International Journal of Thermophysics, Vol. 26, No. 3, May 2005 (© 2005)
DOI: 10.1007/s10765-005-5580-8

Thermodynamic and Mechanical Properties of Skeletal Muscle Contraction

Yu. I. Prylutskyy,[1,2] A. M. Shut,[1] M. S. Miroshnychenko,[1] and A. D. Suprun[3]

Received June 27, 2003

Thermodynamic parameters such as the change of entropy, internal energy, and enthalpy were calculated as a function of the relative skeletal muscle strain within the framework of a proposed thermodynamic model. A value for the Young's modulus for the skeletal muscle was also estimated. The obtained theoretical values are in a good agreement with available experimental results for the frog skeletal muscle contraction.

KEY WORDS: Pmechanical properties; skeletal muscle contraction; thermodynamic properties.

1. INTRODUCTION

Muscle, as a complex biophysical system, draws the attention of many researchers. It is conditioned mainly by newly received experimental data [1–4] on muscle contraction, in particular of a force, which is developed by a fiber of skeletal muscle under loading (the so-called *equation of state*) and electrical stimulation and its dependence on length, speed, and other physical parameters. It was determined that the obtained experimental results did not quite match the postulates of a model of skeletal muscle contraction, known as the theory of sliding [5]. Therefore, it is needed to explain these experimental facts within the framework of a correct mechanism of contraction and to develop an adequate mathematical formulation.

[1] Department of Biophysics, Kyiv National Shevchenko University, Volodymyrska Str., 64, 01033 Kyiv, Ukraine.
[2] To whom correspondence should be addressed. E-mail: prylut@biocc.univ.kiev.ua
[3] Department of Physics, Kyiv National Shevchenko University, Volodymyrska Str., 64, 01033 Kyiv, Ukraine.

First of all, it should be noted that all contraction models in one way or another are connected with the dynamics of the myosin–actin complex within the sarcomere (the smallest moving unit of skeletal muscle). For example, an active movable unit of a sliding model [6] is a heavy fraction of myosin (the head of a myosin molecule). In addition, the sliding model has two submodels, one of which is based on the inactivity of a light fraction of myosin and the activity of its heavy fraction, while the other one, on the contrary, is based on the contracting activity of a light fraction with a heavy fraction functioning as a connector of myosin and actin filaments. According to another mechanism [7], the contraction of skeletal muscle is a result of twisting of myosin filaments into the tubiform structures, formed by actin filaments. The contraction is possible because of the interdomain motion of two molecule heads, which, in turn, move. Pollack's model [1] is based on the "stepwise" contraction of muscle fiber. Davydov's model [8] is based on motion as well, but that of a soliton, which stimulates the reciprocal movement of both myosin and actin filaments. There is another model [9], which is based on stimulation of α-helical segments of albumin, but unlike Davydov's model, it is focused not on the soliton motion, but on a deformation reaction of α-helix to stimulation. Although the concepts concerning the mechanism of contraction show considerable differences, all the existing models are connected with the motion ("sliding," "twisting," "stepwise," "soliton," etc.). In addition, this motion should be asynchronous in different parts of a sarcomere and in different points of time to provide (during the process of contraction) constant interaction between actin and myosin. Such asynchronism means simultaneous presence in a sarcomere of all possible impulse values of moving elements, independent of what is meant under the "moving element," that is, regardless of the model. Besides, these are the elements, which can be considered as a one-dimensional gas of non-interacting particles (at least to a first approximation). Therefore, it's obvious that to explain experimental data on skeletal muscle contraction, one should use methods of statistical physics for a one-dimensional gas of non-interacting particles.

2. MODEL AND DISCUSSION

Let's consider a biological system – sarcomere (its length $\sim 2.5\,\mu$m), stimulation of which results in contraction. In consequence, in such a continuum – one-dimensional gas, emerge movements with continuous or quasi-continuous set of impulses $\boldsymbol{p} = \hbar \boldsymbol{k}$ ($\hbar$ is Planck's constant and $\boldsymbol{k}$ is a wave vector), which represents the sarcomere function.

