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INFLUENCE OF SHEAR STRAIN ON STABILITY OF 2D TRIANGULAR LATTICE

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Stability of 2D triangular lattice under finite arbitrary strain is investigated. The lattice is considered infinite and consisting of particles which interact by pair force central potential. Dynamic stability criterion is used: frequency of elastic waves is required to be real for any real wave vector. Two stability regions corresponding to horizontal and vertical orientations of the lattice are obtained. It means that a structural transition, which is equal to the change of lattice orientation, is possible.

Keywords: stability, triangular lattice, finite strain, biaxial strain, pair potential, elastic wave, structural transition.

1. Introduction

In work [1] stability of plane triangular lattice under finite biaxial strain was investigated. Two stability regions, which correspond to vertical and horizontal orientations of the lattice, were obtained both analytically and using MD simulation. It was shown that taking more than one coordination sphere into account leads to a new effect: possibility of structural transition, which is equal to the change of lattice orientation. In this work shear strain is added. Modeling based on discrete atomistic methods [2] is proposed. The medium is represented by a set of particles interacting by a pair force central potential, in particular Lennard-Jones and Morse. Direct tensor calculus [3] is used.

Following [1, 4, 5], let us introduce the following notation to describe the geometry:

$$\underline{a}_k = \underline{r}_k - \underline{r}_0, \tag{1}$$

where $\underline{r}_k$ is radius vector of a particle k, $\underline{r}_0$ is radius vector of reference particle. If a lattice is simple, then any particle can be named "reference", each particle k has a pair $-k$ and $\underline{a}_{-k} = -\underline{a}_k$. Triangular lattice is simple and close-packed: it coincides with its Bravais lattice and possesses maximum concentration of nods in elementary volume V_0 with the given minimum distance between the nods. Let us refer to the geometry which is described by $\underline{r}_k$ and $\underline{a}_k$ as reference configuration.

Let $\overset{\circ}{\nabla}$ and ∇ be Hamilton's operators in reference and current configurations [3]:

$$\overset{\circ}{\nabla} = \underline{e}_i \frac{\partial}{\partial x_i}, \qquad \nabla = \underline{e}_i \frac{\partial}{\partial X_i}. \tag{2}$$

Vectors $\underline{e}_i$ form an orthonormal basis. If vector $\underline{r}$ has projections x_i in reference configuration, then in current configuration $\underline{r}$ will turn into $\underline{R}$ with projections X_i in the same basis.

Suppose that the lattice is subject to strain characterized by $\overset{\circ}{\nabla}\underline{R}$. According to long-wave approximation [2, 6]

$$\underline{A}_k = \underline{R}\left(\underline{r} - \underline{a}_k\right) - \underline{R}\left(\underline{r}\right) \approx \underline{a}_k \cdot \overset{\circ}{\nabla}\underline{R}. \tag{3}$$

Long-wave approximation takes into account those wave lengths that are much greater than the interatomic distance. The thermal motion is neglected.

Morse and Lennard-Jones potentials are used in this work to describe the interaction between particles

$$\Pi(r) = D\left[e^{-2\theta\left(\frac{r}{a}-1\right)} - 2e^{-\theta\left(\frac{r}{a}-1\right)}\right], \quad \Pi_{LJ}(r) = D\left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^{6}\right]. \tag{4}$$

Here a is equilibrium distance in the system of two particles, D is the depth of potential well, θ characterizes the width of the well. If $\theta = 6$, these potentials coincide in the elastic zone. Morse potential is preferable in this work, because, firstly, it decreases faster, so less particles may be taken into consideration, secondly, if $r \to 0$ Morse potential remains finite.

Let $F_k = F(A_k) = -\Pi'(A_k)$ be interaction force and $C_k = C(A_k) = \Pi''(A_k)$ be the bond stiffness, both calculated in current configuration. Then we can introduce

$$\underline{\underline{A}}_k = \underline{A}_k\underline{A}_k, \quad {}^4\underline{\underline{A}}_k = \underline{A}_k\underline{A}_k\underline{A}_k\underline{A}_k, \quad \underline{\underline{a}}_k = \underline{a}_k\underline{a}_k, \quad {}^4\underline{\underline{a}}_k = \underline{a}_k\underline{a}_k\underline{a}_k\underline{a}_k$$
$$\Phi_k = -\frac{F_k}{A_k}, \quad \mathcal{B}_k = \frac{1}{A_k^2}(C_k - \Phi_k), \quad \underline{\underline{\Phi}} = \frac{1}{2}\sum_k \Phi_k\underline{\underline{A}}_k, \quad {}^4\underline{\underline{\mathcal{B}}} = \frac{1}{2}\sum_k \mathcal{B}_k{}^4\underline{\underline{A}}_k. \tag{5}$$

2. Stability criterion and deformation of triangular lattice

In the previous works [1, 4, 5] the following stability criterion was applied

$$\Omega > 0, \tag{6}$$

where Ω is determined from equation

$$\det\left[\underline{\underline{D}} - \Omega\underline{\underline{E}}\right] = 0. \tag{7}$$

Here

$$\underline{\underline{D}} = {}^4\underline{\underline{C}}\cdot\cdot\,\underline{\underline{K}}, \quad {}^4\underline{\underline{C}} = \underline{\underline{E}}\,\underline{\underline{\Phi}} + {}^4\underline{\underline{\mathcal{B}}}, \quad \underline{\underline{K}} = \underline{K}\,\underline{K}.$$

$\underline{K}$ is a real wave vector. This means that frequency of elastic waves is required to be real for any real wave vector.

