

Nonlinear equations of deformation of atomic lattices

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THIS PAPER PRESENTS VECTOR, scalar and variational forms of motion/equilibrium equations of atomic lattices. An automated method is suggested for constructing the matrices and vectors of equations based on summing the corresponding local matrices and vectors of atomic pairs. The exact expression for the tangential stiffness matrix of an atomic pair is obtained where both the change in the segment length of a straight line connecting atoms in this pair and rotation of the segment are taken into account.

1. Introduction

ACCORDING TO PRESENT-DAY IDEAS of solid-state physics (cf., [1]), many solids under common conditions are either single crystals or polycrystals. The single crystal is some spatial atomic lattice with an ordered structure, and the polycrystal is a set of single crystals with various spatial orientations.

A solution of nonlinear problems of deformation of atomic lattices is a pertinent question, for example, in connection with an attempt to describe adequately the initiation and propagation of the crack in a solid under tensile and shear loads. In the context of continuum mechanics, phenomenological models of solid fracture offer no correct pattern of stress and strain distribution in the vicinity of a crack. In particular, the solution of the problems in the framework of linear fracture mechanics leads to infinite values of stresses and strains at the crack tip for the linear-elastic material model. There is thus a conflict between these results and finite values of interaction forces between atoms that make up the solid. The attempts to construct a more correct model of solid fracture result in the description of initiation and propagation of a crack at the atomic level [2, 3] when buckling of an atomic lattice induces the initiation of a crack. A wide difference between tensile failure loads obtained experimentally and theoretical tensile failure loads is due to the presence of foreign atoms and vacancies in an atomic chain [4].

The objective of the present work is to develop various novel formulations of motion/equilibrium equations for atomic lattices. Vector, scalar and variational formulations of the equations are given. One of the complicated things in

constructing a motion/equilibrium system of equations for an atomic lattice is to obtain the matrices and vectors of such a system. KORUBEYNIKOV [5, 6] has proposed to apply a well-developed technique for numerical solution of nonlinear problems of solid mechanics by the FEM (finite element method) (cf., [7–10]) for formulating nonlinear problems of deformation of atomic lattices. In doing so, each atomic pair is considered as a ‘finite element’ for which formulations of the tangential stiffness matrix and vector of internal forces have been obtained. Application of the FEM technique is based on using scalar forms of the motion/equilibrium equations, but the matrices and vectors obtained are finally used to yield a system of equations in vector, scalar and variational formulations.

In [5, 6], the tangential stiffness matrix of an atomic pair is obtained with allowance for change only in the segment length directed along the line of action of the central force of interaction between the atoms. In the present work, a refined formulation of this matrix is developed with allowance for rotation of this segment.

2. Statement of the problem of deformation of an atomic lattice

The ordered set of the atoms (molecules) in equilibrium state (by “equilibrium state” we generally mean both static and dynamic states of a lattice) under the action of internal (interatomic) and external forces (at dynamic equilibrium state the inertial forces are included in the external ones) will be termed an atomic lattice. In the present work, we will consider the internal forces corresponding only to central forces of interaction between atoms. Suppose the action of the central atomic forces follows from the potential

$$(2.1) \quad f = \frac{\partial V(r)}{\partial r}, \quad r \in (0, \infty),$$

where $V(r)$ is the potential energy of the central atomic force at the distance r between atoms in an atomic pair (Fig. 1a).

We consider two kinds of this function (cf., [1]):

- the Lennard–Jones (12-6) potential

$$V(r) = D \left[\left(\frac{r_e}{r} \right)^{12} - 2 \left(\frac{r_e}{r} \right)^6 \right],$$

- and the Morse potential

$$(2.2) \quad V(r) = D \left[e^{-2\alpha(r-r_e)} - 2e^{-\alpha(r-r_e)} \right],$$

where D is the energy of an atomic bond (the depth of a potential hole), r_e is the distance between atoms corresponding to the minimum of potential energy

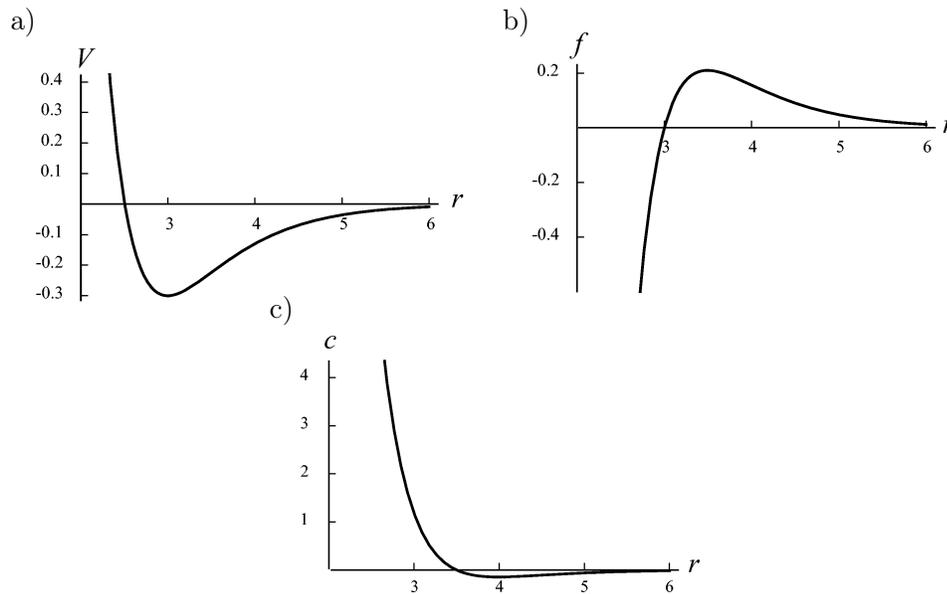


FIG. 1. Potential V , force f , and value c versus the distance r between atoms (dependences for the Morse potential with constants: $r_e = 3$, $\alpha = 1.4$, $D = 0.3$ are given):

a) V versus r , b) f versus r , c) c versus r .

of the atomic bond, and α is the prescribed value determining the potential form (cf., Eq. (2.2)).