As is known [10], the physical behavior of any system is determined by its statistical sum Z, taken over all probable states. In this case, these states are determined by the value of a wave number k. In other words, the statistical sum is given by the formula

$$Z = \sum_k e^{-\frac{E(k)}{\Theta}}, \tag{1}$$

where the energy of a system may be written as

$$E(k) = \frac{\hbar^2 k^2}{2m}. \tag{2}$$

Here, m is a mass of an active motor element and $\Theta = k_B T$, where k_B is the Boltzmann constant and T is an absolute temperature.

Substituting Eq. (2) into Eq. (1), we get

$$Z = \sum_k e^{-\frac{\hbar^2 k^2}{2m\Theta}}. \tag{3}$$

Equation (3) is used to find the statistical sum. Since the problem is one-dimensional, in this formula we can change from summing to integration by area, where values of k have physical significance: $\frac{4\pi}{l} \le |k| \le \frac{\pi}{2a}$, where l is a length of a region under review (length of a sarcomere) and a is the smallest area in a system (it varies in different models). Then

$$Z = \frac{l}{\pi} \int_{\frac{4\pi}{l}}^{\frac{\pi}{2a}} e^{-\frac{\hbar^2 k^2}{2m\Theta}} dk. \tag{4}$$

Assuming

$$\frac{\hbar^2 k^2}{2m\Theta} = X^2 \tag{5}$$

we get

$$Z = 4\frac{\Phi(X_2) - \Phi(X_1)}{X_1}, \tag{6}$$

where

$$X_1 = \frac{4\pi\hbar}{l\sqrt{2m\Theta}} = \frac{l_0}{l}, \tag{7}$$

$$X_2 = \frac{\pi\hbar}{2a\sqrt{2m\Theta}} = \frac{l_0}{8a}, \tag{8}$$

$$\Phi(X) = \int_0^X e^{-t^2} dt. \tag{9}$$

Here $l_0 = \frac{4\pi\hbar}{\sqrt{2m\Theta}}$ is a parameter, which has a dimension of length and can equal or be proportional to the initial length of a sarcomere. This implies that the length of a sarcomere depends on temperature as in

$$l \sim \frac{1}{\sqrt{T}}. \tag{10}$$

Let's estimate the value of X_2 and the function $\Phi(X_2)$, assuming $l_0 \sim 2.5\,\mu$m and $a \sim 20$ nm (this value corresponds to the length of the head of a myosin molecule [6] and to the length of a "skip" in Pollack's model [1]): $X_2 \sim 15.6$ and $\Phi(15.6) \sim \Phi(\infty) = \frac{\sqrt{\pi}}{2} = 0.89$.

With regard to the function $\Phi(X_1)$, we decompose into a Taylor series to the second non-zero term inclusive, that is,

$$\Phi(X_1) = X_1 - \frac{X_1^3}{3}. \tag{11}$$

Then the statistical sum (Eq. (3)) is

$$Z = 4\frac{0.89 - X_1 + \frac{X_1^3}{3}}{X_1},$$

or, taking into account Eq. (7),

$$Z = 4\left\{0.89\frac{l}{l_0} - 1 + \frac{1}{3}\left(\frac{l}{l_0}\right)^2\right\}. \tag{12}$$

Using the calculated statistical sum (Eq. (12)), we find the free energy of the system;

$$F = -\Theta \ln Z = -\Theta \ln 4 - \Theta \ln\left\{0.89\frac{l}{l_0} - 1 + \frac{1}{3}\left(\frac{l}{l_0}\right)^2\right\}. \tag{13}$$

Since the change of a muscle volume as a function of its strain at isobaric conditions ($P = \text{const}$) is insignificant ($P\Delta V \approx 0$), the change of the Helmholtz free energy of the system can be written as

$$\Delta F \approx -f\Delta l - S\Delta T, \tag{14}$$

where the contraction force f is concentrated in the opposite direction from the direction of muscle contraction and is a function of its relative deformation, $\varepsilon = \frac{\Delta l}{l_0}$

$$f(\varepsilon) = -\left(\frac{\partial F}{\partial l}\right)_T = f_0\varphi(\varepsilon),$$