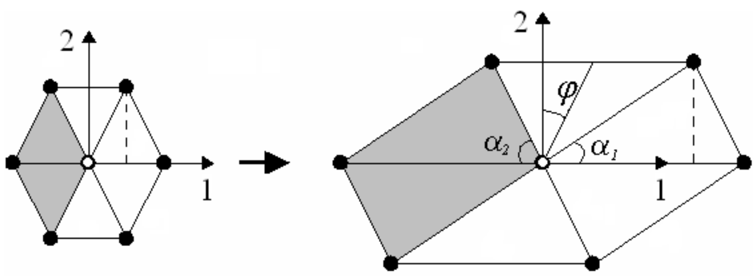

Fig. 1. Reference and current configurations

Fig. 1 shows the typical part of triangular lattice before and after deformation. In reference configuration $\alpha_1 = \alpha_2 = 60°$. It is sufficient to take only $0 \le \varphi \le 30°$ in account due to symmetry and infiniteness of the lattice. It was shown in [1, 5] that at least two coordination spheres should be considered.

In 2D case (7) takes the form

$$\Omega^2 - \Omega\,\mathrm{tr}\,\underline{\underline{D}} + \det\underline{\underline{D}} = 0. \tag{8}$$

According to (6) roots of equation (8) are positive for stable current configurations. Thus, stability criterion is

$$\operatorname{tr}\underline{\underline{D}} > 0, \qquad \det\underline{\underline{D}} > 0, \qquad 2\operatorname{tr}\underline{\underline{D}}^2 - \left(\operatorname{tr}\underline{\underline{D}}\right)^2 \geq 0. \tag{9}$$

Inequality $2\operatorname{tr}\underline{\underline{D}}^2 - \left(\operatorname{tr}\underline{\underline{D}}\right)^2 \geq 0$ is always true in 2D.

Let $\underline{\underline{G}} = \underline{\underline{E}}\cdot\cdot{}^4\underline{\underline{C}}$. The equations (9) yield

$$\begin{aligned} &\operatorname{tr}\underline{\underline{D}} > 0 \Leftrightarrow G_{11}K_1^2 + G_{12}K_1K_2 + G_{22}K_2^2 > 0,\\ &\det\underline{\underline{D}} > 0 \Leftrightarrow AK_1^4 + BK_1^2K_2^2 + CK_2^4 + DK_1^3K_2 + EK_1K_2^3 > 0, \end{aligned} \tag{10}$$

where

$$\begin{gathered} G_{11} = C_{11} + C_{21}, \quad G_{12} = C_{14} + C_{24}, \quad G_{22} = C_{12} + C_{22},\\ A = C_{11}C_{21} - C_{41}^2, \quad B = 4C_{14}C_{24} + C_{11}C_{22} + C_{12}C_{21} - 2C_{41}C_{42} - 4C_{44}^2,\\ C = C_{12}C_{22} - C_{42}^2, \quad D = 2C_{11}C_{24} - 4C_{41}C_{44} + 2C_{14}C_{21},\\ E = 2C_{12}C_{24} + 2C_{14}C_{22} - 4C_{42}C_{44}. \end{gathered} \tag{11}$$

Here C_{ij} are the components of tensor ${}^4\underline{\underline{C}}$.

The left part of $\operatorname{tr}\underline{\underline{D}} > 0$ is a quadratic form in the components of the wave vector K_1 and K_2. It is positive definite, if

$$G_{11} > 0, \quad 4G_{11}G_{22} - G_{12}^2 > 0. \tag{12}$$

The left part of $\det\underline{\underline{D}} > 0$ is a homogeneous polynomial of degree four. In this case, a general analytical criterion cannot be constructed.

Due to the fact that both K_1 and K_2 may be equal to zero, two necessary stability conditions are obtained, which help to narrow down the set of current configurations $\varepsilon_1,\ \varepsilon_2,\ \varphi$

$$A > 0, \quad C > 0. \tag{13}$$

Then, there are two ways to obtain sufficient conditions:

(1) For each ε_1, ε_2, φ we can construct $\det\underline{\underline{D}}$, and check it for a set of K_1 and K_2 (Monte Carlo method). The inequality is homogeneous and even, so it is sufficient to consider only $-1 \leq K_1 \leq 1$ and $0 \leq K_2 \leq 1$, which increases the efficiency.

(2) We can divide $\det\underline{\underline{D}}$ by K_2^4 and look into the problem of determining the coefficients so that a fourth-degree equation has no real roots, again for each ε_1, ε_2, φ. This method is much faster, but it causes a problem of distinguishing between complex and real roots, which leads to inaccurate results at the border.