A typical dependence of the central force f of atom interaction in an atomic pair of a lattice at the distance r between atoms is shown in Fig. 1b (cf., [1]). For $r = r_e$ (the equilibrium state in the absence of the external forces acting on an atomic pair), the central force of interaction between atoms is equal to zero; for $r < r_e$, a (negative) repulsion force acts between the atoms; for $r > r_e$, a (positive) attractive force acts between the atoms, the force taking the maximum value f_m at some distance r_m , so that the central force of interaction between atoms is weaker as the atoms move away from each other and this force decreases by one order of magnitude from its maximum value at distance $2r_e$.

In conformity with Eq. (2.1), the first derivative of the potential $V(r)$ suggests the expression of the central force of interaction between atoms. Further we need the second derivative of the potential

$$(2.3) \quad c \equiv \frac{\partial f}{\partial r} = \frac{\partial^2 V(r)}{\partial r^2},$$

that characterizes the rate of change in the central force f depending on r

(Fig. 1 c). We find explicit expressions of f , c , r_m and f_m for the considered potential functions:

- the Lennard–Jones (12–6) function

$$f = \frac{12D}{r} \left[\left(\frac{r_e}{r} \right)^6 - \left(\frac{r_e}{r} \right)^{12} \right], \quad c = \frac{12D}{r^2} \left[13 \left(\frac{r_e}{r} \right)^{12} - 7 \left(\frac{r_e}{r} \right)^6 \right],$$

$$r_m = \sqrt[6]{\frac{13}{7}} r_e, \quad f_m = \frac{72D}{13r_e} \left(\frac{7}{13} \right)^{7/6},$$

- the Morse function

$$f = 2D\alpha [e^{-\alpha(r-r_e)} - e^{-2\alpha(r-r_e)}], \quad c = 2D\alpha^2 [2e^{-2\alpha(r-r_e)} - e^{-\alpha(r-r_e)}],$$

$$r_m = r_e + \frac{\ln 2}{\alpha}, \quad f_m = \frac{D\alpha}{2}.$$

Suppose that the atomic lattice consists of K atoms. Each atom in the atomic lattice is under the action of both central forces (short-range interaction $r \approx r_e$ follows from the nearest neighbors; long-range interaction $r \gtrsim 2r_e$ results from more remote neighbors) and external forces (Fig. 2).

It is noted that the character of external forces is of no importance for solving the problem of deformation of a lattice; in particular, these forces may also be the central forces of interaction between atoms, which are not included in the atomic lattice considered in the statement of the problem. It is assumed that the external forces are known, i.e. both their magnitude and direction of their action. The vector equation of balance of the forces acting on the k -th atom ($k = \overline{1, K}$) in a lattice takes the form

$$(2.4) \quad \sum_{m=1}^{M_k} \mathbf{f}_k^m = \mathbf{R}_k - m_k \ddot{\mathbf{u}}_k.$$

Henceforth, M_k is the number of atoms in a lattice, the action of the internal forces of these atoms on the k -th atom being taken into account; \mathbf{f}_k^m is the central interaction force of the m -th atomic pair; \mathbf{R}_k and $m_k \ddot{\mathbf{u}}_k$ are the vectors of external and inertial forces acting on the k -th atom (m_k is the mass of the k -th atom; \mathbf{u}_k is the displacement vector of the k -th atom; henceforth, a superimposed dot denotes the derivative of the value with respect to time t , i.e., $\ddot{\mathbf{u}}_k$ is the acceleration vector of the k -th atom). Suppose that M_k of the neighbor atoms interact with the k -th atom, the number M_k being arbitrary: the more influence of neighbor atoms (including remote atoms: $r \gtrsim 2r_e$) on behavior of the k -th atom is taken into account, the larger is the number M_k . In most cases, only the action of the nearest neighbors ($r \approx r_e$) can be accounted for. It should be noted that the number M_k may vary from atom to atom.

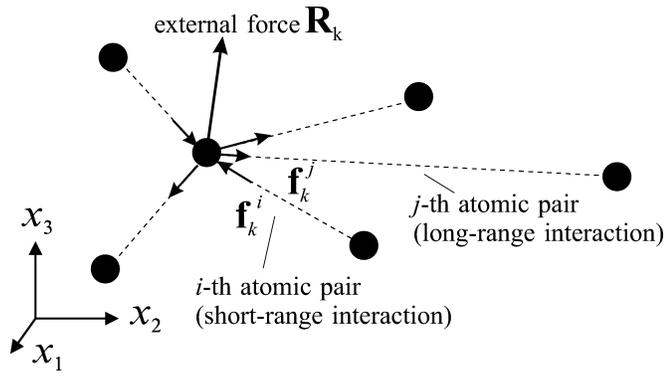


FIG. 2. Internal force \mathbf{f}_k^m and external force \mathbf{R}_k acting on the k -th atom ($1 \leq k \leq K$).

3. Vector form of motion/equilibrium equations of atomic lattice

The motion of each atom in a lattice depends on motions of other atoms. In the general case, since values of the internal forces \mathbf{f}_k^m in Eq. (2.4) are unknown, this equation is not solved separately for each atom. A set of all equations of the form (2.4) yields the system of $N = 3K$ of nonlinear ordinary differential equations relative to the i -th ($i = 1, 2, 3$) components of displacement vectors of the k -th ($k = \overline{1, K}$) atoms. Let us introduce a column vector of atom displacement components in a lattice

$$(3.1) \quad \mathbf{U} = [u_1^1, u_2^1, u_3^1, u_1^2, u_2^2, u_3^2, \dots, u_1^K, u_2^K, u_3^K]^T.$$

