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A CONTRIBUTION TO DYNAMICS OF POLYATOMIC LATTICES

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Using the concept of internal degrees of freedom a new finite difference formulation of polyatomic lattice dynamics is proposed. A transition from the nonlocal equations of motion to the partly local and local ones as well as the possibility of reduction of internal degrees of freedom are shown.

Key words: lattice dynamics, continuum models

1. Introduction

The problem we are to deal with is a modelling of long wave deformation patterns in linear elastodynamics of arbitrary perfect polyatomic lattice systems with a restricted range of binary interactions. The proposed approach constitutes a certain alternative to those given by Brillouin (1946), Born and Huang (1954), Babuška (1959), Künin (1975) or Cielecka (1995), being based on a new averaged finite-difference formulation of the equations of motion for periodic composite mass-point systems. It will be shown that this formulation makes it possible to specify two levels of long wave deformations, yields a simple transition from the nonlocal models to the local ones and leads to the approximate models governed by the monoatomic-type lattice equations. The obtained results can be used for the analysis of wave propagation problems in periodic composite mass-point systems.

Notations. Small and capital bold face characters stand for vectors and second order tensors in 3D-space, respectively. Indices a, b run over $1, \dots, n$

while A and K run over $1, \dots, M$ and $1, \dots, N$, respectively. Superscripts k, l run over $1, \dots, n-1$; the summation convention with respect to k, l holds. Points in the physical space are identified with their position vectors and denoted by \mathbf{x}, \mathbf{z} ; symbol t stands for a time coordinate.

2. Auxiliary concepts

Let Λ be the Bravais lattice with the base vectors $\mathbf{d}^1, \mathbf{d}^2, \mathbf{d}^3$ and Δ stands for the elementary cell spanned on these vectors and having a center at $\mathbf{x} = \mathbf{0}$. For an arbitrary $\mathbf{x} \in \Lambda$ we define $\Delta(\mathbf{x}) \equiv \mathbf{x} + \Delta$ as a translated cell with a center at \mathbf{x} . We assume that in Δ is situated a molecule consisting of n mass-points (atoms) having the equilibrium positions $\mathbf{p}^a \in \Delta$, $a = 1, \dots, n$; $n > 1$. The total mass-point system P under consideration is assumed to be periodic. Hence, $\mathbf{p}^a(\mathbf{x}) \equiv \mathbf{p}^a + \mathbf{x}$, $\mathbf{x} \in \Lambda$, $a = 1, \dots, n$, are the equilibrium positions of mass-points in an arbitrary translated cell $\Delta(\mathbf{x})$, $\mathbf{x} \in \Lambda$. The one-to-one mapping

$$P \xleftrightarrow{1:1} \left\{ \mathbf{z} \in E^3 : \mathbf{z} = \mathbf{p}^a(\mathbf{x}), \mathbf{x} \in \Lambda, a = 1, \dots, n \right\} \quad (2.1)$$

will be referred to as a *parametrization of the mass-point system* P . It means that in the sequel the points of P will be identified with their equilibrium positions; namely $\mathbf{p}^a(\mathbf{x})$ is said to be the a th mass-point in the cell $\Delta(\mathbf{x})$, $\mathbf{x} \in \Lambda$.

Define $\mathbf{d}^0 \equiv \mathbf{0}$ and let $D \equiv (\mathbf{d}^0, \mathbf{d}^1, \dots, \mathbf{d}^M)$, $M \geq 3$, be the $M+1$ -tuple of vectors such that $\mathbf{d}^0, \mathbf{d}^1, \dots, \mathbf{d}^M \in \Lambda$ and if $\mathbf{d} \in D$ then $-\mathbf{d} \notin D$. We assume that all interactions between mass-points of P are binary and that the mass-points in an arbitrary cell $\Delta(\mathbf{x})$, $\mathbf{x} \in \Lambda$, can interact only with those in cells $\Delta(\mathbf{x} \pm \mathbf{d}^A)$, $A = 0, 1, \dots, M$. Let N stand for a number of binary interactions between points in an arbitrary cell $\Delta(\mathbf{x})$, $\mathbf{x} \in \Lambda$, and those in all cells $\Delta(\mathbf{x} + \mathbf{d}^A)$; $A = 0, 1, \dots, M$; due to the periodic structure of the system, the number N is independent of the choice of $\mathbf{x} \in \Lambda$. Let φ be a function