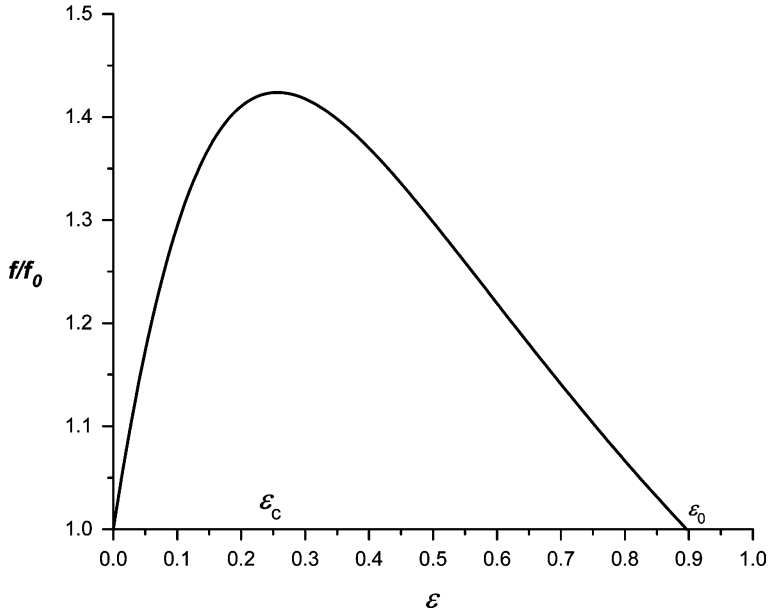

Fig. 1. Force of the muscle contraction (referenced to the amplitude value f_0) as a function of relative deformation ε using Eq. (16).

where

$$f_0 = \frac{k_B T}{l_0}, \tag{15}$$

$$\varphi(\varepsilon) = \frac{0.223 + 1.78\varepsilon + 3.56\varepsilon^2 + 0.89\varepsilon^3}{0.223 + 0.89\varepsilon + 2.34\varepsilon^2 + 2.56\varepsilon^3 + 0.89\varepsilon^4}. \tag{16}$$

Equation (16) is plotted in Fig. 1. As we can see, it has a maximum value at $\varepsilon_c = 0.25$, which, although the phases of contraction and relaxation are simultaneous, divides them. This value corresponds to the "physiological" muscle length $1.25l_0$. The increase of this length can lead to irreversible changes in the muscle, which, under such conditions, loses its ability to contract. The maximum possible lengthening of a muscle in our case is $1.9l_0(\varepsilon_0 = 0.9)$. The theoretical curve in Fig. 1 agrees qualitatively with the data of well-known classical experiments on stress–strain properties of a frog skeletal muscle, as cited in Refs. 1 and 6.

From Eqs. (15) and (10) we note that the contraction force of a muscle depends on temperature,

$$f \sim k_B T^{3/2}. \tag{17}$$

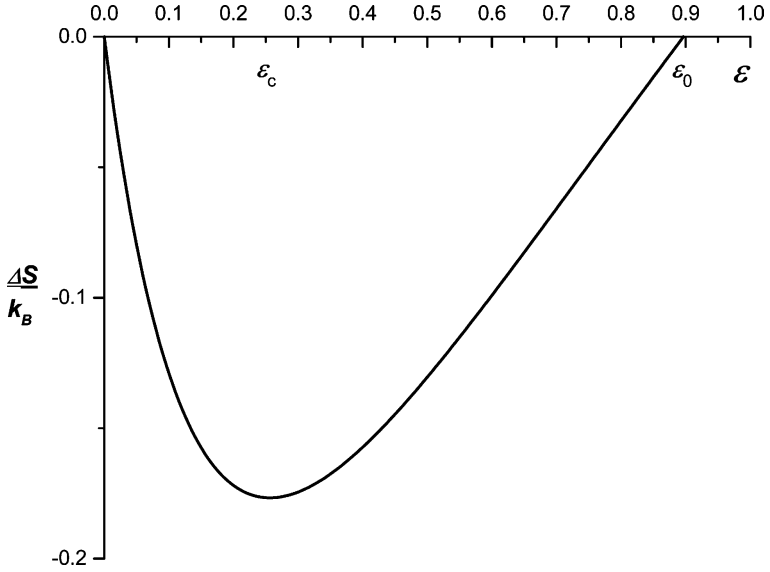

Fig. 2. Change of system entropy (referenced to the Boltzmann constant k_B) as a function of relative deformation ε using Eq. (20).