Henceforth, the upper index T denotes a transposition operation and u_i^k is the i -th component of the displacement vector of the k -th atom in an atomic lattice. The sought system of equations with initial conditions can be written in the form of a single vectorial nonlinear motion equation of an atomic lattice

$$(3.2) \quad \mathbf{F}(\mathbf{U}) = \mathbf{R} - \mathbf{M}\ddot{\mathbf{U}}, \quad \mathbf{U}(0) = \mathbf{U}_0, \quad \dot{\mathbf{U}}(0) = \mathbf{V}_0.$$

Here \mathbf{F} is the internal force vector of a lattice, \mathbf{R} is the external force vector of a lattice, $\ddot{\mathbf{U}}$ is the acceleration vector of a lattice; \mathbf{U}_0 and \mathbf{V}_0 are the prescribed vectors of initial values of the displacement vector \mathbf{U} and velocity vector $\dot{\mathbf{U}}$ of an atomic lattice, respectively; and \mathbf{M} is the diagonal positive definite mass matrix of a lattice

$$\text{diag}(\mathbf{M}) = [m_1, m_1, m_1, m_2, m_2, m_2, \dots, m_K, m_K, m_K].$$

If inertial forces may be neglected, Eq. (3.2) is reduced to the nonlinear vectorial algebraic equilibrium equation (to the system of N scalar algebraic equations) of an atomic lattice

$$(3.3) \quad \mathbf{F}(\mathbf{U}) = \mathbf{R}.$$

It should be noted that the number N of scalar equations in systems (3.2) and (3.3) is independent of the values M_k ($k = \overline{1, K}$) corresponding to the number of neighbors being considered for the k -th atom.

Components u_i^k of the vector \mathbf{U} in Eqs. (3.2) and (3.3) are assumed to be independent degrees of freedom. These equations should be modified if restrictions are imposed on the degrees of freedom of some atoms. Denoting a degree of freedom u_i^k ($i = 1, 2, 3, k = \overline{1, K}$) by U_n ($n = \overline{1, N}$), we can rewrite expression (3.1) for the vector \mathbf{U} in the form

$$\mathbf{U} = [U_1, U_2, \dots, U_N]^T.$$

Let the restrictions on some degrees of freedom of an atomic lattice be imposed in the form

$$(3.4) \quad U_j(t) = U_j^*(t) \quad (1 \leq j \leq N),$$

where the asterisk denotes a prescribed value. To illustrate such restrictions, we give the following example. Let prescribed values be assigned to six components of the displacement vector in order to eliminate the motion of a lattice as a single rigid whole (three components of the displacement vector and three rotations relative to the axes of the Cartesian coordinate system). It is necessary to apply such elimination for solving the system (3.3), and it is useful but not necessary to apply elimination for solving the system (3.2).

The inclusion of restrictions (3.4) into Eqs. (3.2) and (3.3) can be performed in different ways. First, the restrictions (3.4) can be introduced directly into Eqs. (3.2) and (3.3) by rejection of the j -th equations from these systems and modifying the remaining equations (transferring the members containing U_j values from the left-hand sides of equations to the right-hand ones). Following [9], this method of inclusion of restrictions can be referred to as the condensation of a system of equations. Rejecting the prescribed components with numbers j ($1 \leq j \leq N$) from the vector \mathbf{U} and renumbering the remaining independent degrees of freedom, we introduce a condensed displacement vector of an atomic lattice

$$\hat{\mathbf{U}} = [U_1, U_2, \dots, U_{NEQ}]^T$$

where $NEQ = N - J$ is the number of independent degrees of freedom of an atomic lattice (J is the total number of restrictions of the form (3.4)). The condensation method allows restrictions in Eq. (3.4) to be taken exactly into account. But the method is complicated enough in practical realization and it does not allow to define the reaction forces corresponding to the prescribed displacements.

Second, restrictions (3.4) can be taken into account also by using the classical methods of introducing restrictions into equations, such as the methods of

Lagrangian multiplier or penalty function (cf., [7, 8]). The Lagrangian multiplier method provides a faithful inclusion of restrictions and determination of the reaction forces, but it is inconvenient in practical realization and, moreover, the method leads to an increase in the number of unknown values since J unknown Lagrangian multipliers are added to the sought N independent degrees of freedom (in this method, U_j degrees of freedom in Eq. (3.4) are assumed to be independent). The total number of both the degrees of freedom and scalar equations in Eqs. (3.2) and (3.3) becomes equal to $NEQ = N + J$. The penalty function method is more efficient. When using this method, equations in systems (3.2) and (3.3) corresponding to the j -th degrees of freedom in Eq. (3.4) are modified, the total number of these equations being unchanged (i.e., $NEQ = N$). The reaction forces are also defined. However, restrictions in Eq. (3.4) are satisfied approximately.

In order to avoid introduction of additional notation, the modified systems of equations of the order NEQ (as a result of restrictions being accounted by one of the presented methods) are written in the same form as it was shown before in Eqs. (3.2) and (3.3). It is difficult to obtain an expression of the internal force vector \mathbf{F} by a direct composition of vectors of the forces applied to atoms in a lattice. It is simpler to derive an expression for this vector based on the scalar form of the motion/equilibrium equations, which are given in the following section.

4. Scalar form of motion/equilibrium equations of an atomic lattice

Taking the scalar product of both the left- and right-hand sides of vector equation (3.2) by the arbitrary vector $\mathbf{W} \in R^{NEQ}$, we obtain the scalar equation

$$(4.1) \quad \mathbf{W}^T \mathbf{F}(\mathbf{U}) = \mathbf{W}^T \mathbf{R} - \mathbf{W}^T \mathbf{M}\ddot{\mathbf{U}} \quad \forall \mathbf{W} \in R^{NEQ}.$$

On the contrary, matching special expressions of vectors \mathbf{W} , we may obtain each scalar equation in the system (3.2) from Eq. (4.1). That is, vector equation (3.2) and scalar equation (4.1) are equivalent (cf., [9]).