$$\varphi : \{1, \dots, N\} \ni K \rightarrow \varphi(K) \equiv (a, b, A) \in \{1, \dots, n\}^2 \times \{0, 1, \dots, M\} \quad (2.2)$$

such that for every $\mathbf{x} \in \Lambda$ points $\mathbf{p}^a(\mathbf{x})$ and $\mathbf{p}^b(\mathbf{x} + \mathbf{d}^A)$ can interact if and only if $(a, b, A) = \varphi(K)$ for some $K \in \{1, \dots, N\}$. It can be seen that $(a, b, 0) = (b, a, 0)$. The mapping (2.2) represents a *parametrization of the binary interactions* in P .

Using the above parametrizations we shall denote by m_a the mass of a th point in an arbitrary cell $\Delta(\mathbf{x})$, $\mathbf{x} \in \Lambda$, and by κ_K the elastic modulus determining the K th interaction. It means that if e^K is a change of a distance between the mass-points $\mathbf{p}^a(\mathbf{x})$ and $\mathbf{p}^b(\mathbf{x} + \mathbf{d}^A)$, where $(a, b, A) = \varphi(K)$, then $\kappa_K e^K$ is the value of mutual interaction between these points. At the same time it has to be understood that $|e^K|$ are small as compared to the corresponding distances between the mass-points $\mathbf{p}^a(\mathbf{x})$ and $\mathbf{p}^b(\mathbf{x} + \mathbf{d}^A)$, where $(a, b, A) = \varphi(K)$. Denoting

$$\mathbf{t}_a^K \equiv \begin{cases} \frac{\mathbf{p}^b(\mathbf{d}^A) - \mathbf{p}^a}{|\mathbf{p}^b(\mathbf{d}^A) - \mathbf{p}^a|} & \text{if } \varphi(K) = (a, b, A) \\ \mathbf{0} & \text{otherwise} \end{cases} \quad (2.3)$$

we conclude that $\kappa_K e^K \mathbf{t}_a^K$ is a force acting on $\mathbf{p}^a(\mathbf{x})$ from $\mathbf{p}^b(\mathbf{x} + \mathbf{d}^A)$.

For an arbitrary function $f(\mathbf{x})$, $\mathbf{x} \in \Lambda$, we introduce the denotations

$$\Delta_A f(\mathbf{x}) \equiv f(\mathbf{x} + \mathbf{d}^A) - f(\mathbf{x}) \quad \bar{\Delta}_A f(\mathbf{x}) \equiv f(\mathbf{x}) - f(\mathbf{x} - \mathbf{d}^A) \quad (2.4)$$

for the right- and left-hand side differences of $f(\cdot)$, respectively, provided that $A \neq 0$; for $A = 0$ we have $\Delta_A f = 0$.

3. Finite difference formulations

Let $\mathbf{u}^a = \mathbf{u}^a(\mathbf{x}, t)$, $\mathbf{x} \in \Lambda$, be a displacement vector at an instant t of an arbitrary mass-point from its equilibrium position $\mathbf{p}^a(\mathbf{x})$. The change of the distance between the points $\mathbf{p}^a(\mathbf{x})$ and $\mathbf{p}^b(\mathbf{x} + \mathbf{d}^A)$, for which $(a, b, A) = \varphi(K)$ for some $K \in \{1, \dots, N\}$, is equal to

$$e^K = \Delta_A \mathbf{u}^b \cdot \mathbf{t}_a^K + (\mathbf{u}^b - \mathbf{u}^a) \cdot \mathbf{t}_a^K \quad \varphi(K) = (a, b, A) \quad (3.1)$$

for the sake of simplicity here and in the sequel arguments $\mathbf{x} \in \Lambda$ and t are neglected. Functions $e^K = e^K(\cdot, t)$ defined on Λ will be called strains of the system under consideration. Hence within the framework of linearized elastodynamics function $\Phi = \Phi(\Delta_A \mathbf{u}^a, \mathbf{u}^b)$, given by

