

STRUCTURE OF FIBROIN MOLECULE IN NATURAL SILK FIBER

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Abstract

This article provides information on the composition and structure of the fibrillar protein-fibrion macromolecule, which makes up the composition of natural silk fiber. The primary structure of these proteins depends on the nature of the natural cocoon, the diet of the silkworm, time and other biological factors.

Keywords: Fibroin, Sericin, natural silk, polypeptide chain, conformational diversity, α -helix, β -structure, crystalline part, amorphous part, hydrophilic, hydrophobic, disulfide bridge, hydrogen bond.

Fibroin and sericin are fibrillar proteins that form the polymer base of natural silk. The primary structure of these proteins depends on the nature of the natural cocoon, the diet of the silkworm, time and other biological factors. The largest amount of mass in fibroin macromolecule corresponds to Gly, Ala, Tyr, Ser groups. In addition, there is a very small amount (<1 %) of Cys per fibroin macromolecule. The polypeptide chain of fibroin contains hydrophilic and hydrophobic amino acid groups in a ratio of 6.3:1. The sequence of amino acid groups in the crystal parts of fibroin macromolecule is arranged in the following order:



The average molecular mass of fibroin is $M_w=(2.5\div 3.8)\cdot 10^5$. Both fibroin and sericin macromolecules are characterized by conformational diversity, i.e., the polymer chain consists of consecutive α -helix and β -structural parts. Since natural silk does not contain sulfur amino acids, waves do not appear in the silk fiber. X-rays of natural silk show that this fiber is made up of crystalline areas - fibrils, which is why it is called fibroin. Amorphous parts of other proteins are also present between the fibrils. Fibroin has a layer-by-layer secondary structure, and the molecular chains are antiparallel. The distances between the molecular chain layers are repeated in the form of 0.35-0.57 nm.

Fibroin is a protein with poor water solubility, while sericin is well soluble in water. It is observed that macromolecules in the swollen state move to the following conformation, which rotates to each other under conditions of high mobility. α -spiral \leftrightarrow tubercle \leftrightarrow β -structure α -helix - is distinguished by its side substituents and is composed of repeating groups of amino acids. The distance between atoms of the same type in a helix (helix pitch) is 1.5 Å. The angle between the spirals is 26°. One turn of the helix consists of 3.6 amino acid residues. If these residues are converted from a helical to a linear configuration, this distance is 5.4 Å. If the

protein is subjected to external deformation forces, a layered β -structure is formed. Tertiary structure of fibroin in the solid state is formed by parallel and antiparallel elongated polypeptide chains on the basis of β -structures packed in parallel. The distance between these layers corresponds to $3.5\div 3.8\text{\AA}$.

Polypeptide chains are interconnected by intensive intermolecular bonds, both in each ribbon and between layers. These ribbons are an elementary component of the fibroin base of natural silk and are wound in a spiral form. Hydrothermal treatment of natural silk-cocoon is a thread wound under intensively suffocated conditions. In this case, the spun thread forms a single coil with the help of 2 fibroin fibers sericin layers with a very complex morphological structure. If the layer of sericin between the fibers is washed by 25%, a silk fiber product is obtained; If it is washed up to 4-5%, the silk fiber becomes natural silk. Polypeptide chains in natural cocoons have a primary structure depending on their function (silk is mainly fibroin or the connecting layer between them is sericin). If the amount of hydrophobic amino acid groups in these polypeptide chains is high, fibroin is formed, if the amount of hydrophobic amino acid groups is low, sericin is formed.

The connection between fibroin and sericin is formed by disulfide and complex ether bridges, intermolecular hydrogen bonds, and non-protein components, such as monooses. The orderly arrangement (crystallization) of polypeptide chains in the system increases with decreasing water content. In addition, heating the fiber in an inert environment also leads to an increase in the degree of crystallization.

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