If by the ‘vector \mathbf{W} ’ we mean a vector of possible (virtual) velocities of lattice atoms (the velocities do not necessarily satisfy the motion equations (3.2)), then Eq. (4.1) expresses the equality of virtual power balance: the virtual power of internal forces is equal to that of external forces (including inertial forces). If by the ‘vector \mathbf{W} ’ we mean a vector of virtual displacement of an atomic lattice $\delta\mathbf{U}$, then Eq. (4.1) can be rewritten as

$$(4.2) \quad \delta\mathbf{U}^T \mathbf{F}(\mathbf{U}) = \delta\mathbf{U}^T \mathbf{R} - \delta\mathbf{U}^T \mathbf{M}\ddot{\mathbf{U}} \quad \forall \delta\mathbf{U} \in R^{NEQ}.$$

In mechanics, scalar equation (4.1) given in the form of Eq. (4.2) is commonly referred to as an equation of the virtual work principle. This principle is formulated as follows: virtual work of the internal forces (work of the internal forces at virtual displacements) is equal to that of the external forces (including the inertial forces).

The virtual power of internal forces of an atomic lattice w is expanded additively into virtual powers of the internal forces of all atomic pairs w_m ($m = \overline{1, M}$), i.e.,

$$(4.3) \quad w = \sum_{m=1}^M w_m,$$

where M is the total number of atomic pairs of a lattice that are considered in the mathematical model. The following notations are introduced here

$$(4.4) \quad w \equiv \mathbf{W}^T \mathbf{F}(\mathbf{U}), \quad w_m \equiv \mathbf{W}^T \tilde{\mathbf{F}}^m(\mathbf{U}) \quad \forall \mathbf{W} \in R^{NEQ},$$

where $\tilde{\mathbf{F}}^m(\mathbf{U})$ is the internal force vector of an atomic pair. From Eqs. (4.3) and (4.4) and taking the vector \mathbf{W} as arbitrary, we have

$$(4.5) \quad \mathbf{F}(\mathbf{U}) = \sum_{m=1}^M \tilde{\mathbf{F}}^m(\mathbf{U}).$$

The equality in Eq. (4.5) allows to pass from the definition of the internal force vector \mathbf{F} of an atomic lattice to the definition of the internal force vector $\tilde{\mathbf{F}}^m$ of the m -th atomic pair. It is more appropriate to define this vector by going from the global approach to a local one (cf., [9]). Since only two atoms are needed to define a virtual power of the internal force of an atomic pair, the definition of virtual power of the internal force w_e of the e -th ($1 \leq e \leq M$) atomic pair may be written as

$$(4.6) \quad w_e = \mathbf{W}^{eT} \mathbf{F}^e(\mathbf{U}^e),$$

where $\mathbf{W}^e \in R^6$ is an arbitrary vector of the form

$$\mathbf{W}^e \equiv [W_1, W_2, W_3, W_4, W_5, W_6]^T,$$

so that W_1, W_2, W_3 are components of the virtual velocity vector of the first atom, and W_4, W_5, W_6 are the same components of the second atom in the atomic pair being considered (Fig. 3).

Note that numbers #1 and #2 are assigned to atoms arbitrarily. The displacement vector $\mathbf{U}^e \in R^6$ of an atomic pair is defined as follows:

$$(4.7) \quad \mathbf{U}^e \equiv [u_1^1, u_2^1, u_3^1, u_1^2, u_2^2, u_3^2]^T = [U_1, U_2, U_3, U_4, U_5, U_6]^T,$$

where u_j^i is the j -th ($j = 1, 2, 3$) component of the displacement vector \mathbf{u}_i of the i -th ($i = 1, 2$) atom in the considered atomic pair. Note that in Eq. (4.7) the local numbering is used, which is generally not coincident with the global numbering of the degrees of freedom of an atomic lattice.

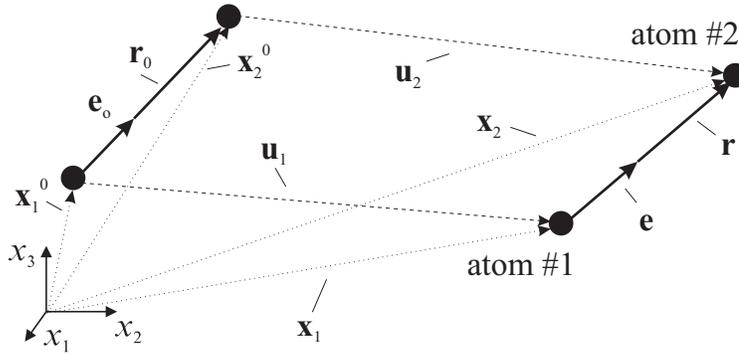


FIG. 3. Initial and deformed configurations of the k -th atomic pair.

The power of the internal forces of an atomic pair is defined as follows:

$$(4.8) \quad w_e = f\dot{r}.$$

For r , we have the expression:

$$(4.9) \quad r \equiv \sqrt{\mathbf{r}^T \mathbf{r}} = \sqrt{r_k r_k} \quad (k = 1, 2, 3).$$

Henceforth, summing is extended over repeated indices (indices run over all their values for which they are defined), r_k is the k -th component of a vector

$$(4.10) \quad \mathbf{r} \equiv \mathbf{x}_2 - \mathbf{x}_1 \Leftrightarrow \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} x_1^2 \\ x_2^2 \\ x_3^2 \end{bmatrix} - \begin{bmatrix} x_1^1 \\ x_2^1 \\ x_3^1 \end{bmatrix}.$$

Here \mathbf{x}_i is the position vector of the i -th ($i = 1, 2$) atom, and x_j^i ($j = 1, 2, 3$) are its components (Fig. 3). From Eq. (4.9), we obtain

$$(4.11) \quad \dot{r} = \frac{1}{r} r_k \dot{r}_k = e_k \dot{r}_k = \mathbf{e}^T \dot{\mathbf{r}},$$

where $e_k = r_k/r$ ($k = 1, 2, 3$) are components of the unit length vector $\mathbf{e} = [e_1, e_2, e_3]^T$

$$(4.12) \quad \mathbf{e} \equiv \mathbf{r}/r,$$

directed along the segment connecting atoms #1 and #2 (Fig. 3).

