

DISLOCATION MODEL OF MUSCULAR CONTRACTION

L.A. BULAVIN, YU.F. ZABASHTA, S.V. SEVERYLOV

UDC 577.3:532:577.11:
538.951-405Taras Shevchenko Kyiv National University, Faculty of Physics
(6, Academician Glushkov Ave., Kyiv 03127, Ukraine; e-mail: severylov@univ.kiev.ua)

© 2004

The model describing the contraction of an ensemble of interacting muscular fibers has been developed on the basis of the continuum theory of dislocations. In the framework of this model, the evaluation of a strained state of the principal element of the cardiovascular system, the aortic ventricle of heart, has been carried out, and its qualitative interpretation has been made.

Introduction

The muscle is known to be an ensemble of muscular fibers. A muscular fiber consists of fibrils, which contain a certain number of macromolecules. Accordingly, when studying the structure of muscular tissue, the sequence of spatial scales is considered: the size of the muscle, L , the characteristic size of a fiber, l , etc.

On the spatial scale, whose unit of measurement Δx satisfies the condition

$$l \ll \Delta x \ll L, \quad (1)$$

the phenomenological theory is actual. Then, the zero-order approximation with respect to a small parameter $l/\Delta x$ is taken into account, which brings us to a continuum model, where the thickness of the fiber l should be considered as an infinitesimal value.

Both the phenomenological [1, 2] and microscopic [3–5] approaches are applied when studying the muscular contraction. The main feature of the earlier publications on the muscular contraction is that the object of research in them was an isolated fiber or a fibril. However, in a real system, namely muscular tissue, fibers are not isolated. They interact with one another, and therefore their contractions should occur in coordination. How will this circumstance affect the deformation of muscular tissue? This work is devoted to the search for the answer to this question.

1. Construction of a Muscular Contraction Model

1.1. Emergence of Dislocation Loops upon the Contraction of Muscular Fibers

The basic idea of the work consists in considering the contraction of a muscular fiber as the emergence of some defect. This idea brings us to the necessity for using the continuum theory of defects [6]. We shall take advantage of the considerations that are traditional to this theory in constructing a physical model which would describe the contraction of muscles.

Consider an isolated fiber A (Fig. 1). Let the size of the section ac , after the contraction which occurs owing to some biochemical processes, become equal to ac' (Fig. 1, *a*). Such a change in the size can be considered as the removal of a section $\Delta = ac - ac'$ in length from the fiber (Fig. 1, *b*) and the following glueing of the cut edges (Fig. 1, *c*). As a result, the volume of the fiber decreases and its density grows.

Now, let fiber A try to contract, being surrounded by other fibers. In accordance with Fig. 1, the contraction is reduced to the procedure of “removing the material plus glueing the edges of the cut”. But the recurrence of this procedure (Figs. 2, *b* and *c*) results in the appearance of an edge dislocation with a Burgers vector $\vec{\Delta}$. The dislocation line is closed, i.e. such a procedure results in the emergence of a dislocation loop [7] which surrounds fiber A . A displacement, which would arise in an isolated fiber owing to the contraction induced by biochemical processes, will be designated further by \vec{W} .

1.2. Continuous Distribution of Dislocations in Muscular Tissue

The structure of the system in the accepted approximation will be characterized by the field of a director $\vec{n}(\vec{r})$, i.e. a unit vector, whose direction coincides with that of the axis of a fiber at the given point. The displacement $\vec{W}(\vec{r})$ is expressed as