$$\Phi \equiv \frac{1}{2} \sum_{K=1}^N \kappa_K (e^K)^2 = \frac{1}{2} \sum_{K=1}^N \kappa_K [\Delta_A \mathbf{u}^b \cdot \mathbf{t}_a^K + (\mathbf{u}^b - \mathbf{u}^a) \cdot \mathbf{t}_a^K]^2 \quad (3.2)$$

where $(a, b, A) = \varphi(K)$, represents the strain energy assigned to an arbitrary cell. Using Eq (3.2) we shall introduce the generalized internal forces by means of

$$\mathbf{s}_A^a = \frac{\partial \Phi}{\partial \Delta_A \mathbf{u}^a} \quad \mathbf{s}^b = \frac{\partial \Phi}{\partial \mathbf{u}^b} \quad (3.3)$$

We also define the inertia matrix setting

$$M^{ab} = \begin{cases} m_a & \text{if } a = b \\ 0 & \text{otherwise} \end{cases} \quad (3.4)$$

while $\mathbf{f}^a = \mathbf{f}^a(\mathbf{x}, t)$ denote the external force acting at an instant t on the a th mass-point in a cell $\Delta(\mathbf{x})$. Under the aforementioned denotations it can be proved that functions $\mathbf{u}^a(\mathbf{x}, \cdot)$, $a = 1, \dots, n$, $\mathbf{x} \in \Lambda$, have to satisfy the equations

$$\overline{\Delta}_A \mathbf{s}_A^a - \mathbf{s}^a + \mathbf{f}^a - M^{ab} \ddot{\mathbf{u}}^b = \mathbf{0} \quad a = 1, \dots, n \quad (3.5)$$

where the summation convention over $A = 1, \dots, N$ and $b = 1, \dots, n$ holds and the internal forces are defined by Eq (3.3).

The aim of this section is to obtain an alternative formulation of the finite difference equations (3.5). To this end we define $m = m^1 + \dots + m^n$ and introduce the *averaged displacements* $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$, $\mathbf{x} \in \Lambda$, setting

$$\mathbf{u} \equiv \frac{1}{m} \sum_{a=1}^n m_a \mathbf{u}^a \quad (3.6)$$

Moreover, let h^{ak} , $(a, k) \in \{1, \dots, n\} \times \{1, \dots, n-1\}$, be real numbers satisfying the conditions

$$\sum_{a=1}^n m_a h^{ak} = 0 \quad k = 1, \dots, n-1 \quad (3.7)$$

and such that $\det[h^{ab}] \neq 0$, where $h^{an} \equiv 1$ for $a = 1, \dots, n$. In the subsequent considerations an arbitrary motion of the lattice system will be described in terms of functions $\mathbf{u}(\mathbf{x}, \cdot)$, $\mathbf{v}^k(\mathbf{x}, \cdot)$ of time, which for every $\mathbf{x} \in \Lambda$ are interrelated with functions $\mathbf{u}^a(\mathbf{x}, \cdot)$, by means of the one-to-one mapping (summation over $k = 1, \dots, n-1$ holds)

$$\mathbf{u}^a = \mathbf{u} + l h^{ak} \mathbf{v}^k \quad (3.8)$$

where $l > 0$ is a certain length parameter. The new unknowns $\mathbf{v}^k(\mathbf{x}, \cdot)$ will be called the *internal degrees of freedom*. It can be seen that

$$\mathbf{e}^K = \Delta_A \mathbf{u} \cdot \mathbf{t}_a^K + l(h^{bk} - h^{ak}) \mathbf{v}^k \cdot \mathbf{t}_a^K + l h^{bk} \Delta_A \mathbf{v}^k \cdot \mathbf{t}_a^K \quad (3.9)$$

for $\varphi(K) = (a, b, A)$. Hence, the strain energy function, now denoted by $W = W(\Delta_A \mathbf{u}, \mathbf{v}^k, \Delta_A \mathbf{v}^k)$, is equal to

