)/2].
 \tag{5.15}$$

Depending on the sign of equation (5.15), the group velocity associated with optical branch may take positive or negative values around  $\xi = 0$ . If the foregoing equation is positive, i.e.,

$$(1 - \gamma)^2\kappa_2 + \gamma^2\kappa_1 > \gamma(1 - \gamma)/2,
 \tag{5.16}$$

the function  $\Omega_{op}(\xi)$  takes its minimum value at  $\xi = 0$ . Another words, the frequency of the wave increases with increasing wave number. However, if (5.15) satisfies the restriction

$$(1 - \gamma)^2\kappa_2 + \gamma^2\kappa_1 < \gamma(1 - \gamma)/2,
 \tag{5.17}$$

the point  $\xi = 0$  is a maximum point for  $\Omega_{op}$ . If this latter condition is valid, then the frequency decreases with increasing wave number. It should be noted that in the former (latter) case the group velocity is positive (negative).

## Conclusion

Starting from a generalized continuum model (directed continuum) the field equations and the constitutive relations of a diatomic solid are derived through the use of a variational principle. An example problem concerning the one-dimensional harmonic wave propagation in such a medium shows that the field equations presented here give wave solutions that are dispersive. Moreover, depending on the positive or negative values of a function  $f(E_{11}, E_{12}, E_{22}, \rho, \rho_2)$  the group velocity may take positive or negative values (see equations (5.16) and (5.17)). It is particularly interesting to note that this relation depends also on mass densities of the medium under investigations.

Here we have presented a simple application of generalized continuum theories to diatomic solids. Similar ideas may be extended to formulate the field equations and constitutive relations of multi-atomic solids.

## Appendix. Dispersion relations of one-dimensional diatomic lattices

In the main part of this study we have needed the dispersion relation of one-dimensional diatomic lattices. In the Born model for NaCl, the interactions of only the nearest atoms are taken into account. For our purposes, however, we should consider the interactions of next nearest atoms as well as those of nearest atoms.

We assume that the atoms of all kinds are spaced at equal distance, say  $d/2$ , so that the cell length is  $d$ , Figure 2. The particles of mass  $M_2$  will be numbered by even integers ( $2n, 2n + 2$ , etc.), the ones of mass  $M_1$  by odd integers ( $2n - 1, 2n + 1$ , etc.). The spring constants associated with interatomic forces are shown in Figure 2. Let the displacements of these particles be denoted by  $u_{2n+1}^{(1)}$  and  $u_{2n}^{(2)}$ . Thus the motions of two different types of particles may be given by

$$M_1 \ddot{u}_{2n+1}^{(1)} = k_3(u_{2n+2}^{(2)} + u_{2n}^{(2)} - 2u_{2n+1}^{(1)}) + k_1(u_{2n+3}^{(1)} + u_{2n-1}^{(1)} - 2u_{2n+1}^{(1)}), \quad (\text{A-1})$$

$$M_2 \ddot{u}_{2n}^{(2)} = k_3(u_{2n+1}^{(1)} + u_{2n-1}^{(1)} - 2u_{2n}^{(2)}) + k_2(u_{2n+2}^{(2)} + u_{2n-2}^{(2)} - 2u_{2n}^{(2)}). \quad (\text{A-2})$$

In harmonic approximation, the displacements are expressed as

$$u_{2n+1}^{(1)} = U_1 \exp\{i[\omega t - (2n + 1)\eta_1]\}, \quad u_{2n}^{(2)} = U_2 \exp\{i[\omega t - 2n\eta_1]\}, \quad (\text{A-3})$$

where  $\omega$  is the angular frequency,  $\eta_1 = kd/2$  ( $k$  is the wave number), and  $U_1$  and  $U_2$  are the complex amplitudes of the wave.

Introducing (A-3) into (A-1, 2) the following homogeneous equations are obtained:

$$\left[ \rho_1 \omega^2 - \left( \frac{4E_{11}}{d^2} \sin^2 \eta_1 + \frac{2E_{12}}{d^2} \right) \right] U_1 + \left( -\frac{4E_{12}}{d^2} \sin^2 \eta_{1/2} + \frac{2E_{12}}{d^2} \right) U_2 = 0, \quad (\text{A-4})$$

$$\left( -\frac{4E_{12}}{d^2} \sin^2 \eta_{1/2} + \frac{2E_{12}}{d^2} \right) U_1 + \left[ \rho_2 \omega^2 - \left( \frac{4E_{22}}{d^2} \sin^2 \eta_1 + \frac{2E_{12}}{d^2} \right) \right] U_2 = 0, \quad (\text{A-5})$$

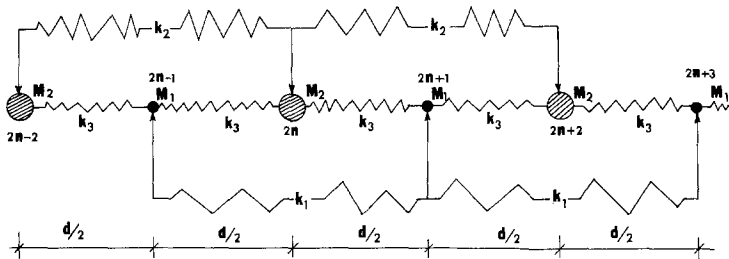


Figure 2. One dimensional diatomic lattice.

where  $E_{11} = k_1d$ ,  $E_{22} = k_2d$ , and  $E_{12} = k_3d$  are the partial Young's moduli, and  $\rho_1 \equiv M_1/d$ ,  $\rho_2 = M_2/d$  are the partial mass densities of the diatomic solid under investigation.

In local continuum theories we assume that the wave length is very large, or the wave number is very small, as compared to the cell length  $d$ . If  $\eta_1 = kd \ll 1$ , the function  $\sin(kd/2)$  may then be approximated by  $kd/2$ . With this assumption, the equations (A-4) and (A-5) take the following form

$$\left[ \rho_1 \omega^2 - \left( E_{11} k^2 + \frac{2E_{12}}{d^2} \right) \right] U_1 + \left[ -\frac{E_{12}}{4} k^2 + \frac{2E_{12}}{d^2} \right] U_2 = 0, \tag{A-6}$$

$$\left[ -\frac{E_{12}}{4} k^2 + \frac{2E_{12}}{d^2} \right] U_1 + \left[ \rho_2 \omega^2 - \left( E_{22} k^2 - \frac{2E_{12}}{d^2} \right) \right] U_2 = 0. \tag{A-7}$$

These equations, in their present form, are not convenient to compare with equations (5.2) and (5.3). Noting the relation  $U_2 = U_1 + W_1$  (see equation (4.21)) and summing up the equations (A-6) and (A-7) side by side, we have

$$[\rho \omega^2 - (E_{11} + E_{22} + E_{12/2})k^2]U_1 + [\rho_2 \omega^2 - (E_{22} + E_{12/4})k^2]W_1 = 0, \tag{A-8}$$

$$[\rho_2 \omega^2 - (E_{22} + E_{12/4})k^2]U_1 + [\rho_2 \omega^2 - (E_{22}k^2 + 2E_{12}/d^2)]W_1 = 0, \tag{A-9}$$

where  $\rho = \rho_1 + \rho_2$  is the total mass density.

This is the dispersion relation for a wave propagating in a diatomic solid viewed as a directed continuum.

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