$$\vec{W}(\vec{r}) = W(\vec{r}) \vec{n}(\vec{r}). \quad (2)$$

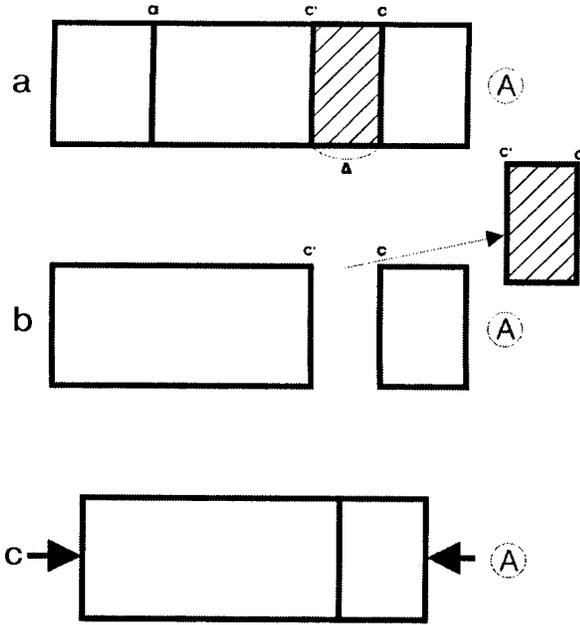


Fig. 1. Diagram of the contraction of an isolated muscular fiber

The dislocation loop, whose emergence is represented in Fig. 2, collapses to a point in the zero-order approximation mentioned above. Then, it is natural to turn to a continuous distribution of dislocations by introducing the dislocation density tensor which is connected to the tensor of incompatibility η [8].

It is essential that the continuum model introduced here allows the interaction of muscular fibers with one another to be taken into account. Consider first an ideal situation, where the interaction between the fibers of the ensemble is absent. The contraction results in the appearance of the field $\vec{W}(\vec{r})$ in such a system. It is obvious that, after switching on the interaction between the fibers, the field of displacements does not remain equal to $\vec{W}(\vec{r})$ but has to change, because, generally speaking, the tensor of incompatibility η , which must be equal to zero for a continuum, is not zero in this case for an arbitrary field $\vec{W}(\vec{r})$, namely,

$$\eta = -\text{Rot}q \neq 0, \quad (3)$$

where q_{ik} is the strain tensor, whose components are determined by the known expression

$$q_{ij} = \frac{1}{2} \left(\frac{\partial W_i}{\partial x_j} + \frac{\partial W_j}{\partial x_i} \right), \quad (4)$$

and the operator Rot is defined as

$$\text{Rot}_{mni} = \text{rot}_{mi} \text{rot}_{nj}, \quad \text{rot}_{ik} \equiv e_{ijk} \frac{\partial}{\partial x_j}, \quad (5)$$

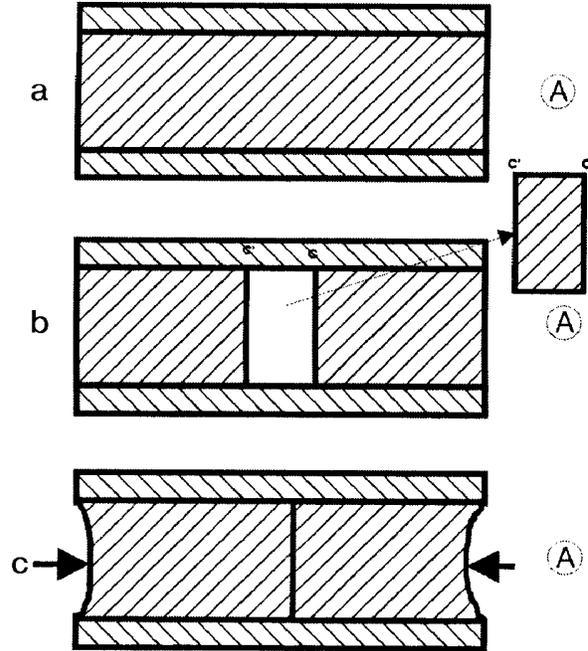


Fig. 2. Diagram of the contraction of a muscular fiber surrounded by other fibers

e_{ijk} being the antisymmetric unit tensor.

In the framework of the continuum model introduced here, the influence of the interaction between fibers will be taken into account, if the real field $\vec{U}(\vec{x})$ is found, for which the condition

$$\text{Rot}\varepsilon = 0, \quad (6)$$

where

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right). \quad (7)$$

is satisfied. This field preserves the continuity of the system after the contraction of the fibers, which, provided that the latter are isolated, is determined by the function $\vec{W}(\vec{r})$.

