BUCKLING CRITERIA OF ATOMIC LATTICES

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ABSRACT

In the present work buckling criteria of atomic lattices are established. An external force is considered to be dead (the vector of this force does not change a direction during deformation of a lattice). It is supposed that deformation of a lattice is initiated from its natural state (in this state forces of atomic interaction are equal to zero in all atomic pairs of a lattice). Singular points of two types of integral curves are considered: turning points (corresponding to the maximum loads) and bifurcation points of solutions of a quasi-static deformation problem. The assumption that the singular point may be both a turning point and a bifurcation point simultaneously is admitted. A loss of stability of solutions of the equilibrium equations of atomic lattices is investigated. Stability criteria of equilibrium states with respect to dynamic perturbation introduced into the lattice through specifying the initial velocity vector are obtained. It is shown that unstable, according to Lyapunov, equilibrium equation solutions arise under quasi-static deformation of an atomic lattice just after the singular points occur on the integral curve. Post-critical deformation of an atomic lattice corresponds to its buckling after the loss of stability of the solution takes place.

1 INTRODUCTION

The necessity of the solution of nonlinear problems on the deformation of atomic lattices arises in connection with an attempt to describe adequately the initiation and evaluation of a crack in a solid undergoing stretching and shift loads. Phenomenological models of fracture of solid bodies do not give a correct pattern of distribution of stresses and strains near the crack within the framework of continuum mechanics. In particular, the solution of problems within the framework of linear fracture mechanics results in infinite values of stresses and strains in the tip crack for a linear elastic material model. This fact does not agree with finite values of interaction forces of atoms, of which the solid body consists.

The attempts to create a more correct model of fracture of solids result in the initiation and evaluation of the crack at an atomic level [1,2] when the initiation of the crack is induced by the buckling of an atomic lattice. A great difference between the strength obtained experimentally and a theoretical one is due to foreign atoms and vacancies in an atomic chain [3]. The buckling of a four-atoms cell as the mechanism of monocrystal destruction is considered in [4]. By 'buckling phenomena' we mean: the achievement of maximum interatomic forces [1], the branching solutions of equilibrium equations [2,3], and the achievement both of the maximum by external force on the 'atom displacements vs. external force' curve and of the forces which concern the branching solutions of equilibrium equations [4].

General formulations of the equations on quasi-static deformation of an atomic lattice are presented in [5,6], and the maximum and bifurcation loads correspond to singular points of integral curves of these equations when the tangential stiffness matrix of an atomic lattice degenerates. Here the turning points of the integral curve (where the maximum load is reached) may coincide with those of bifurcation. The algorithm on numerical solution of problems on quasi-static deformation of an atomic lattice is developed. The solutions of some problems on deformation of atomic chains and cells are obtained. In these solutions, singular points of integral curve are obtained. It is found that they are both turning points and bifurcation ones. It is noted that more complex forms of monocrystal destruction, in comparison with those obtained in [4], correspond to such points. Vector, scalar and variational forms of the nonlinear equilibrium/motion equations of

atomic lattices are presented in [7]. Obtained in more exact form than in [5, 6], the expression of a tangential stiffness matrix of an atomic lattice allows us to take into account both change of length of the straight line segment connecting atoms in pair and its rotation.

In the present work, a loss of stability of solutions of the equilibrium equations of atomic lattices is investigated. Stability criteria of equilibrium states with respect to dynamic perturbation introduced into the lattice through specifying the initial velocity vector are obtained. External forces are assumed to be dead. It is shown that unstable, according to Lyapunov, equilibrium equation solutions arise under quasi-static deformation of an atomic lattice just after the singular points occur on integral curve. Post-critical deformation of an atomic lattice corresponds to its buckling after the loss of stability of the solution takes place.

2 THE NONLINEAR EQUATIONS ON DEFORMATION OF ATOMIC LATTICES

The motion equations of an atomic lattice in a vector form are as follows [7]

$$\mathbf{M}\ddot{\mathbf{U}} + \mathbf{F}(\mathbf{U}) = \mathbf{R}, \quad \mathbf{U}(0) = \mathbf{U}_0, \dot{\mathbf{U}}(0) = \mathbf{V}_0. \tag{1}$$

Here $\mathbf{M}$ is a diagonal positive defined mass matrix of a lattice; $\mathbf{U} \in R^{NEQ}$ is a displacement vector of atoms of lattice

$$\mathbf{U} = [U_1, U_2, \ldots, U_{NEQ}]^T; \tag{2}$$

$\mathbf{R}$ is a vector of external forces; the index 'T' designates transposition operation; the point above value designates its derivative on time t; $\mathbf{U}_0$ 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.

