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Myosin, numerical position determination and mechanical properties

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Myosin is a superfamily of molecular motor [3]. Especially, myosin II is able to generate force for a muscle contraction by sliding on an actin filament. To extract energy, the myosin motor has to hydrolyze adenosine triphosphate (ATP) to adenosine diphosphate (ADP). The energy is used for the power stroke.

We use three state mathematical model based on three connected Fokker-Planck equations [1]

$$\frac{\partial \rho_i}{\partial t} = D\frac{\partial}{\partial x}\left[\frac{1}{k_B T}\left(V_i'(x) + F_{Load}\right)\rho_i\right] + D\frac{\partial^2 \rho_i}{\partial x^2} + \sum_{j=1}^{N} k_{ij}\rho_j - \sum_{j=1}^{N} k_{ji}\rho_i, \tag{1}$$

where ρ is probability density function of a presence of a single myosin head at actin filament x in a time t. D is a diffusion coefficient, which describes Brownian motion in an aqueous solution (the myosin characteristic size is in nanometers—thus, myosin is also a kind of Brownian particle). k_B denotes the Boltzmann constant and T thermodynamic temperature. Their product is a characteristic value of thermal fluctuations. V is the active potential energy produced by the chemical reaction in a given state. The parameter F_{Load} is the external load force on myosin motor. The index i is used as a marker for a single state [1]. Equation (1) is solved by the WPE algorithm [5] for space variables x and by the MATLAB function ode15s for the time variable t.

The three states are known as unbound, weakly-bound and post-power-stroke [2]. None of these states does include the power stroke itself. The key step for obtaining mechanical properties of such system is the determination of the generation of the force. The force generated by a single myosin F has to be calculated based on the probability density distribution as

$$F = \int_0^L x\rho \mathrm{d}x, \tag{2}$$

where $L = 36\,\mathrm{nm}$, which is characteristic myosin II step. Other mechanical properties, like work W, can be obtained by its definition, for example,

$$W = \int F\mathrm{d}x. \tag{3}$$

In case of determination myosin head state and position, it is still possible to calculate these classical mechanical properties. In our model, the determination is simulated by a pseudorandom number generator provided by MATLAB. The generated number provides both the state and position. We presume the procedure is not error-less [4]. The error has a Gaussian form

$$\rho_e = \frac{1}{\sqrt{2\pi\sigma^2}} \exp -\frac{(x-y)^2}{2\sigma^2}, \tag{4}$$

where the variance $\sigma^2 = 5\,\mathrm{m}^2$.

The next system evolution is started after determination myosin position with a new initial condition. The condition is created via Bayes' theorem.

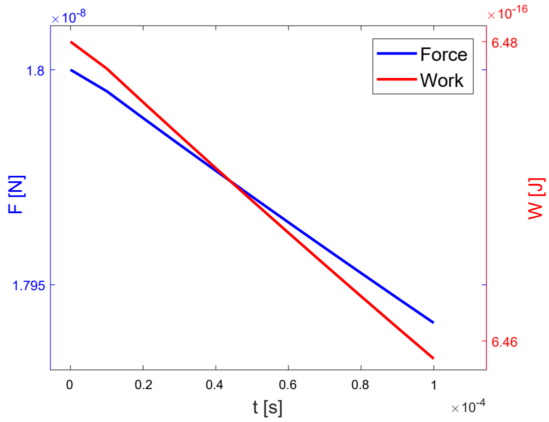

Fig. 1. Generated force and work before myosin state and position determination. The initial condition is the canonical one

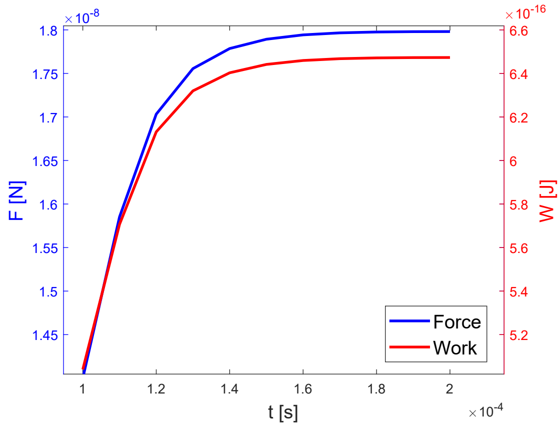

Fig. 2. Force and work after myosin state and position determination. The determined state is the unbound one

In Fig. 1 is visible the biggest value of force F and work W is in the equilibrium state. In the time of position and state determination is the system very disturbed. Its next values of mechanical properties are given of the myosin position mostly. For the unbound state we obtained an increase of the mechanical properties, see Fig. 2. For other states, we obtained different characteristics. For the weakly-bound state, there are almost constant and for post-power-stroke are decreasing, respectively.

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