10. COMPUTER MODELLING OF THE QUASI-CRYSTALLOID BIOPOLYMER STRUCTURE IV.

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Abstract

This paper deals with the computer modelling of the single filament, and the α-helix composed of pentagon dodecahedrane units. The method is nearly the same as in our previous papers (1995, 1996, 1997), only the modelling of the superficial network together with the superficial points of symmetry was omitted. In particular the different kinds of points of symmetry of the single α-helix seem to be useful in the interpretation of our partially degraded recent and fossil biopolymer systems.

Key words: Plant cell, biopolymer system, computer modelling.

Introduction

Filaments as one of the earliest biological structure were published by PFLUG (1965 a,b) isolated from the Algonkian. Helical Precambrian organic microfossils (*Spirillinema bentori*) from Sinai were described by SHIMRON and HOROWITZ (1972). Filaments are essential components of the cytoskeleton (KOBAYASHI, FUKUDA and SHIBAOKA, 1987). ROWLEY (1967) published fibrils, microtubules and lamellae from the pollen grains. HESLOP-HARRISON, Y. and HESLOP-HARRISON, J. (1982) investigated the microfibrillar components of the intine. Radially oriented chain-molecules were described at the ontogenetically different layers (ectexine and endexine) of the partially dissolved pollen grains of *Pinus griffithii* MCCLELL by KEDVES, TÓTH, KÁROSSY and VARGA (1996). Following MACKAY (1990) α-helix was demonstrated at the structures of the amino-acids by PAULING and COREY (1951). ROWLEY, J. R., DAHL and ROWLEY, J. S. (1980) described first the helical subunits from the exine of *Artemisia* pollen grains. Later ROWLEY, J. R., DAHL, SENGUPTA and ROWLEY, J. S. (1981) published a model for the exine substructure. ROWLEY, J. R., EL-GHAZALY and ROWLEY, J. S. (1987) described the subunits of the microchannels of the pollen exine. Fossil helical biopolymer unit was published from the Jurassic carbonate manganese layers by KEDVES (1987). During the three dimensional modelling of the quasi-crystalloid biopolymer structures (KEDVES 1991, 1992) the filaments and the helical structures were also the subject of our investigations.

It was emphasized previously that to investigate several characters of the quasi-crystalloid biopolymer systems and the stabilizing molecular structures the computer modelling is the unique method. In this way the aim of this contribution is to investigate with this method these two very important structures.