The scalar form of the motion equations has the form [7]

$$\mathbf{W}^T[\mathbf{M}\ddot{\mathbf{U}} + \mathbf{F}(\mathbf{U})] = \mathbf{W}^T\mathbf{R} \quad \forall\, \mathbf{W} \in R^{NEQ}. \tag{3}$$

We consider the potential law of atomic (molecular) interaction in pair

$$f = \frac{\partial V^e(r)}{\partial r}, \tag{4}$$

where V^e is the potential energy (for example, Lennard – Jones) of atomic pair when only the central forces of interaction of atoms f depending on their distance r are taken into account. In [7], it is offered to define a vector $\mathbf{F}$ of internal forces of an atomic lattice using the scalar form of the motion equations and assembly operation [8] of the vectors of internal forces for all atomic pairs of a lattice. The vector of internal forces for atomic pair has the form [5-7]

$$\mathbf{F}^e = f\,\mathbf{B}^T, \quad \mathbf{B} \equiv [-\mathbf{e}, \mathbf{e}]^T, \tag{5}$$

where $\mathbf{e}$ is the unit length vector directed along the segment connecting atoms in the pair in the current (deformed) state. Potential energy of an atomic lattice $V(\mathbf{U})$ is defined by summing potential energy of all atomic pairs

$$V(\mathbf{U}) = \sum_{m=1}^{M} V^m, \tag{6}$$

where M is a total number of all atomic pairs of a lattice.

We obtain the equilibrium equations from Equation (1) by omitting inertial forces

$$\mathbf{F}(\mathbf{U}) = \mathbf{R}. \tag{7}$$

Let us assume the external force to be *dead* (i.e., this vector does not change its direction during deformation) such as

$$\mathbf{R} = l\,\mathbf{R}_0, \tag{8}$$

where $\mathbf{R}_0$ is the constant vector due to distribution of external forces in a lattice and l is the parameter describing intensity of the application of external forces.

We define a total potential energy of an atomic lattice as

$$e(\mathbf{U}) \equiv V(\mathbf{U}) - l\,\mathbf{U}^T\,\mathbf{R}_0. \tag{9}$$

We find the differential of total potential energy [7]

$$de(\mathbf{U}, d\mathbf{U}) = d\mathbf{U}^T[(\mathbf{F}(\mathbf{U}) - l\,\mathbf{R}_0], \quad d\mathbf{U} \in R^{NEQ}. \tag{10}$$

The variational formulation of the equilibrium equations is reduced to the scalar equation

$$de(\mathbf{U}, d\mathbf{U}) = 0 \quad \forall d\mathbf{U} \in R^{NEQ}. \tag{11}$$

This equation coincides with the equation obtained from Equation (3) by omitting inertial forces

$$d\mathbf{U}^T[\mathbf{F}(\mathbf{U}) - l\,\mathbf{R}_0] = 0 \quad \forall d\mathbf{U} \in R^{NEQ}. \tag{12}$$

The stationarity principle of total potential energy of an atomic lattice [7] confirms equivalence of the equilibrium equation

$$\mathbf{F}(\mathbf{U}) = l\,\mathbf{R}_0 \tag{13}$$

and variational Equations (11) or (12).

3 EQUATIONS ON QUASI-STATIC DEFORMATION OF AN ATOMIC LATTICE

Let us introduce a monotonously growing parameter t describing quasi-static deformation of an atomic lattice (e.g., this parameter may be taken as the value l in Equation (13), as the prescribed displacement of some atom, etc). Differentiating the left- and right-hand sides of (13) with respect to t and adding initial conditions, we obtain

$$\mathbf{K}(\mathbf{U})\mathbf{U}' = l'\mathbf{R}_0, \quad \mathbf{U}(0) = \mathbf{U}_0, \tag{14}$$

where the prime designates derivative of the value with respect to the parameter t. Here $\mathbf{K}(\mathbf{U})$ is a symmetric tangential stiffness matrix of an atomic lattice

$$\mathbf{K} \equiv \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \frac{\partial^2 V}{\partial \mathbf{U} \partial \mathbf{U}} \quad \Leftrightarrow \quad K_{ij} \equiv \frac{\partial F_i}{\partial U_j} = \frac{\partial^2 V}{\partial U_i \partial U_j} \quad (i, j = \overline{1, NEQ}). \tag{15}$$

