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PROTEIN MECHANICS: FROM AMINO ACID TO SWIMMING CELLS

Patrick Onck

Micromechanics, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

Abstract

This proceedings paper contains a review of the work presented in the Sectional Lecture in Solids on August 25 at ICTAM 2016. -- Proteins are long polypeptide chains of amino acids and their structure and biological function are directly related to their amino acid sequence. I will discuss three different biological functions that are dominated by protein mechanics, each at their own specific time and length scale. To relate structure to function, multiscale computational models have been developed for (i) cilia and flagella, (ii) actin filament networks and (iii) the nuclear pore complex.

Peer-review under responsibility of organizing committee of the 24th International Congress of Theoretical and Applied Mechanics

Keywords: proteins; computational biomechanics; biophysics; molecular dynamics, actin networks, nuclear pore complex, cilia and flagella.

1. Introduction: Proteins

Proteins are often referred to as the building blocks of life, playing critical roles in almost all structures and activities in biology. Fig. 1 provides an overview of the different length scales of proteins discussed in this review, starting from the atomic scale and ending at the scale of cells. At the smallest, atomic length scale, proteins consist of amino acids. There are 20 different amino acids, each with their own atomic structure, chemical and physical properties. The amino acids form peptide bonds that form long polypeptide chains consisting of hundreds and sometimes thousands of amino acids. Depending on the specific amino-acid sequence (primary structure) the polypeptide chains fold into regular structures, such as α-helices and β-sheets (secondary structure). At a larger spatial level of organization, α-helices and β-sheets will fold into three-dimensional (tertiary) structures, i.e., the actual protein molecule. Finally, protein molecules can combine to form large protein complexes (quaternary structures). In this Proceedings paper I will discuss three different quaternary structures: (i) cilia and flagella in section 2.1, (ii) actin filament networks in section 2.2 and (iii) the nuclear pore complex (NPC) in section 2.3.

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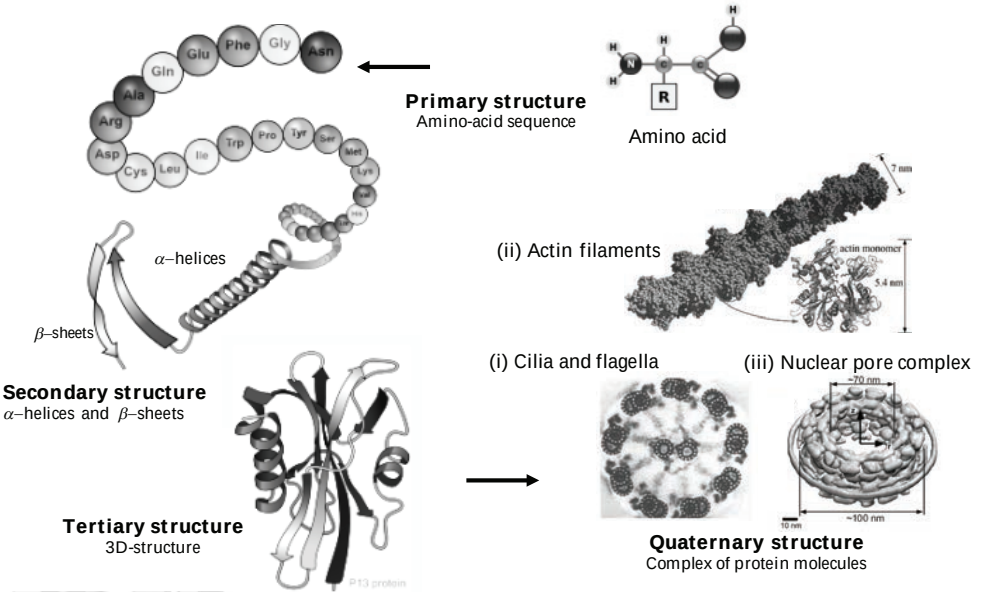

Fig. 1. Overview of the different length scales of proteins. Proteins consist of long polypeptide chains consisting of hundreds of amino-acids. The amino-acids is the smallest building block of proteins, consisting of 10 atoms on average. These amino-acid sequences form the primary structure of proteins. Depending on the specific amino-acid sequence the polypeptide chains fold into ordered structures: α-helices and β-sheets, the secondary structure of proteins. At an even larger spatial level the secondary structures combine into the three-dimensional (tertiary) structure, often referred to as the actual protein molecule or subunit. Finally, the protein molecules can combine into large protein complexes (quaternary structures), such as actin filaments, cilia and flagella, and the nuclear pore complex (NPC). Image sources: [1-4].

2.1 Cilia and flagella

At the largest length scale, we focus on cilia and flagella, long hair-like projections from the surface of cells that play an important role in cell motility [5], see Fig. 2. Cells and micro-organisms use cilia and flagella to propel themselves or to propel the fluid surrounding them. Examples are the beating tails (flagella) of sperm cells (see Fig. 2c), or the cilia that line the respiratory tract to propel mucus out of the lungs. The beating of cilia and flagella is enabled by their internal microstrucure, the axoneme (see Fig. 2b), a big protein complex (tens of μm long and 250 nm wide) that is powered by a dense distribution of motor proteins, called dyneins (Fig. 2a). Motor proteins constitute an important class of proteins that, powered by the hydrolysis of ATP, undergo

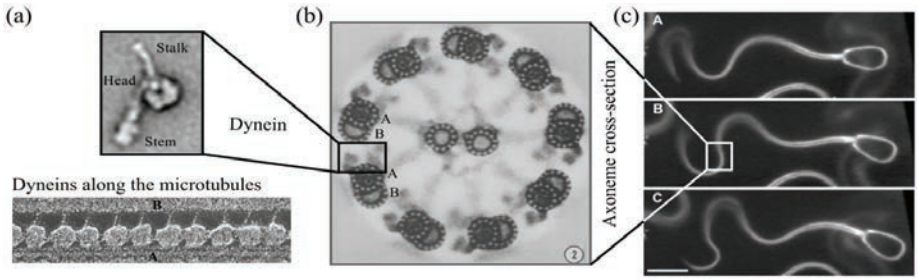

Fig. 2.: (a) Structure of an axonemal dynein (top). Dyneins at a regular spacing along the microtubules (bottom) (from [6]). (b) An electron micrograph of an axoneme cross-section (from [7]). (c) Flagellar beating of a spermatozoon. The three images (A-C) are 200 ms apart (from[8]). The total figure appeared before in [9].