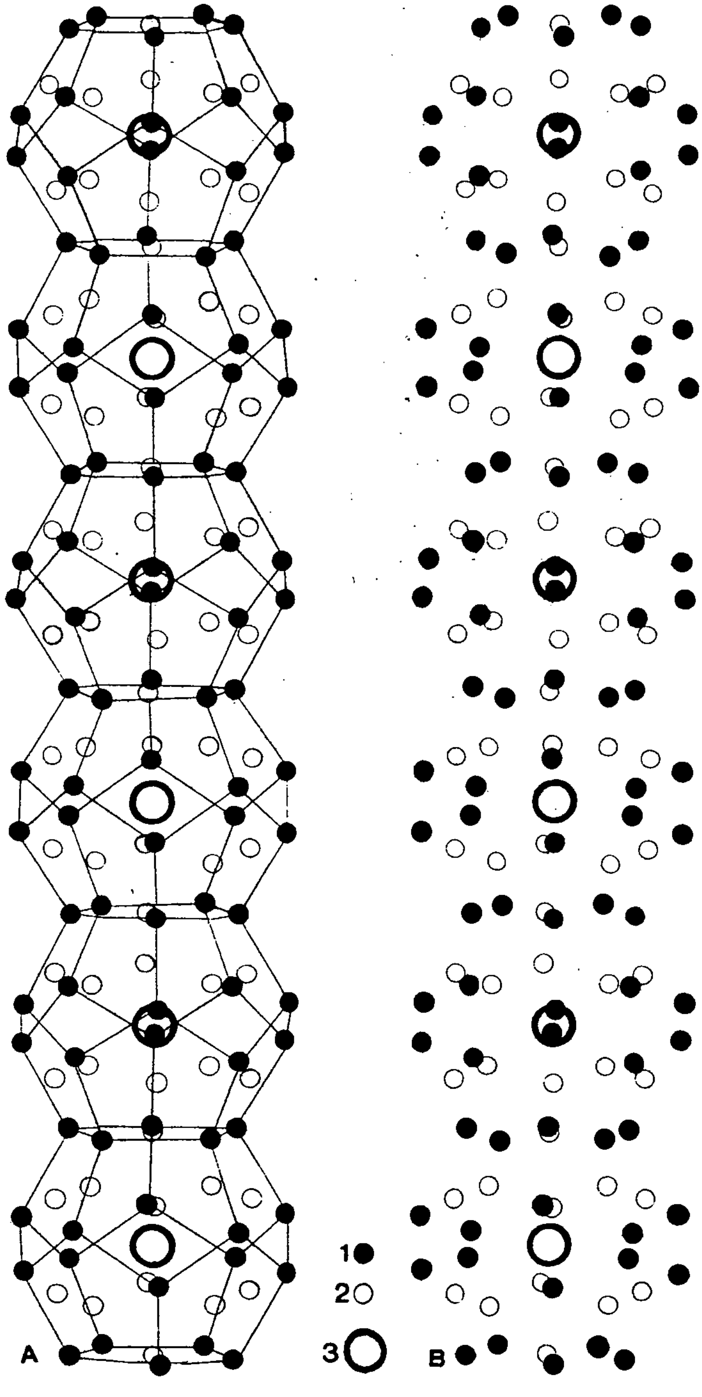

Plate 10.1.

Methods

The basic method was elaborated and described in our previous papers (1994, 1995). The symbols are also the same as in the previous publications. The following characteristic features of symmetry were the subject of this contribution: 1. The network of the quasi-crystalloid skeleton together of the three kinds of points of symmetry. 1.1. The centrum of the pentagon dodecahedrane. 1.2. The points of symmetry of the edges of the pentagonal planes, 1.3. The centrum of the pentagonal planes. 2. The points of symmetry of the quasi-crystalloid biopolymer system without network.

Results

1. FILAMENT (Text-fig. 10.1 A,B)

A so-called single filament was modelled. Text-fig. 10.1A represents the lateral view of the quasi-crystalloid skeleton and all points of symmetry, including the central stabilizing units also. The regular alterning characteristic features of the skeletal network of the pentagon dodecahedrane units and the different kinds of points of symmetry are well shown. Particularly the central stabilizing globular units are interesting. In two dimensions, the schema of each second central stabilizing unit surrounds two points of symmetry of the edges of the quasi-crystalloid skeleton. At the other stabilizing units the two points of symmetry are near the central unit in the axial line of the filament. In lateral view the part of the quasi-crystalloid skeleton around the central stabilizing units is a rhombus form.

The points of symmetry of the single filament without network (Text-fig. 10.1B). The axial points of symmetry represent the following alterations. In the axis there are six nearby points of the edges of the pentagons. At each second "pentagon dodecahedrane unit" two of them are surrounded by the contour of the central stabilizing unit as it was discussed previously. Perpendicular to the axis of the filament two different kinds of patterns of points of symmetry are characteristic which follow the regular alterations of the central points of symmetry.

2. SINGLE α-HELIX (Text-figs. 10.2., 10.3.)

The computer model of this simple helical structure of pentagon dodecahedrane units well demonstrates the complexity of this problem. First of all the arrangements of the different kinds of points of symmetry and the network of the quasi-crystalloid skeleton depend from the orientation of the helical unit. By the different orientation of the single helical structure several different patterns of network, and points of symmetry may be obtained. We have chosen a lateral view, which may be useful in the interpretation of the biopolymer structure of the microchannels also. Text-fig. 10.2. well illustrates the position in the quasi periodic system every skeletal and the central stabilizing biopolymer system of the pentagon dodecahedrane unit. Without quasi-crystalloid network, the results of the pattern of the different kinds of points of symmetry may be summarized as follows:

Text-fig. 10.1.

Computer model of the single filament composed of pentagon dodecahedrane units. Legends: 1. Points of symmetry of the edges of the pentagon dodecahedrane units. 2. The centres of the regular pentagon planes. 3. The centrum of the pentagon dodecahedrane units.