Elements of this matrix are defined following the scalar form of Equation (14)

$$\mathbf{W}^T\mathbf{K}(\mathbf{U})\mathbf{U}' = l'\mathbf{W}^T\,\mathbf{R}_0, \quad \forall\,\mathbf{W} \in R^{NEQ} \tag{16}$$

and assembly operation [8] of tangential stiffness matrices of all atomic pairs. The expression of a tangential stiffness matrix of the atomic pair is presented in [5,6] with allowance for the change of length of a segment connecting atoms. The refined matrix expression taking into account rotation of this segment is presented in [7].

We introduce a scalar function of a velocity vector of an atomic lattice

$$I(\mathbf{U}') \equiv \frac{1}{2}\mathbf{U}'^T\mathbf{K}\,\mathbf{U}' - l'\,\mathbf{U}'^T\mathbf{R}_0, \quad \mathbf{U}' \in R^{NEQ}. \tag{17}$$

Let us define the differential

$$dI(\mathbf{U}', d\mathbf{U}') = d\mathbf{U}'^T(\mathbf{K}\,\mathbf{U}' - l'\mathbf{R}_0), \quad d\mathbf{U}' \in R^{NEQ}. \tag{18}$$

The variational formulation of the quasi-static deformation equations is

$$dI(\mathbf{U}', d\mathbf{U}') = 0 \quad \forall d\dot{\mathbf{U}} \in R^{NEQ} \tag{19}$$

or

$$d\mathbf{U}'^T(\mathbf{K}\,\mathbf{U}' - l'\mathbf{R}_0) = 0 \quad \forall d\mathbf{U}' \in R^{NEQ}. \tag{20}$$

These equations are equivalent to the vector form of Equation (14).

4 SINGULAR POINTS OF INTEGRAL CURVES OF QUASI-STATIC DEFORMATION EQUATIONS OF AN ATOMIC LATTICE

The points of an integral curve when a matrix $\mathbf{K}$ degenerates, i.e., the equality

$$\det \mathbf{K} = 0, \tag{21}$$

is satisfied, are named as singular. Let $\mathbf{W}_i$ $(i = \overline{1, I},\ I \geq 1)$ be the vectors constituting a basis for the null-space of a matrix $\mathbf{K}$.

Identifying consecutively a vector $\mathbf{W}$ in (16) with vectors $\mathbf{W}_i$, we obtain the conditions for existence of the solution of Equation (14) at singular point

$$l' \mathbf{W}_i^T \mathbf{R}_0 = 0 \quad (i = \overline{1, I}). \tag{22}$$

Let us $I = 1$, i.e., the basis for the null-space of a matrix $\mathbf{K}$ consists of a unique vector $\mathbf{W}_1$. Then the following variants are possible [9]

$$(1)\ l' = 0,\ \mathbf{W}_1^T \mathbf{R}_0 \neq 0, \quad (2)\ l' \neq 0,\ \mathbf{W}_1^T \mathbf{R}_0 = 0. \tag{23}$$

In the first case, the singular point is a turning point, and in the second case, the singular point is a bifurcation point. In the latter case, for one point of an integral curve it is possible to define two vectors $\dot{\mathbf{U}}$ corresponding to two solution continuations.

At $I > 1$, we admit that the singular point may be both a turning point and a bifurcation one simultaneously [5,6]. Let $I = 2$, then in this case

$$l' = 0, \mathbf{W}_1^T \mathbf{R}_0 \neq 0, \mathbf{W}_2^T \mathbf{R}_0 = 0. \tag{24}$$

Let us introduce the quadratic form

$$J(\mathbf{W}) \equiv \frac{1}{2} \mathbf{W}^T \mathbf{K}(\mathbf{U}) \mathbf{W}, \quad \mathbf{W} \in R^{NEQ}. \tag{25}$$

Let the equilibrium state of an atomic lattice satisfy Equation (13). Continuation of the solution from this equilibrium state satisfies Equation (14). If condition (21) is fulfilled for such equilibrium state, it is named as eigenstate. We formulate a sufficient condition of absence of eigenstates.