The entropy of the system is given by the formula:

$$S(\varepsilon) = -\left(\frac{\partial F}{\partial T}\right)_l = k_B \ln \phi(\varepsilon),$$

$$\phi(\varepsilon) = \frac{0.893 + 2.68\varepsilon + 6.68\varepsilon^2 + 3.56\varepsilon^3}{(1+\varepsilon)^2}. \tag{18}$$

The change of internal energy and enthalpy is given by the formula

$$\Delta U(\varepsilon) \approx \Delta H = -f\,\Delta l + T\,\Delta S, \tag{19}$$

where, using Eqs. (10) and (17), the isothermal change of the entropy of a system can be written as

$$\Delta S(\varepsilon) = -\int_{f_0\varphi(\varepsilon)}^{f_0} \left(\frac{\partial l}{\partial T}\right)_f df \sim -\frac{k_B}{2} \ln \varphi(\varepsilon). \tag{20}$$

Equation (20) is plotted in Fig. 2. As we can see, on the strain of the muscle, the value of entropy decreases and reaches its minimum value at the point $\varepsilon_c = 0.25$. However, the tendency of a strained muscle to contract is

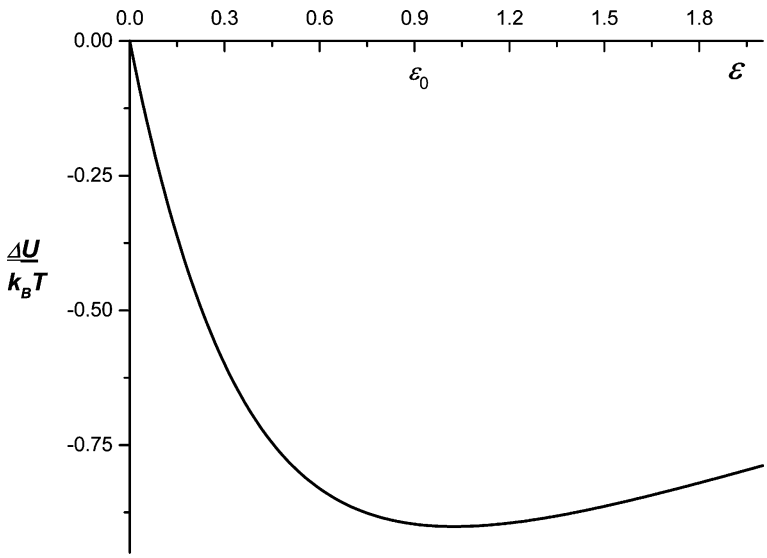

Fig. 3. Change of system internal energy (referenced to the thermal energy $k_B T$) as a function of relative deformation ε using Eq. (21).

determined by a spontaneous tendency of the entropy to increase, which occurs at $\varepsilon_c < \varepsilon \leq \varepsilon_0$.

Substituting Eq. (20) into Eq. (19), we get

$$\Delta U(\varepsilon) \approx \Delta H \sim -k_B T \psi(\varepsilon),$$
$$\psi(\varepsilon) = \varepsilon\varphi(\varepsilon) + \frac{\ln \varphi(\varepsilon)}{2}. \tag{21}$$

Equation (21) is shown in Fig. 3. As we can see, its minimum value is at $\varepsilon_0 = 0.9$, which corresponds to the maximum possible muscle strain $1.9 l_0$. In the investigated area of a length change of relative muscle deformation, the change of enthalpy $\Delta H < 0$, in other words, the system, evolves heat.