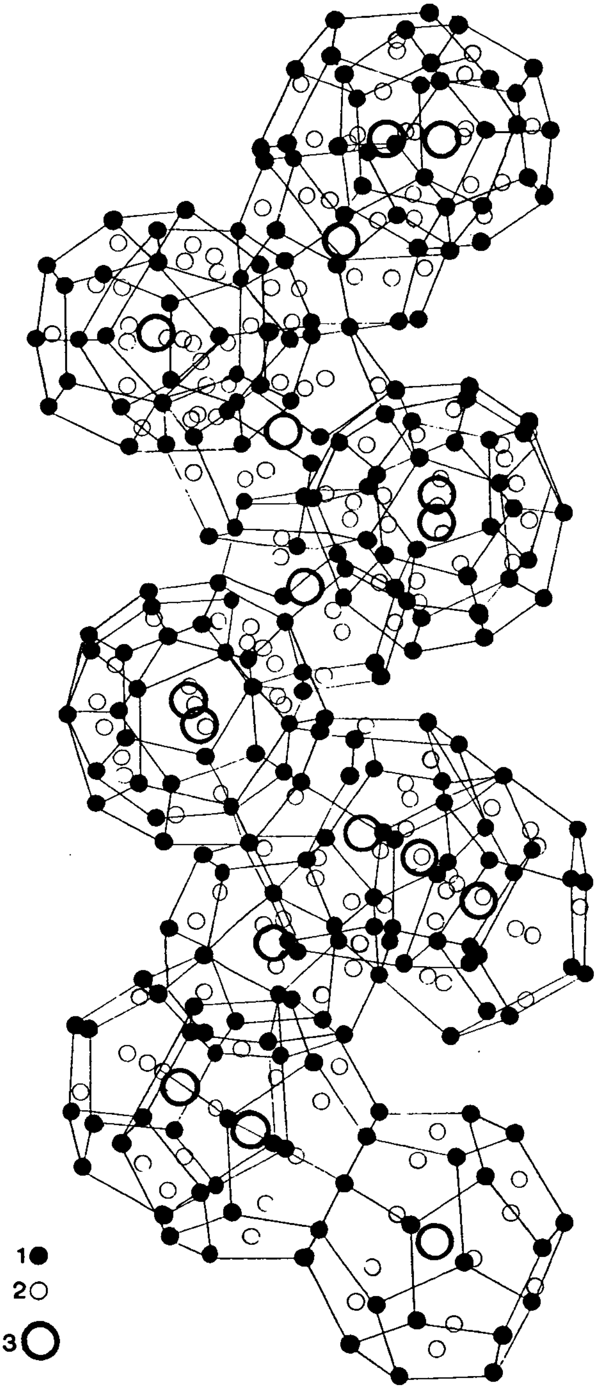

Plate 10.2.

Plate 10.3.

2.1. The schemas of the central stabilizing biopolymer form a zigzag. In two dimension the skeletal biopolymer points of symmetry are arranged in different patterns.

2.2. It seems as the most important the pattern of the points of symmetry of the edges and the centrum of the pentagonal planes. In optimal view may be observed the connections of two pentagonal polygon by five points of the edges, and two times five points of the centrum of the planes. As the other kind of pattern we would like to emphasize the following:

2.2.1. Pairs of points of symmetry.

2.2.2. Threefold groups of points of symmetry.

2.2.3. Linear arrangement, which may be simple or ramified.

2.2.4. Further regular or irregular groups of points of symmetry.

Discussion and Conclusions

1. The quasi-crystalloid skeleton of the single (primary) filament was investigated by the three dimensional modelling (KEDVES, 1992). The alterations of symmetry of the consecutive pentagon dodecahedrane units were analyzed by this method also. To this in the first place the symmetry of the central stabilizing unit and its surrounding skeletal and further points of symmetry modelled by the computer method may be pointed out. To this the computer modelling is the unique method. The pattern of the skeletal points of symmetry is very useful in the interpretation of the TEM pictures of the partially degraded or dissolved cell walls. Particularly after the different kinds of rotations we have observed such arrangements of biopolymer units. To this our newest results may be mentioned (KEDVES, TRIPATHI, VÉR, PÁRDUTZ and ROJIK, 1998, KEDVES and BORBOLA, 1998).

2. The three dimensional model of the quasi-crystalloid skeleton of the single helical or microfibrillar structure was investigated in different aspects previously (KEDVES, 1991, p. 72., plate 7.3.). At this first modelling, the points of symmetry of the edges of the pentagons were only illustrated together with the pentagon dodecahedrane units. At this kind of investigation the complexity of the pattern of points of symmetry depending from the aspect of the investigation was clear. The computer modelling added two kinds of points of symmetry to the previous method. This was the reason that for the first time one aspect was investigated only from the helical unit by the computer method. Here also the points of symmetry of the α–helix without network are very important in the interpretation of our TEM pictures before and after different kinds of rotation. In this way for example linear biopolymer structures may also be present as a part of the helical quasi-crystalloid biopolymer structures.

Finally it is necessary to emphasize that the computer and other modelling and investigations of the biopolymer system of the living and fossil plant cell walls is not yet finished. The helical system by its complexity needs also further investigations.

Text-fig. 10.2.

Computer model of the single α-helix composed of pentagon dodecahedrane units.

Text-fig. 10.3.

Computer model of the single α-helix composed of pentagon dodecahedrane units without network.

Acknowledgements

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