Theorem 1 (Sufficient condition of absence of eigenstates). If the quadratic form $J(\mathbf{W})$ is positive defined, i.e.,

$$J(\mathbf{W}) \geq 0 \quad \forall\, \mathbf{W} \in R^{NEQ} \quad \text{and} \quad J(\mathbf{W}) = 0 \Leftrightarrow \mathbf{W} = 0, \tag{26}$$

then the equilibrium state is not eigenstate.

5 STABILITY OF EQUILIBRIUM STATES OF ATOMIC LATTICES

Let an atomic lattice be in an equilibrium state so that Equation (13) holds. Let this lattice be deviated from an equilibrium state by a small perturbation, i.e., the prescribed initial velocity $\mathbf{V}_0$. We investigate the perturbed motion of the atomic lattice in the vicinity of this equilibrium state. Let $\bar{\mathbf{U}}$ designate a displacement vector of the perturbed motion so that motion equation (1) holds, i.e.,

$$\mathbf{M}\ddot{\bar{\mathbf{U}}} + \mathbf{F}(\bar{\mathbf{U}}) = l\, \mathbf{R}_0, \quad \bar{\mathbf{U}}(0) = 0, \dot{\bar{\mathbf{U}}}(0) = \mathbf{V}_0. \tag{27}$$

If the equilibrium configuration with a displacement vector $\mathbf{U}$ is considered as a point of the integral curve of Equation (14), then described by Equation (27), the process of perturbed atomic lattice motion is supposed to develop in natural time t. Here the parameter of deformation t is fixed.

We introduce a designation

$$\mathbf{q} \equiv \bar{\mathbf{U}} - \mathbf{U}. \tag{28}$$

From Equations (13) and (27), we obtain the following homogeneous equation with respect to a vector $\mathbf{q}$

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{F}(\bar{\mathbf{U}}) - \mathbf{F}(\mathbf{U}) = 0, \quad \mathbf{q}(0) = 0, \dot{\mathbf{q}}(0) = \mathbf{V}_0. \tag{29}$$

Let us define a total energy of an atomic lattice

$$E \equiv T + e, \tag{30}$$

where T is kinetic energy of an atomic lattice

$$T(\dot{\mathbf{U}}) \equiv \frac{1}{2}\dot{\mathbf{U}}^T \mathbf{M}\,\dot{\mathbf{U}}. \tag{31}$$

For an equilibrium configuration we obtain

$$E(\mathbf{U},\dot{\mathbf{U}}) = e(\mathbf{U}) = V(\mathbf{U}) - l\,\mathbf{U}^T\,\mathbf{R}_0 = const, \tag{32}$$

and for the perturbed motion we get

$$E(\bar{\mathbf{U}},\dot{\bar{\mathbf{U}}}) = T(\dot{\bar{\mathbf{U}}}) + e(\bar{\mathbf{U}}) = T(\dot{\bar{\mathbf{U}}}) + V(\bar{\mathbf{U}}) - l\,\bar{\mathbf{U}}^T\,\mathbf{R}_0. \tag{33}$$

Let us define

$$\Delta E \equiv E(\bar{\mathbf{U}},\dot{\bar{\mathbf{U}}}) - E(\mathbf{U},\dot{\mathbf{U}}) = \frac{1}{2}\dot{\mathbf{q}}^T\mathbf{M}\dot{\mathbf{q}} + \Delta e. \tag{34}$$

Let us find expression for Δe

$$\Delta e \equiv e(\bar{\mathbf{U}}) - e(\mathbf{U}) = \mathbf{q}^T\left(\frac{\partial e}{\partial \mathbf{U}}\right) + \frac{1}{2}\mathbf{q}^T\left(\frac{\partial^2 e}{\partial \mathbf{U}\,\partial \mathbf{U}}\right)\mathbf{q} + \ldots = \mathbf{q}^T(\mathbf{F} - l\,\mathbf{R}_0) + \frac{1}{2}\mathbf{q}^T\,\mathbf{K}\,\mathbf{q} + \ldots = \frac{1}{2}\mathbf{q}^T\,\mathbf{K}\,\mathbf{q} + \ldots \tag{35}$$