Finally, muscle tension is given by the formula,

$$\sigma(\varepsilon) = \frac{f}{s} = \frac{f_0}{s}\varphi(\varepsilon). \tag{22}$$

From this we obtain the formula for its Young's modulus,

$$E = \left.\frac{d\sigma}{d\varepsilon}\right|_{\varepsilon=0} \approx 4\frac{f_0}{s}, \tag{23}$$

where s is a squire of a muscle crosscut. From experiments [3, 11] we know that $\frac{f_0}{s} \approx (0.1 - 0.3)$ MPa (the maximum value of isometric strain of a frog

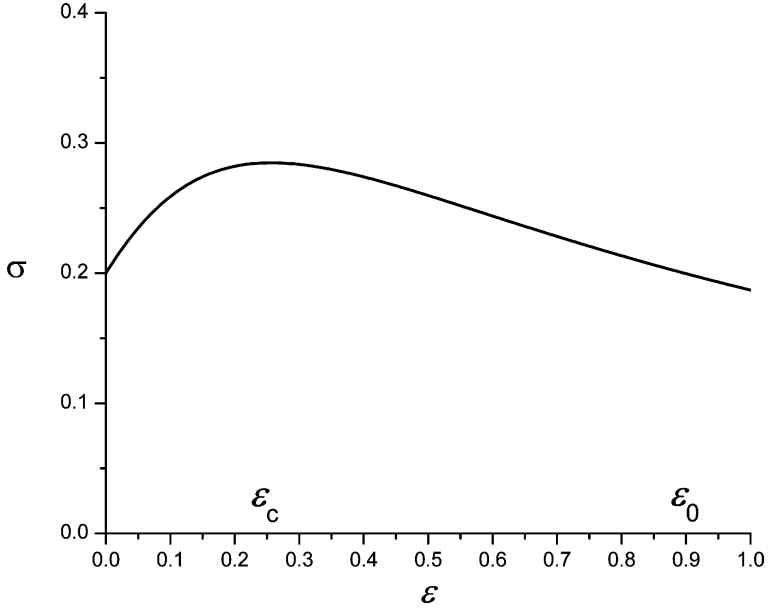

Fig. 4. Muscle tension as a function of relative deformation ε using Eq. (24).

skeletal muscle). Consequently, we have $E \approx (0.4\text{–}1.2)$ MPa (for comparison: $E \approx 8$ MPa for rubber).

The calculated muscle tension by the equation,

$$\sigma(\varepsilon) \approx \frac{\langle E \rangle}{4} \varphi(\varepsilon) \tag{24}$$

is given in Fig. 4 (here $\langle E \rangle = 0.8$ MPa). As one can see, the obtained $\sigma(\varepsilon)$ dependence for the $f(\varepsilon)$ function (Fig. 1) has a maximum value at $\varepsilon_c = 0.25$, and further it falls with an increase of lengthening muscle.

3. CONCLUSION

Within the framework of the proposed model of the skeletal muscle contraction, which is based on the general principles of statistical physics, it was possible first to analytically calculate a change in the internal energy and enthalpy of this system and to estimate its Young's modulus. The obtained theoretical results agree qualitatively with the known classical experiments from the study of the mechanical properties of the frog skeletal muscle contraction. One particularly interesting result, in our opinion, is the establishment of the temperature dependence of the sarcomere

length and force of the muscle contraction, which requires further experimental examination.

REFERENCES

1. G. H. Pollack, *Muscles and Molecules: Uncovering the Principles of Biological Motion* (AIP, New York, 1990).
2. P. A. Wahr and J. M. Metzger, *J. Physiol.* **85**:76 (1998).
3. K. A. P. Edman, *J. Physiol.* **519**:515 (1999).
4. M. S. Miroshnichenko, I. A. Zaloilo, D. M. Nozdrenko, and Yu. I. Prylutskyy, *Phys. Alive* **9**:71 (2001).
5. V. I. Deshcherevskiy, *Mathematical Models of Muscle Contraction* (Nauka, Moscow, 1977).
6. J. Bendoll, *Muscles, Molecules and Motion* (Mir, Moscow, 1970).
7. M. S. Miroshnichenko and M. F. Shuba, *Usp. fiziol. nauk* (in Russian) **21**:3 (1990).
8. A. S. Davydov, *Solitons in the Molecular Systems* (Naukova Dumka, Kiev, 1988).
9. A. D. Suprun and Yu. B. Atmagha, *Visnyk Kyiv Univ.* (in Ukrainian) **3**:470 (2000).
10. E. M. Lifshits and L. P. Pitaevskiy, *Statistical Physics* (Nauka, Moscow, 1978).
11. R. L. Lieber, M. E. Leonard, C. G. Brown, and C. L. Trestik, *Am. J. Physiol.* **261**:86 (1991).