Since

$$\mathbf{x}_i = \mathbf{x}_i^0 + \mathbf{u}_i, \quad \mathbf{x}_i^0 \equiv \mathbf{x}_i(0),$$

using Eq. (4.10), the vector \mathbf{r} can be written in the form

$$(4.13) \quad \mathbf{r} = \mathbf{r}_0 + \mathbf{u}_2 - \mathbf{u}_1, \quad \mathbf{r}_0 \equiv \mathbf{r}(0) = \mathbf{x}_2^0 - \mathbf{x}_1^0.$$

Here \mathbf{x}_i^0 is the position vector of the i -th ($i = 1, 2$) atom at the initial time $t = 0$. From Eq. (4.13), we obtain

$$(4.14) \quad \dot{\mathbf{r}} = \dot{\mathbf{u}}_2 - \dot{\mathbf{u}}_1.$$

We introduce a matrix

$$\mathbf{D} \equiv [-\mathbf{I}, \mathbf{I}], \quad \mathbf{I} \equiv \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

such that expression

$$(4.15) \quad \dot{\mathbf{r}} = \mathbf{D}\dot{\mathbf{U}}^e$$

is valid. Substituting $\dot{\mathbf{r}}$ from Eq. (4.15) into Eq. (4.11), we obtain

$$(4.16) \quad \dot{r} = \mathbf{B}\dot{\mathbf{U}}^e = \dot{\mathbf{U}}^{eT} \mathbf{B}^T,$$

where a row vector is introduced

$$(4.17) \quad \mathbf{B} \equiv \mathbf{e}^T \mathbf{D} = [-e_1, -e_2, -e_3, e_1, e_2, e_3].$$

Replacing the velocity vector $\dot{\mathbf{U}}^e$ in Eq. (4.16) with an arbitrary virtual velocity vector of an atomic pair $\mathbf{W}^e \in R^6$, substituting \dot{r} into Eq. (4.8) with regard to Eq. (4.6) and in view of the fact that \mathbf{W}^e is arbitrary, we obtain

$$(4.18) \quad \mathbf{F}^e(\mathbf{U}^e) = f\mathbf{B}^T.$$

Note that nonlinear dependence of the vector \mathbf{F}^e on the vector \mathbf{U}^e in Eq. (4.18) is implicit.

We use the standard FEM technique [7–10] to turn from definition of the internal force vector of an atomic pair \mathbf{F}^e in local variables to a definition of this vector $\tilde{\mathbf{F}}^e$ in the global ones. We introduce a Boolean localization matrix (the elements of which consist of zeros and units) of an atomic pair \mathbf{A}^e such that [9, 10]

$$(4.19) \quad \mathbf{U}^e = \mathbf{A}^e \mathbf{U}, \quad \mathbf{W}^e = \mathbf{A}^e \mathbf{W}.$$

From Eqs. (4.4), (4.6) and (4.19), we obtain an expression relating internal force vectors of an atomic pair applying both the local and global approaches

$$(4.20) \quad \tilde{\mathbf{F}}^e = \mathbf{A}^{eT} \mathbf{F}^e.$$

Following the definition of internal force vectors $\tilde{\mathbf{F}}^e$ of all atomic pairs, the internal force vector \mathbf{F} of a lattice is defined from Eq. (4.5).

Summing operation of internal force vectors of atomic pairs \mathbf{F}^e to get the internal force vector \mathbf{F} using localization matrices \mathbf{A}^e is referred to as an assembly operation in the FEM literature. The symbol 'A' is frequently used for this operation (cf., [9]), so that Eq. (4.5) may be rewritten as

$$(4.21) \quad \mathbf{F}(\mathbf{U}) = \sum_{m=1}^M \mathbf{A}^m \mathbf{F}^m(\mathbf{U}^m) \quad \Leftrightarrow \quad \mathbf{F}(\mathbf{U}) = \sum_{m=1}^M \mathbf{A}^{mT} \mathbf{F}^m(\mathbf{A}^m \mathbf{U}).$$

Vector equation (3.3) is equivalent to the scalar equilibrium equation

$$(4.22) \quad \mathbf{W}^T \mathbf{F}(\mathbf{U}) = \mathbf{W}^T \mathbf{R} \quad \forall \mathbf{W} \in R^{NEQ},$$

which is obtained by rejection of the last summand in the right-hand side of Eq. (4.1).

5. The variational formulation of equilibrium equations of an atomic lattice

Scalar equilibrium equation (4.22) and, hence, vector equation (3.3) can be derived using a stationarity principle of the total potential energy (the variational formulation of equilibrium equations) of an atomic lattice. The stationarity principle is formulated below.

Consider the total potential energy of an atomic lattice

$$E(\mathbf{U}) = V(\mathbf{U}) - \mathbf{U}^T \mathbf{R},$$

which is the sum of potential energies of the internal forces $V(\mathbf{U})$ and the external forces $-\mathbf{U}^T \mathbf{R}$ of an atomic lattice. The potential energy of an atomic lattice $V(\mathbf{U})$ is equal to the sum of potential energies of central forces of interatomic interactions in all atomic pairs

$$(5.1) \quad V(\mathbf{U}) = \sum_{m=1}^M \tilde{V}^m(\mathbf{U}),$$

where

$$(5.2) \quad \tilde{V}^m(\mathbf{U}) \equiv V^m[r(\mathbf{U}^m)] = V^m(\mathbf{U}^m) = V^m(\mathbf{A}^m \mathbf{U})$$

is the potential energy of the m -th atomic pair (see Sec. 2). Here $\tilde{V}^e(\mathbf{U})$ ($1 \leq e \leq M$) is the potential energy of an atomic pair that is expressed in terms of the components of the global displacement vector \mathbf{U} of an atomic lattice, and $V^e(\mathbf{U}^e)$ is the potential energy of this pair expressed in terms of the displacement vector \mathbf{U}^e of an atomic pair using dependence $r(\mathbf{U}^e)$ that is obtained with the help of Eqs. (4.9) and (4.13).