From Equations (33) and (34), using smallness of $\mathbf{q}$, we obtain

$$\Delta E = T(\dot{\mathbf{q}}) + J(\mathbf{q}). \tag{36}$$

Let the condition (26) of positive definiteness of the quadratic form $J(\mathbf{q})$ be satisfied for a concerned equilibrium configuration. Then

(1) $(\Delta E)^{\cdot} = 0$ for $0 < t < \infty$;

(2) $\Delta E > 0 \quad \forall \mathbf{q},\dot{\mathbf{q}} \in R^{NEQ}(\mathbf{q} \neq 0 \text{ or } \dot{\mathbf{q}} \neq 0)$;

(3) $\Delta E = 0 \text{ for } \mathbf{q} = \dot{\mathbf{q}} = 0$.

Hence, it is possible to identify ΔE with Lyapunov function [10]. From this it follows that we can prove Theorem 2 by using Lyapunov's second (direct) method.

Theorem 2 (Sufficient condition of stability of equilibrium state of an atomic lattice). If the quadratic form $J(\mathbf{W})$ is positive defined, i.e., Equation (26) is valid, then the solutions of Equations (13) are stable in the sense of Lyapunov.

We assume that investigating Lyapunov stability of solution (13) of Equation (29) may be performed on a first approximation. Stability research on a first approximation is reduced to definition of stability of the trivial solution

$$\mathbf{q} = 0 \tag{37}$$

with the help of the equation

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}(\mathbf{U})\mathbf{q} = 0, \quad \mathbf{q}(0) = 0, \dot{\mathbf{q}}(0) = \mathbf{V}_0, \tag{38}$$

obtained due to linearization of Equation (29).

The analysis of stability of solution (37) on Lyapunov's first approximation does not reveal the stability of source nonlinear system in case the quadratic form J is positive defined or semi-defined. If the quadratic form J is not defined (there is at least one vector $\mathbf{W} \in R^{NEQ}$ such that $J(\mathbf{W}) < 0$), then solution (13) is unstable according to Lyapunov.

Summarizing investigations of stability of the solution $\mathbf{U}$ of nonlinear Equation (29), we obtain the following criterion of stability of solution (13) according to Lyapunov's second method and on a first approximation approach:

$$J(\mathbf{W}) \text{ is } \begin{cases} \text{positive defined} \\ \text{positive semi-defined} \\ \text{undefined} \end{cases} \Rightarrow \text{equilibrium state is } \begin{cases} \text{stable} \\ \text{undefined}. \\ \text{unstable} \end{cases} \tag{39}$$

6 COMPARISON OF CRITERIA FOR ABSENCE OF EIGENSTATES AND STABILITY OF EQUILIBRIUM STATES

From formulations of Theorems 1 and 2 it follows that the condition of positive definiteness of the quadratic form $J(\mathbf{W})$ is simultaneously sufficient condition of both absence of eigenstates and stability of equilibrium states. At the same time this condition is also necessary for stability of equilibrium states (except for those ones where the quadratic form is semi-defined), but for absence of eigenstates this condition is unnecessary. To confirm it, the condition of negative definiteness of $J(\mathbf{W})$ may be presented as a sufficient condition of absence of eigenstates.

It is possible to deduce the important practical conclusion from coincidence of the above sufficient conditions: in solving a problem of quasi-static deformations of an atomic lattice under dead load, the status of equilibrium states (points of an integral curve) with respect to Lyapunov stability criteria is automatically determined. If quasistatic deformation of a lattice is initiated from a natural configuration (forces of atomic interaction f are equal to zero in all atomic pairs), then equilibrium configurations are stable, according to Lyapunov, before bifurcation points or turning ones occur on an integral curve.

7 CONCLUSION

It is presented that in achieving singular points of an integral curve the regime of quasi-static deformation of an atomic lattice may be maintained only by a special way. In a general case, in achieving singular points (bifurcation and turning points) the solutions of static equilibrium problems are unstable according to Lyapunov and at a small perturbation a quasi-static regime of deformation of the atomic lattice changes into a dynamic one.

The supports from Russian Foundation for Basic Research (Grant Nos. 02-01-00195 and 04-01-00191), Integration Project of RAS No. 3.11.1 and Grant of Russian President No. SS-319.2003.1 are gratefully acknowledged.

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