$$W = \frac{1}{2} \sum_{K=1}^N \kappa_K [\Delta_A \mathbf{u} \cdot \mathbf{t}_a^K + l(h^{bk} - h^{ak})\mathbf{v}^k \cdot \mathbf{t}_a^K + lh^{bk} \Delta_A \mathbf{v}^k \cdot \mathbf{t}_a^K]^2 \quad (3.10)$$

where $\varphi(K) = (a, b, A)$. Setting

$$m^{kl} \equiv \sum_{a=1}^n m_a h^{ak} h^{al} \quad \mathbf{f} \equiv \sum_{a=1}^n \mathbf{f}^a \quad \mathbf{g}^k \equiv \sum_{a=1}^n h^{ak} \mathbf{f}^a$$

and introducing the new generalized internal forces

$$\mathbf{s}_A = \frac{\partial W}{\partial \Delta_A \mathbf{u}} \quad \mathbf{h}^k = \frac{\partial W}{\partial \mathbf{v}^k} \quad \mathbf{h}_A^k = \frac{\partial W}{\partial \Delta_A \mathbf{v}^k} \quad (3.11)$$

we can prove the following assertion.

Assertion 1. A motion of the system represented by averaged displacements $\mathbf{u}(\mathbf{x}, \cdot)$ and internal degrees of freedom $\mathbf{v}^k(\mathbf{x}, \cdot)$, $k = 1, \dots, n-1$, $\mathbf{x} \in \Lambda$, satisfies the equations

$$\begin{aligned} \overline{\Delta}_A \mathbf{s}_A + \mathbf{f} - m\ddot{\mathbf{u}} &= \mathbf{0} \\ \overline{\Delta}_A \mathbf{h}_A^k - \mathbf{h}^k + l\mathbf{g}^k - l^2 m^{kl} \ddot{\mathbf{v}}^l &= \mathbf{0} \quad k = 1, \dots, n-1 \end{aligned} \quad (3.12)$$

where the summation convention over $A = 1, \dots, N$ and $l = 1, \dots, n-1$ holds and the internal forces are defined by (3.11).

The equations of motion (3.12) together with Eqs (3.10), (3.11) constitute the basis for the subsequent analysis. It can be seen that the generalized internal forces (3.11) are related to those represented by Eq (3.3) by means of

$$\mathbf{s}_A = \sum_{a=1}^n \mathbf{s}_A^a \quad \mathbf{h}_A^k = \sum_{a=1}^n \mathbf{s}_A^a h^{ak} \quad \mathbf{h}^k = \sum_{a=1}^n \mathbf{s}^a h^{ak}$$

The main feature of the equations of motion (3.12) is the fact that deformations of the system, given by functions $\mathbf{u}(\cdot, t)$, $\mathbf{v}^k(\cdot, t)$ for an arbitrary but fixed time t , are defined on the Bravais lattice Λ .

4. Long wave deformations

Let us take into account a class of deformations $\mathbf{u}(\cdot, t)$, $\mathbf{v}^k(\cdot, t)$ depending on the length parameter l , $l > 0$, such that for every $\mathbf{x} \in \Lambda$ the conditions $\Delta_A \mathbf{u} \in O(l)$, $\Delta_A \mathbf{v}^k \in O(l)$ and $l \mathbf{v}^k \in O(l)$ hold. Hereafter we shall confine ourselves to deformations for which terms of a higher order $O(l^2)$ in Eq (3.9) can be neglected and hence the strains e^K are approximated by $\tilde{e}^K = \Delta_A \mathbf{u} \cdot \mathbf{t}_a^K + l(h^{bk} - h^{ak})\mathbf{v}^k \cdot \mathbf{t}_a^K \in O(l)$, $\varphi(K) = (a, b, A)$. It follows that the strain energy function will be given by

$$\widetilde{W} = \frac{1}{2} \sum_{K=1}^N \kappa_K [\Delta_A \mathbf{u} \cdot \mathbf{t}_a^K + l(h^{bk} - h^{ak})\mathbf{v}^k \cdot \mathbf{t}_a^K]^2 \quad (4.1)$$