Now we find the differential of the total potential energy of an atomic lattice in the form

$$(5.3) \quad dE(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T \frac{\partial V}{\partial \mathbf{U}} - d\mathbf{U}^T \mathbf{R},$$

or in the component form

$$dE(U_i, dU_j) = \frac{\partial V}{\partial U_k} dU_k - R_k dU_k \quad (i, j, k = \overline{1, NEQ}).$$

The potential energy gradient of internal forces of an atomic lattice $\partial V / \partial \mathbf{U}$ is defined using Eqs. (5.1) and (5.2):

$$dV(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T \frac{\partial V}{\partial \mathbf{U}} = \sum_{m=1}^M d\tilde{V}^m(\mathbf{U}) = \sum_{m=1}^M dV^m(\mathbf{U}^m).$$

Define now the differential of the potential energy of internal force of the e -th ($1 \leq e \leq M$) atomic pair. From Eq. (5.2), we obtain

$$(5.4) \quad dV^e(\mathbf{U}^e, d\mathbf{U}^e) = \frac{\partial V^e(r)}{\partial r} \frac{\partial r}{\partial U_i} dU_i \quad (i = \overline{1, 6}),$$

where U_i are displacement vector components of an atomic pair (see Eq. (4.7)). Equation (2.1) can be rewritten as

$$(5.5) \quad f = \frac{\partial V^e(r)}{\partial r}.$$

From Eqs. (4.9) and (4.12), we obtain

$$(5.6) \quad \frac{\partial r}{\partial U_i} = \frac{1}{r} r_k \frac{\partial r_k}{\partial U_i} = e_k \frac{\partial r_k}{\partial U_i} \quad (k = 1, 2, 3, i = \overline{1, 6}).$$

Rewrite Eq. (4.13)₁ in the component form

$$(5.7) \quad r_k = r_k^0 + u_k^2 - u_k^1 \quad (k = 1, 2, 3).$$

Using Eqs. (4.7) and (5.7), from Eq. (5.6) we obtain

$$(5.8) \quad \begin{aligned} \frac{\partial r}{\partial U_1} &= -e_1, & \frac{\partial r}{\partial U_2} &= -e_2, & \frac{\partial r}{\partial U_3} &= -e_3, \\ \frac{\partial r}{\partial U_4} &= e_1, & \frac{\partial r}{\partial U_5} &= e_2, & \frac{\partial r}{\partial U_6} &= e_3. \end{aligned}$$

Substituting expressions (5.5) and (5.8) into Eq. (5.4) and using Eqs. (4.17) and (4.18), we obtain

$$dV^e = f\mathbf{B} d\mathbf{U}^e = \mathbf{F}^{eT} d\mathbf{U}^e = d\mathbf{U}^{eT} \mathbf{F}^e.$$

From Eq. (4.19)₁, we have

$$(5.9) \quad d\mathbf{U}^e = \mathbf{A}^e d\mathbf{U}.$$

Then from Eqs. (4.20), (5.2), and (5.9), we get

$$(5.10) \quad dV^e(\mathbf{U}^e, d\mathbf{U}^e) = dV^e(\mathbf{A}^e \mathbf{U}, \mathbf{A}^e d\mathbf{U}) = d\tilde{V}^e(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T \tilde{\mathbf{F}}^e.$$

From Eqs. (4.21), (5.1) and (5.10), we obtain

$$(5.11) \quad dV(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T \mathbf{F}(\mathbf{U}).$$

Since (see Eq. (5.3))

$$(5.12) \quad dV(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T \frac{\partial V}{\partial \mathbf{U}},$$

then from Eqs. (5.11), (5.12) and in view of the fact that the vector $d\mathbf{U}$ is arbitrary, we obtain

$$(5.13) \quad \frac{\partial V}{\partial \mathbf{U}} = \mathbf{F}(\mathbf{U}) \quad \Leftrightarrow \quad \frac{\partial V}{\partial U_i} = F_i \quad (i = \overline{1, NEQ}).$$

Using Eq. (5.13), we rewrite Eq. (5.3) for the differential of the total potential energy of an atomic lattice

$$(5.14) \quad dE(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T [\mathbf{F}(\mathbf{U}) - \mathbf{R}] \quad \mathbf{U}, d\mathbf{U} \in R^{NEQ}.$$

Let us formulate and prove the theorem on stationarity of the total potential energy of an atomic lattice.

THEOREM 1. *For an atomic lattice to be in equilibrium state it is necessary and sufficient that its total potential energy should take a stationary value.*

P r o o f. Necessity. Let an atomic lattice be in the equilibrium state, so that system (3.3) is realized. Then using Eq. (5.14), we obtain

$$(5.15) \quad dE(\mathbf{U}, d\mathbf{U}) = 0 \quad \forall d\mathbf{U} \in R^{NEQ},$$

i.e., the function $E(\mathbf{U})$ takes the stationary value at the equilibrium point.

Sufficiency. Let the total potential energy take a stationary value at some point $\mathbf{U} \in R^{NEQ}$, i.e. Eq. (5.15) is realized. From Eqs. (5.14) and (5.15), we have

$$(5.16) \quad d\mathbf{U}^T[\mathbf{F}(\mathbf{U}) - \mathbf{R}] = 0 \quad \forall d\mathbf{U} \in R^{NEQ}.$$

By virtue of the fact that vector $d\mathbf{U}$ is arbitrary, Eq. (3.3) follows from Eq. (5.16). \square

Note. The stationarity condition (5.16) is equivalent to the scalar equilibrium equation (4.22). This statement follows from identification of the $d\mathbf{U}$ and \mathbf{W} vectors.

6. Equations of quasistatic deformation of an atomic lattice

Vector equation (3.3) or the equivalent scalar equation (4.22) determine the equilibrium of an atomic lattice to which external forces are applied and/or displacements of some atoms are prescribed. Since in the general case, the uniqueness of solutions of these equations is not provided, it is more advantageous to reformulate the problem of definition of equilibrium of a lattice as a problem of quasistatic deformation of a lattice by defining in succession all the equilibrium configurations in the range from the initial to final ones.