2. An Example of the Model Application: Calculation of the Strained State of the Aortic Ventricle of Heart

2.1. Simulation Model of the Ventricle: the Cylindrical Field of the Director and the Emergence of a Wedge Disclination

In accordance with [9], the ventricle can be regarded in calculations as a thick-walled pipe. Let r_0 and R be,

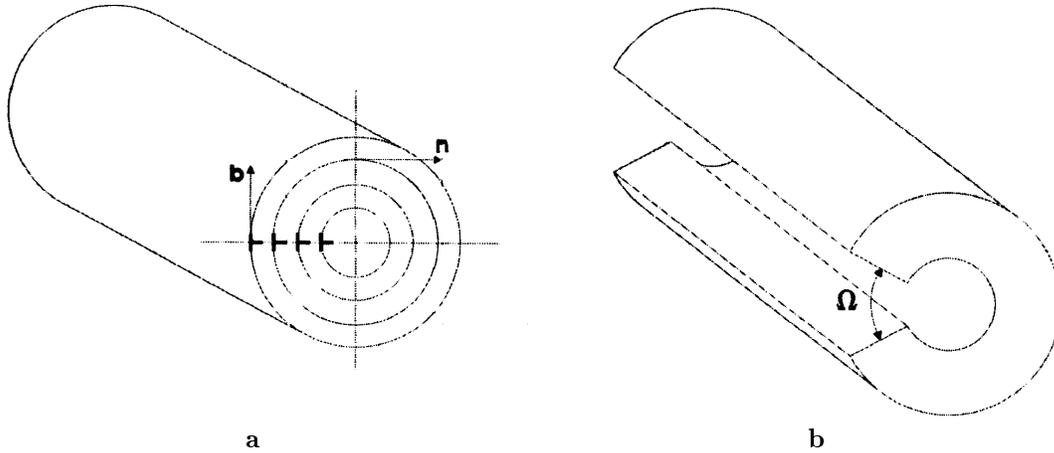


Fig. 3. *a* — appearance of the wall of edge dislocations upon the reduction of the director lines; *b* — appearance of a wedge disclination

respectively, the internal and external radii of the pipe. We introduce the cylindrical coordinates (r, φ, z) , with the z -axis directed along the axis of the pipe. The lines of the director are assumed to have the form of the concentric circles located in a plane perpendicular to the z -axis. The contraction of the material occurs under identical conditions, i.e. the corresponding relative contractions along the director have the same value designated as κ . The emergence of the field of displacements $\vec{W}(r, \varphi, z)$ results in a decrease of the length of the corresponding line of the director by the value $b = 2\pi r\kappa$. This result can be considered as a consequence of the appearance of the edge dislocation with a vector $b\vec{e}_\varphi$. Considering each line of the director in a similar manner, we come to the conclusion that, owing to the contraction, a wall of edge dislocations arises along the pipe radius (Fig. 3,*a*). According to [8], the dislocation wall is equivalent to a wedge disclination (Fig. 3,*b*). The contraction of the pipe can be therefore regarded as a result of the appearance of the wedge disclination with the angle Ω .

2.2. The Strained State of the Pipe with a Wedge Disclination: Linear Theory

The elastic field of a wedge disclination was calculated in [10]. The displacements U_r, U_φ and the stresses $\sigma_{rr}, \sigma_{\varphi\varphi}$, and σ_{zz} are described by the following formulae:

$$U_r = \frac{\Omega}{4\pi} \left(\frac{1-2\sigma}{1-\sigma} \right) r \ln \frac{r}{R} + \left(ar + \frac{b}{r} \right),$$

$$U_\varphi = \frac{\Omega\varphi}{2\pi} r, \tag{8}$$

$$\sigma_{rr} = \frac{\mu\Omega}{2\pi} \frac{1}{1-\sigma} \left[\ln \frac{r}{R} - \frac{(1-r^2/R^2)}{(1-r_0^2/R^2)} \left(\frac{r_0}{r} \right)^2 \ln \frac{r_0}{R} \right],$$

$$\sigma_{\varphi\varphi} = \frac{\mu\Omega}{2\pi} \frac{1}{1-\sigma} \left[1 + \ln \frac{r}{R} + \frac{(1+r^2/R^2)}{(1-r_0^2/R^2)} \left(\frac{r_0}{r} \right)^2 \ln \frac{r_0}{R} \right],$$

$$\sigma_{zz} = \frac{\mu\Omega}{2\pi} \frac{\sigma}{1-\sigma} \left[1 + 2 \ln \frac{r}{R} + \frac{2(r_0/R)^2}{(1-r_0^2/R^2)} \ln \frac{r_0}{R} \right], \tag{9}$$

where σ is Poisson's ratio, and μ is the shear modulus.