In Fig. 2 stability regions, obtained by inequalities (12) and (13) and by the second method, are drawn. Here ε_1 and ε_2 are linear parts of Cauchy-Green tensor. There are several points, marked black, which were added by the first method. The stability regions are symmetric with respect to the plane $\operatorname{tg}\varphi = 0$. Two major areas correspond to horizontal and vertical orientations of the lattice [1]. Two additional small stability areas are connected with square lattices at $\varphi \approx 0°$ and $\varphi \approx 26°$ (see Fig. 3).

Let us draw a series of stress-strain diagrams, e.g. Fig. 4. According to [2] Cauchy stress tensor has the form

$$\underline{\underline{\sigma}} = \frac{1}{2V}\sum_k \underline{A}_k\underline{F}_k, \tag{14}$$

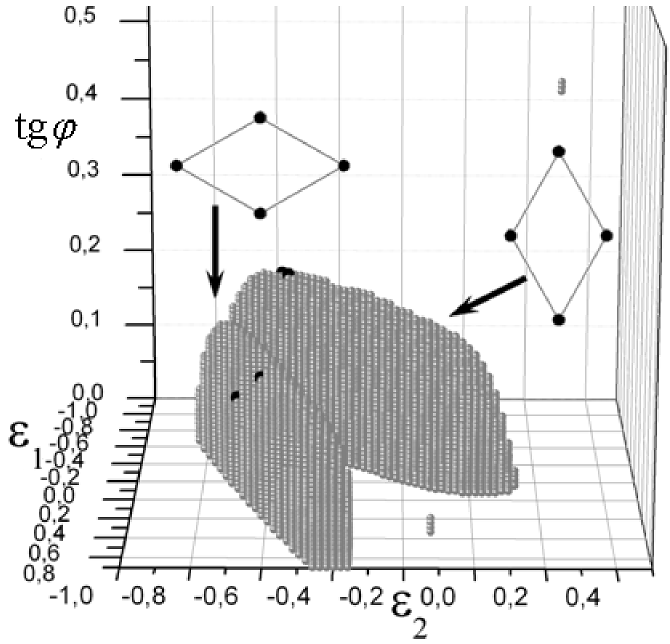

Fig. 2. Stability regions

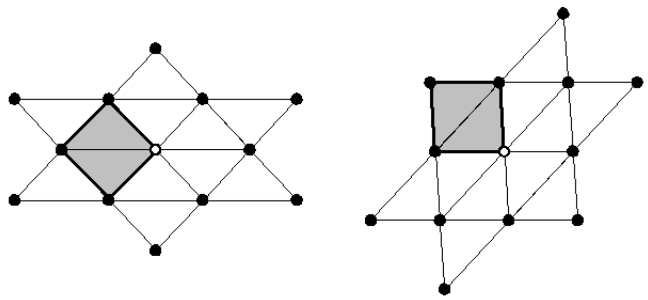

Fig. 3. Square lattices at $\varphi \approx 0^\circ$ and $\varphi \approx 26^\circ$

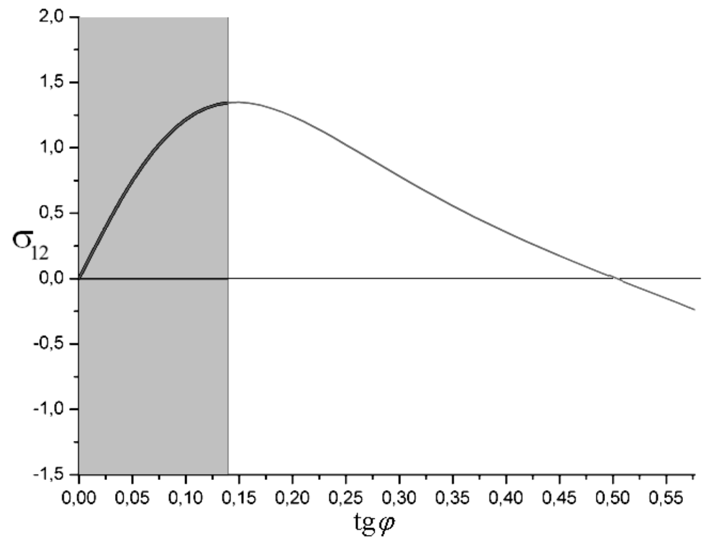

Fig. 4. Pure shear ($\sigma_{11} = \sigma_{22} = 0$)

where $V = \sqrt{3}/2(1+\varepsilon_1)(1+\varepsilon_2)$. Grey zone in Fig. 4 corresponds to stability region, σ_{12} is diagonal component of Cauchy stress tensor.

In Fig. 4 we can see, that the loss of stability is strongly connected with the sign of the first derivative.

3. Concluding remarks

Stability analysis of 2D triangular lattice under finite arbitrary strain was carried out. In addition to [1] shear was taken into account. Two stability regions were obtained, when more than one coordination sphere were regarded, and a possibility of structural transition, which is equal to the change of lattice orientation, was noticed. Monte Carlo and analytical methods were used, and they proved to give practically equal results. Thus, Monte Carlo method can be applied to more complex cases, where it is impossible to accomplish analytical investigation, e.g. 3D lattices.

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