Introduce a certain monotonically increasing parameter of atomic lattice deformation t . The prescribed force, atom displacement, and arc length in the (\mathbf{U}, λ) -space can be used as this parameter (\mathbf{U} is a displacement vector of atoms in a lattice, λ is a scalar parameter describing the external force), etc. Further, for brevity, the parameter t will be termed as time. Note that natural time is always used as the deformation parameter in motion equations (3.2) and (4.1).

Differentiating left- and right-hand sides of Eq. (3.3) with respect to t , we obtain the equilibrium equations in the rate form

$$(6.1) \quad \dot{\mathbf{F}}(\mathbf{U}) = \dot{\mathbf{R}}.$$

Since

$$(6.2) \quad \dot{\mathbf{F}}(\mathbf{U}) = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \dot{\mathbf{U}} \quad \Leftrightarrow \quad \dot{F}_i = \frac{\partial F_i}{\partial U_j} \dot{U}_j \quad (i, j = \overline{1, NEQ}),$$

then introducing the Hesse matrix

$$(6.3) \quad \mathbf{K} \equiv \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \frac{\partial^2 V}{\partial \mathbf{U} \partial \mathbf{U}} \quad \Leftrightarrow \quad K_{ij} \equiv \frac{\partial F_i}{\partial U_j} = \frac{\partial^2 V}{\partial U_i \partial U_j} \quad (i, j = \overline{1, NEQ}),$$

and adding initial conditions to the system (6.1), we get

$$(6.4) \quad \mathbf{K}(\mathbf{U})\dot{\mathbf{U}} = \dot{\mathbf{R}}, \quad \mathbf{U}(0) = \mathbf{U}_0.$$

Herein \mathbf{U}_0 is the prescribed initial displacement vector. Following the terminology adopted in the FEM application to solution of the problems of solid mechanics, the Hesse matrix \mathbf{K} will be termed a *tangential stiffness matrix* of an atomic lattice. The symmetry of this matrix follows from Eq. (6.3): $\mathbf{K}^T = \mathbf{K}$. To define the equilibrium configurations of an atomic lattice, it is necessary to solve the Cauchy problem (6.4) for the system of quasilinear ordinary differential equations.

Elements of the matrix \mathbf{K} are more convenient to define starting from the scalar equation equivalent of the vector equation (6.4):

$$(6.5) \quad \mathbf{W}^T \mathbf{K}(\mathbf{U})\dot{\mathbf{U}} = \mathbf{W}^T \dot{\mathbf{R}} \quad \forall \mathbf{W} \in R^{NEQ}.$$

From Eqs. (5.1) and (6.3), we obtain

$$(6.6) \quad \mathbf{K} = \sum_{m=1}^M \tilde{\mathbf{K}}^m, \quad \tilde{\mathbf{K}}^m \equiv \frac{\partial \tilde{\mathbf{F}}^m}{\partial \mathbf{U}} = \frac{\partial^2 \tilde{V}^m}{\partial \mathbf{U} \partial \mathbf{U}},$$

where the tangential stiffness matrix of an atomic pair $\tilde{\mathbf{K}}^m$ ($1 \leq m \leq M$) is introduced when the global approach is used to form the matrices and vectors of an atomic pair. By v denote the left-hand side of equality (6.5):

$$v \equiv \mathbf{W}^T \mathbf{K}(\mathbf{U})\dot{\mathbf{U}}.$$

From (6.6) we get

$$(6.7) \quad v = \sum_{m=1}^M \tilde{v}_m, \quad \tilde{v}_m \equiv \mathbf{W}^T \tilde{\mathbf{K}}^m(\mathbf{U})\dot{\mathbf{U}}.$$

Using the local approach to form the matrices and vectors of an atomic pair, first we define the tangential stiffness matrix of an atomic pair. We have

$$(6.8) \quad v_e = \mathbf{W}^{eT} \mathbf{K}^e(\mathbf{U}^e)\dot{\mathbf{U}}^e (= \tilde{v}_e) \quad (1 \leq e \leq M),$$

where

$$\mathbf{K}^e \equiv \frac{\partial \mathbf{F}^e}{\partial \mathbf{U}^e} = \frac{\partial^2 V^e(\mathbf{U}^e)}{\partial \mathbf{U}^e \partial \mathbf{U}^e}.$$

The elements of \mathbf{K}^e matrix can be expressed based on the equality

$$(6.9) \quad \dot{\mathbf{F}}^e(\mathbf{U}^e) = \frac{\partial \mathbf{F}^e}{\partial \mathbf{U}^e} \dot{\mathbf{U}}^e = \mathbf{K}^e \dot{\mathbf{U}}^e \Leftrightarrow \dot{F}_i^e = \frac{\partial F_i^e}{\partial U_j} \dot{U}_j = K_{ij}^e \dot{U}_j \quad (i, j = \overline{1, 6}).$$

From Eq. (4.18), we have

$$(6.10) \quad \dot{\mathbf{F}}^e = \dot{f} \mathbf{B}^T + f \dot{\mathbf{B}}^T.$$

From Eqs. (2.3) and (4.16), we obtain

$$(6.11) \quad \dot{f} = \frac{\partial f}{\partial r} \dot{r} = c \mathbf{B} \dot{\mathbf{U}}^e.$$

To define elements of the row vector $\dot{\mathbf{B}}$, it is necessary to determine the \dot{e}_k ($k = 1, 2, 3$) values in terms of Eq. (4.17). Using the definition of a unit length vector \mathbf{e} in Eq. (4.12) and equalities (4.14) and (4.16), we obtain

$$(6.12) \quad \dot{e}_k = \left(\frac{r_k}{r} \right) \dot{\cdot} = \frac{\dot{r}_k}{r} - \frac{r_k}{r^2} \dot{r} = \frac{1}{r} (\dot{u}_k^2 - \dot{u}_k^1 - e_k \mathbf{B} \dot{\mathbf{U}}^e).$$