2.3. The Strained State of the Pipe with a Wedge Disclination: Nonlinear Theory

In real systems, the deformation is of the order of unity, which demands the application of a nonlinear theory. In the present work, we use the following approximation. The reference and actual configurations of the system are known to be distinguished in a nonlinear theory. We designate the position of a small particle of the system, which corresponds to the first configuration, by $\vec{\rho}_0$. For the particle position in the second configuration, we introduce the notation $\vec{\rho}$. The vector of displacements \vec{U} is defined, correspondingly, as the difference:

$$\vec{U} = \vec{\rho} - \vec{\rho}_0. \tag{10}$$

We consider the transition from the reference configuration to the actual one as a sequence of steps, every step corresponding to a small increase \vec{U} . The actual configuration obtained at the end of every step is regarded as a reference one for the following step, which makes eligible the application of the formulae of the linear theory of infinitesimal deformations, including (8) and (9), to the calculations carried out at every step.

In so doing, we consider the material of the wall to be quasilinear.

According to this approach, the calculation procedure is presented as a sequence of the following steps:

1. The complete angle of the wedge dislocation is divided into N equal parts of the size ω so that the condition $N \gg 1$ be satisfied.

2. The initial thickness of the pipe wall $h = R - r_0$ is divided into M equal intervals with the thickness $\Delta h = h/M$: $[0, h] = [0, \Delta h] \cup \dots \cup [h - \Delta h, h]$, $M \gg 1$. Let us designate the radius-vectors of the edges of each interval by r_i , $i = 1 \div M$. The stresses $\sigma_{rr}(r_i)$, $\sigma_{\varphi\varphi}(r_i)$, and $\sigma_{zz}(r_i)$ and the displacements, which arise owing to the occurrence of the wedge dislocation with the angle ω , are calculated according to formulae (8) and (9) at each of the r_i points.

3. The obtained values of the displacements are used to calculate new internal and external radii of the pipe, as well as new positions and new thicknesses of the intervals, so that $R \rightarrow R^d$, $r_0 \rightarrow r_0^d$, $[0, h] \rightarrow [0, h_d] = [0, \Delta h_1] \cup \dots \cup [h_d - \Delta h_M, h_d]$, $r_i \rightarrow r_i^d$.

4. The stresses, which were calculated in item 2, are recalculated for the new positions of the interval edges in the framework of the formalism of the nonlinear theory of elasticity according to the formulae

$$\begin{aligned} \sigma_{rr}(r_i^d) &= \sigma_{rr}(r_i) \frac{r_i}{r_i^d}, \\ \sigma_{\varphi\varphi}(r_i^d) &= \sigma_{\varphi\varphi}(r_i) \frac{\Delta h}{\Delta h_i}, \\ \sigma_{zz}(r_i^d) &= \sigma_{zz}(r_i) \frac{r_i}{r_i^d} \frac{\Delta h}{\Delta h_i}. \end{aligned} \quad (11)$$

5. The operations described in items 2–4 are repeated iteratively N times, the obtained stresses being summed up.

2.4. Results of Calculations

On the basis of the algorithm described in items 1–5, the computer program in the programming language PASCAL for the automatic calculation of the stress fields arising in the wall of the aortic ventricle of heart has been developed. The numerical values of the used parameters are listed in the table.

The results of calculations, which represent the distribution curves of the stress tensor components along the thickness of the pipe wall, are shown in Fig. 4.