The generalized internal forces are

$$\mathbf{s}_A = \frac{\partial \widetilde{W}}{\partial \Delta_A \mathbf{u}} \quad \mathbf{h}^k = \frac{\partial \widetilde{W}}{\partial \mathbf{v}^k} \quad (4.2)$$

and the equations of motion have the form

$$\overline{\Delta}_A \mathbf{s}_A + \mathbf{f} - m \ddot{\mathbf{u}} = \mathbf{0} \quad l^2 m^{kl} \ddot{\mathbf{v}}^l + \mathbf{h}^k = \mathbf{g}^k \quad (4.3)$$

with the summation convention over $A = 1, \dots, N$. It has to be emphasized that the second one from the above equations (related to the internal degrees of freedom \mathbf{v}^k) is a local one being independent of increments of functions $\mathbf{v}^k(\cdot, t)$. Hence, Eqs (4.2), (4.3) represent a certain *partly-local model* of the system. This model can be used if internal degrees of freedom are slowly varying functions, i.e., increments $\Delta_A \mathbf{v}^k$ can be treated as negligibly small as compared to the values of \mathbf{v}^k . It follows that the related deformations will be called the *long wave internal deformations*.

Let $\mathbf{u}(\cdot, t)$ and $\mathbf{v}^k(\cdot, t)$, $k = 1, \dots, n - 1$, be sufficiently regular functions defined on E^3 for every time t , which under restriction their domain to Λ coincide with averaged displacements and internal degrees of freedom, respectively. Moreover, let Ψ be an arbitrary differentiable function defined on E^3 such that for every $\mathbf{x} \in \Lambda \in E^3$ the following approximations take place

$$\Delta_A \Psi \cong \mathbf{d}^A \cdot \nabla \Psi \quad \overline{\Delta}_A \Psi \cong \mathbf{d}^A \cdot \nabla \Psi$$

Let us assume that $\mathbf{u}(\cdot, t)$, $\mathbf{v}^k(\cdot, t)$ together with all derivatives satisfy the above conditions and let us confine ourselves to the long wave internal deformations. In this case the class of function $\mathbf{u}(\cdot, t)$, $\mathbf{v}^k(\cdot, t)$ under consideration

will be referred to as the *long wave deformations*. For these deformations the strain energy function (4.1) can be approximated by

$$E = \frac{1}{2} \sum_{K=1}^N \kappa_K [(d^A \cdot \nabla \mathbf{u}) \cdot \mathbf{t}_a^K + l(h^{bk} - h^{ak}) \mathbf{v}^k \cdot \mathbf{t}_a^K]^2 \quad (4.4)$$

with $\varphi(K) = (a, b, A)$. Let us introduce the strain energy density function $\varepsilon = \varepsilon(\nabla \mathbf{u}, \mathbf{v}^k)$ by means of $\varepsilon \equiv El^{-3}$, where from now on $l^3 = \text{vol} \Delta$. The related generalized internal forces are

$$\mathbf{T} = \frac{\partial \varepsilon}{\partial \nabla \mathbf{u}} \quad \mathbf{h}^k = \frac{\partial \varepsilon}{\partial \nabla \mathbf{v}^k} \quad (4.5)$$

Let us also define densities $\mathbf{b} \equiv \mathbf{f}l^{-3}$, $\rho \equiv ml^{-3}$, $\mathbf{b}^k \equiv \mathbf{g}^k l^{-3}$ and $\rho^{kl} \equiv m^{kl} l^{-3}$. Under the aforementioned denotations the following statement holds true.

Assertion 2. For the long wave deformations, which for every t are represented by sufficiently regular functions $\mathbf{u}(\cdot, t)$, $\mathbf{v}^k(\cdot, t)$, $k = 1, \dots, n-1$, defined on E^3 , an arbitrary motion of the system is governed by the equations

$$\begin{aligned} \nabla \cdot \mathbf{T} + \mathbf{b} - \rho \ddot{\mathbf{u}} &= \mathbf{0} \\ l^2 \rho^{kl} \ddot{\mathbf{v}}^l + \mathbf{h}^k &= \mathbf{b}^k \quad k = 1, \dots, n-1 \end{aligned} \quad (4.6)$$

with the internal forces defined by Eq (4.5).