Using Eqs. (4.17) and (6.12), we define

$$(6.13) \quad \dot{\mathbf{B}}^T = \frac{1}{r} (\mathbf{P} - \mathbf{B}^T \mathbf{B}) \dot{\mathbf{U}}^e,$$

where the following matrix is introduced:

$$\mathbf{P} \equiv \mathbf{D}^T \mathbf{D} = \begin{bmatrix} \mathbf{I} & -\mathbf{I} \\ -\mathbf{I} & \mathbf{I} \end{bmatrix}.$$

Using Eqs. (6.11) and (6.13), we obtain an expression for the local tangential stiffness matrix of an atomic pair from Eqs. (6.9) and (6.10)

$$(6.14) \quad \mathbf{K}^e = c \mathbf{B}^T \mathbf{B} + \frac{f}{r} (\mathbf{P} - \mathbf{B}^T \mathbf{B}).$$

Let us analyze expression (6.14). Each summand in the right-hand side of Eq. (6.14) is governed by the fact that the corresponding summand in the right-hand side of Eq. (6.10) is accounted for. If the atomic pair is subjected to rigid translation augmented by tension/compression without rotation, i.e., $\dot{e}_k = 0$ ($k = 1, 2, 3$), then the second term in the right-hand side of Eq. (6.10) is equal to zero. Hence, here follows a simple interpretation of summands in expression (6.14) for the local tangential stiffness matrix: the first summand is caused by tension/compression of the segment connecting atoms in a pair, and the second one is due to rotation of the segment. In the previous works of the author [5, 6],

the tangential stiffness matrix of an atomic pair including only the first summand in the right-hand side of Eq. (6.14) was considered, i.e., rotation of this segment was not taken into account. In the present work, the refined matrix expression is given with account for rotation of this segment during its motion.

Equating the right-hand sides of Eqs. (6.8) and (6.7)₂ ($e = m$) and taking into account Eq. (4.19), we obtain

$$\tilde{\mathbf{K}}^e = \mathbf{A}^{eT} \mathbf{K}^e \mathbf{A}^e.$$

Finally, the tangential stiffness matrix of an atomic lattice is defined by assembling (summing) the tangential stiffness matrices of all atomic pairs of the lattice

$$(6.15) \quad \mathbf{K} = \sum_{m=1}^M \tilde{\mathbf{K}}^m.$$

Using the assembly operation, equality (6.15) can be rewritten as

$$\mathbf{K}(\mathbf{U}) = \sum_{m=1}^M \mathbf{A}^m \mathbf{K}^m(\mathbf{U}^m) \Leftrightarrow \mathbf{K}(\mathbf{U}) = \sum_{m=1}^M \mathbf{A}^{mT} \mathbf{K}^m(\mathbf{A}^m \mathbf{U}) \mathbf{A}^m.$$

We advance a variational formulation of quasistatic deformation equations of an atomic lattice. This formulation may be useful when uniqueness and stability of solutions of these equations are studied. Introduce a scalar function of the vector argument

$$(6.16) \quad I(\dot{\mathbf{U}}) \equiv \frac{1}{2} \dot{\mathbf{F}}^T \dot{\mathbf{U}} - \dot{\mathbf{U}}^T \dot{\mathbf{R}}, \quad \dot{\mathbf{U}} \in R^{NEQ}.$$

It follows from Eqs. (6.2) and (6.3) that

$$(6.17) \quad \dot{\mathbf{F}} = \mathbf{K}(\mathbf{U}) \dot{\mathbf{U}}.$$

Using Eq. (6.17) and symmetry of a matrix \mathbf{K} , we rewrite Eq. (6.16) as

$$I(\dot{\mathbf{U}}) = \frac{1}{2} \dot{\mathbf{U}}^T \mathbf{K} \dot{\mathbf{U}} - \dot{\mathbf{U}}^T \mathbf{R}, \quad \dot{\mathbf{U}} \in R^{NEQ}.$$

Let us formulate and prove a theorem.

THEOREM 2. *The velocity vector $\dot{\mathbf{U}}$ is a solution of Eq. (6.4) of quasistatic deformation of an atomic lattice if and only if the scalar function $I(\dot{\mathbf{U}})$ takes a stationary value.*

P r o o f. Let $I(\dot{\mathbf{U}})$ take the stationary value for some fixed displacement vector \mathbf{U} . We define the differential

$$(6.18) \quad dI(\dot{\mathbf{U}}, d\dot{\mathbf{U}}) = d\dot{\mathbf{U}}^T(\mathbf{K}\dot{\mathbf{U}} - \dot{\mathbf{R}}), \quad d\dot{\mathbf{U}} \in R^{NEQ}.$$

Then from the stationarity condition

$$(6.19) \quad dI(\dot{\mathbf{U}}, d\dot{\mathbf{U}}) = 0 \quad \forall d\dot{\mathbf{U}} \in R^{NEQ}$$

it follows that the velocity vector $\dot{\mathbf{U}}$ should satisfy Eq. (6.4).

On the contrary, let $\dot{\mathbf{U}}$ be the solution of Eq. (6.4). Then the fulfillment of the stationarity condition (6.19) follows from Eqs. (6.18) and (6.4). \square

Assuming in Eq. (6.5) $\mathbf{W} = d\dot{\mathbf{U}}$, we note that stationarity condition (6.19) is equivalent to the scalar form of the equations of an atomic lattice quasistatic deformation.

7. Conclusion

The alternative (vector, scalar and variational) forms of motion/equilibrium equations of atomic lattices are presented in the work. On the basis of the scalar form of equations and FEM technique, the automated technique is put forward for constructing matrices and vectors of equations based on the definition of local matrices and vectors of atomic pairs and their assembling into global matrices and vectors of the atomic lattice.

The refined expression (as compared to that reported in works [5, 6]) for the tangential stiffness matrix of an atomic pair is obtained. Thus, not only a change in segment length connecting two atoms in a pair but also its rotation is taken into account.

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