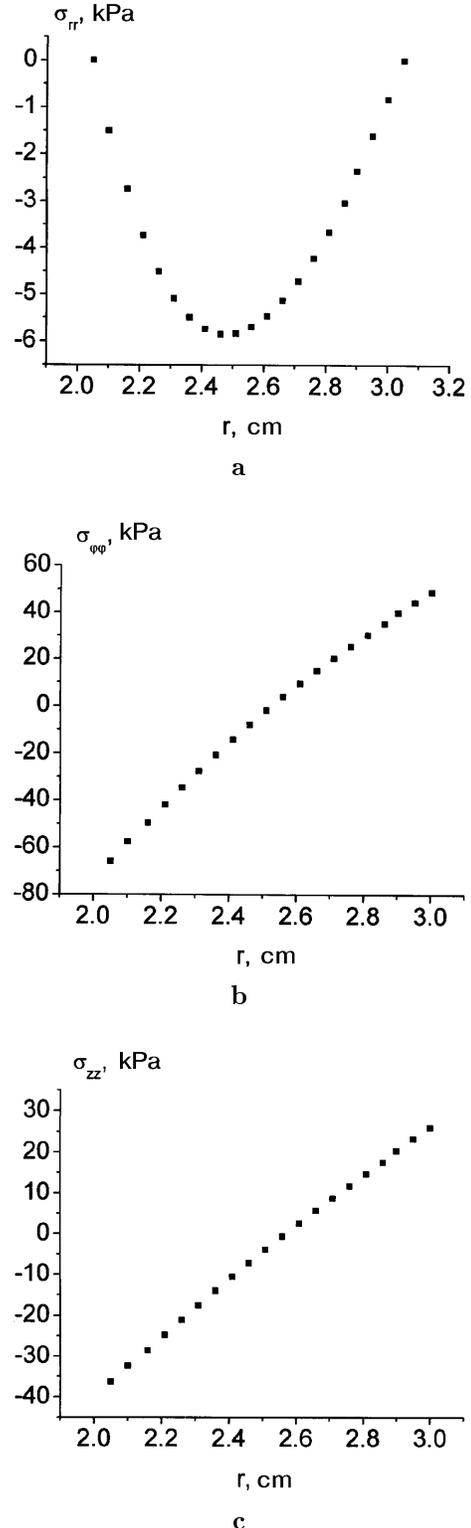


Fig. 4. Stress distributions along the thickness of the pipe wall: σ_{rr} (a), $\sigma_{\varphi\varphi}$ (b), and σ_{zz} (c)

Numerical values of the parameters used for calculations

Shear modulus $\mu \times 10^{-5}$, Pa	5
Internal radius of the ventricle r_0 , cm	2.5
External radius of the ventricle r_0 , cm	3.5
Complete angle of the wedge disclination Ω , rad	1.027

Conclusions

In this work, the model, which allows one to describe the behavior of an ensemble of interacting muscular fibers contracting due to biochemical processes has been suggested for the first time. The capabilities of the model were demonstrated by calculating the field of stresses which arise in the wall of the aortic ventricle of heart. The results of calculations lead to the conclusion that compressive stresses arise in the sections which are adjacent to the internal surface of the ventricle. The obtained result, in the authors' opinion, is worth to be noted for the following reasons. An important factor for the ventricle's normal functioning is a sufficient level of the oxygen supply, which is provided by means of the hemoglobin deoxygenation. The rate of this reaction essentially depends on pressure. Therefore, the significant value of the compressive stresses can essentially worsen the blood supply of those sections which are adjacent to the internal surface of the ventricle. As is known from physiology, such a situation can cause a myocardial infarction in some pathological modes of the heart functioning.

1. *Zima V.L.* // Ukr. Biokhim. Zh.— 1988.— **70**.— P. 23.
2. *Schutt C., Lindberg U.* // Acta phys. Scand.— 1998.— **163**.— P. 307.
3. *Miroshnichenko N.S., Shuba M.F.* // Uspekhi Fiziol. Nauk.— 1991.— **21**.— P. 3.
4. *Mitsui T.* // Adv. Biophys.— 1999.— **36**.— P. 107.
5. *Duke T.* // Proc. Nat. Acad. Sci. USA.— 1999.— **196**.— P. 2770.
6. *Kasevich F.M.* Dislocations in the Theory of Elasticity.— Kyiv: Naukova Dumka, 1976 (in Russian).
7. *Orlov A.N.* Introduction to the Theory of Defects in Crystals.— Moscow: Vysshaya Shkola, 1983 (in Russian).
8. *de Wit R.* Continuum Theory of Disclinations.— Moscow: Mir, 1977 (in Russian).
9. *Rashmer R.* Dynamics of the Cardiovascular System.— Moscow: Meditsyna, 1981 (in Russian).
10. *Lurie A.I.* Theory of Elasticity.— Moscow: Nauka, 1970 (in Russian).

Received 08.01.03.

Translated from Ukrainian by O.I.Voitenko

ДИСЛОКАЦІЙНА МОДЕЛЬ М'ЯЗОВОГО СКОРОЧЕННЯ*Л.А. Булавін, Ю.Ф. Забашта, С.В. Северилов***Резюме**

На основі континуальної теорії дислокацій розроблена модель, що дозволяє описати скорочення колективу взаємодіючих м'язових волокон. За її допомогою зроблено оціночні розрахунки напруженого стану основного елемента серцево-судинної системи — лівого шлуночка серця — і проведено їх якісну інтерпретацію.