The proof of this assertion follows directly from Eqs (4.2), (4.3), after taking into account that \widetilde{W} can be approximated by E and using the relations

$$\frac{\partial E}{\partial \nabla \mathbf{u}} \cong \frac{\partial \widetilde{W}}{\partial \Delta_A \mathbf{u}} \otimes \mathbf{d}^A = \mathbf{s}_A \otimes \mathbf{d}^A \quad \overline{\Delta}_A \mathbf{s}_A \cong \mathbf{d}^A \cdot \nabla \mathbf{s}_A = \nabla \cdot \frac{\partial E}{\partial \nabla \mathbf{u}}$$

where the summation convention over $A = 1, \dots, N$ holds. Eqs (4.5), (4.6) represent a local model of the polyatomic lattice system under consideration.

Let us observe that neglecting in Eqs (4.3) and (4.6) the terms which depend explicitly on l^2 we shall obtain certain approximate models in which internal degrees of freedom can be eliminated from equations of motion. In the partly local model given by Eqs (4.2), (4.3) we obtain for \mathbf{v}^k a system of linear algebraic equations obtained from $\partial \widetilde{W} / \partial \mathbf{v}^k = \mathbf{g}^k$. It can be shown that this system has a unique solution given by $\mathbf{v}^k = \mathbf{D}_A^k \Delta_A \mathbf{u} + \mathbf{v}_0^k$, where \mathbf{D}_A^k are 3×3 matrices and the summation convention over $A = 1, \dots, N$ holds. Substituting

the obtained solution to Eq (4.1) we arrive at the strain energy function in the form $W_0 = W_0(\Delta_A \mathbf{u})$ independent of \mathbf{v}^k . The governing equations for averaged displacements \mathbf{u} will be given by

$$\overline{\Delta}_A \mathbf{s}_A + \mathbf{f} - m\ddot{\mathbf{u}} = \mathbf{0} \quad \mathbf{s}_A = \frac{\partial W_0}{\partial \Delta_A \mathbf{u}} \quad (4.7)$$

The similar procedure can be also applied to the local equations (4.5), (4.6) where after elimination of \mathbf{v}^k we arrive at the strain energy density in the form $\varepsilon_0 = \varepsilon_0(\nabla \mathbf{u})$. In this local model the governing equations for averaged displacements are

$$\nabla \cdot \mathbf{T} + \mathbf{b} - \rho \ddot{\mathbf{u}} = \mathbf{0} \quad \mathbf{T} = \frac{\partial \varepsilon_0}{\partial \nabla \mathbf{u}} \quad (4.8)$$

It can be observed that Eqs (4.7), from the formal point of view, are similar to the equations for monoatomic lattice systems. At the same time, Eqs (4.8) are similar to the equations describing a local model of monoatomic lattice systems and coincide with equations of motion of the linear elasticity. The aforementioned models can be applied only to the problems in which the inertia forces due to oscillatory motions inside every molecule can be neglected.

5. Conclusions

The main results of this contribution are:

- Formulation of the finite difference equations for dynamics of polyatomic lattices systems in the simple form (3.12) with averaged displacements and internal degrees of freedom as basic unknowns.
- Derivation from Eq (3.12) partly local models represented by Eqs (4.3) in which the internal degrees of freedom are governed by local equations.
- Passage from partly local equations (4.3) to the local equations (4.6) which determine a certain continuum model of a periodic composite mass-point system.
- Possibility of elimination of integral degrees of freedom from Eqs (4.2) and (4.3), leading to Eqs (4.7) and (4.8) which reveal the formal resemblance with the equations of monoatomic lattices and their local models, respectively.

More detailed discussion of the obtained results and their applications to the analysis of vibrations and wave propagation problems will be given separately.

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O dynamice sieci wieloatomowych

Streszczenie

Wprowadzając pojęcie wewnętrznych stopni swobody sformułowano nową różnicową postać dynamiki sieci złożonych. Pokazano przejście od równań nielokalnych do modeli częściowo i całkowicie lokalnych oraz zwrócono uwagę na możliwość wyrugowania wewnętrznych stopni swobody.