6. COMPUTER MODELLING OF THE QUASI-CRYSTALLOID BIOPOLYMER STRUCTURE I.

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Abstract

The necessity of using computer modelling for the metastable quasi-crystalloid biopolymer skeleton and its stabilizing molecular system was evident. The computer program was elaborated by the second author based on the TEM data of the partially degraded plant cell walls, and the results of the previous two- and three-dimensional modelling. During the modelling, the following were taken into consideration: 1. The quasi-crystalloid skeleton of the basic dodecahedron units. 2. The points of symmetry of the edges. 3. The points of symmetry of the centre of the regular pentagonal planes. 4. The centre of the dodecahedron. 5. The cavities and/or frustrations (sensu NELSON, 1986), of the metastable quasi-crystalloid skeleton, which are filled by the stabilizing molecular structure. Several, different kinds of modellings have been made so far. In this paper we present four examples. This method seems to be a very useful addition to interpret more precisely our TEM pictures of the partialy degraded plant cell walls, and moreover, it guarantees such opportunities in this field of research which are not possible to do by any other, previousy applied method.

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

Introduction

In the previous number of Plant Cell Biology and Development, which was dedicated to the Tenth Anniversary of the Discovery of The Quasicrystals, an attempt was made to sketch the extreme diversity of the investigations on this subject including the very rapid increasing of publications. On the other hand, a short summary was compiled from the most important results of the laboratory (M. KEDVES, 1994) to attitude the effect of the discovery on rapidly cooled AlMn alloys to Cell Biology.

The quasi-crystalloid biopolymer skeleton of the plant cell wall was first observed on partially degraded pollen grains (*Pinus griffithii* MCCLELL). By the way of the modified MARKHAM rotation method, the PENROSE unit was discovered in 1988 (M. KEDVES). Later a number of two-dimensional models and methods were elaborated, the last one can be seen in this number, M. KEDVES, TÓTH and VÉR (1995). For the better understanding of the metastable skeleton, three-dimensional modelling was also started (M. KEDVES, 1991, 1992, M. KEDVES, TÓTH and FARKAS,

1993). All of these methods are useful to interpret our TEM pictures about the metastable quasi-crystalloid skeleton better.

But the holes or the frustrations (sensu NELSON, 1986) which are filled with the stabilizing molecular system cannot be modelled with methods discussed previously. Regarding the stabilizing molecular system, we have had only one TEM data so far, which we tried to interpret better with the two-dimensional modelling method (cf. M. KEDVES and TÓTH, 1994). Our up-to-date methods are useful to dissolve stabilizing biopolymer structures, but the opposite method, namely the degradation or the dissolution of quasi-crystalloid skeletons is not yet elaborated. Moreover, the three-dimensional modelling of the stabilizing biopolymer system was not accomplished with all of the methods used previously. In this way the computer method seems to be a unique one for the modelling of the stabilizing biopolymer system.

The aim of this first paper is the following:

1. To elaborate and/or give the definition of the basic methodological principles, on the basis of our up-to-date knowledge about biopolymer structures of the sporoderm in angstroem dimension.

2. To present some selected data of our new results concerning this subject, from the point of view of demonstrating the advantages and the opportunities of this method.

Method

As it has been established with the first results, the basic quasi-crystalloid biopolymer unit is a regular pentagon in angstroem dimension; 8–18–22 Å. The further step of organization of the metastable skeleton is the pentagon dodecahedron unit composed of 12 pentagons. The PENROSE-I biopolymer unit (cf. M. KEDVES, 1991, 1992) is composed of a "central" dodecahedron and all its planes are connected with the surrounding further dodecahedrons. This skeleton can be investigated from two basic points of view, as follows.

A = the three-dimensional picture seen in M. KEDVES 1992, Plate 5.4., 1, p. 75: "Quasi-periodic view of the PENROSE-I skeleton. The contour is pentagonal." In the middle there is a plane of a regular pentagon.

B = the three-dimensional picture seen in M. KEDVES 1992, Plate 5.4., 2, p. 75: "The contour is hexagonal, and no central regular pentagon in the centre." In the centrum of the overview, there are three frustrations of an oblique triangle, surrounded with three regular pentagons.

The following characteristics were taken into consideration so far:

1. The quasi-crystalloid skeleton, PENROSE units, or network. Within this, two kinds of methods;
1.1. The complete network of the skeleton, for example, Text-fig. 6.1.
1.2. One side – more or less – the half of the surface (Text-fig. 6.3.).
2. The edges of the regular pentagonal planes (Text-fig. 6.2.).
3. The centrum of the planes of the regular pentagon (Text-fig. 6.2.).
4. The centrum of the pentagon dodecahedron (Text-fig. 6.1.).

5. The holes, and/or the frustrations (sensu NELSON, 1986) of the metastable quasi-crystalloid network.

We need to emphasize that the opportunities of computer modelling are extremely large, we may say endless. We have made several further models which will be published in further papers. But all our models are connected to our TEM data on partially degraded plant cell walls.

Results

THE COMPLETE QUASI-CRYSTALLOID SKELETON OF THE PENROSE-I UNIT, TOGETHER WITH THREE KINDS OF POINTS OF SYMMETRY (Text-fig. 6.1., A, B)

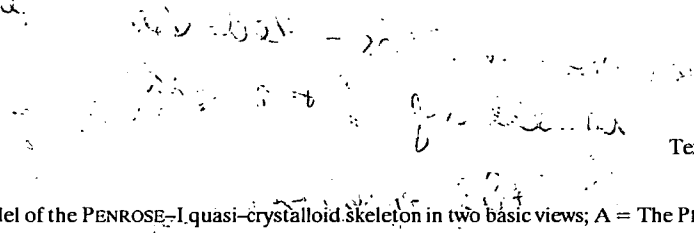
In the centrum there are three central stabilizing units, on the same axis (Text-fig. 6.1., A). Four pentagons in opposite positions are surrounding the centrum. This part is followed by five areas of ten edges. The ten central points of symmetry of the surrounding dodecahedrons are on two "circles". The inner five are touching the fourth ten-angle, the outer ones are near one another on five edges of the outer zone of the angles. All of these units can represent the inner or the central part of the quasi-crystalloid biopolymer system. Within this, the disposition of the three kinds of points of symmetry is interesting.

In the centrum of our figure (Text-fig. 6.1., A) there is a symbol for the centrum of the pentagonal plane, it represents six ones on the same axis. The larger one, the centrum of the dodecahedron represents three ones on the same axis. In this way this centrum is peculiar, we may be say heterogeneous. On the basis of the disposition of the points of symmetry of the edges further areas may be distinguished:

1. Three pentagons on each edge with points of symmetry.
2. Two kinds of radial arrangements.

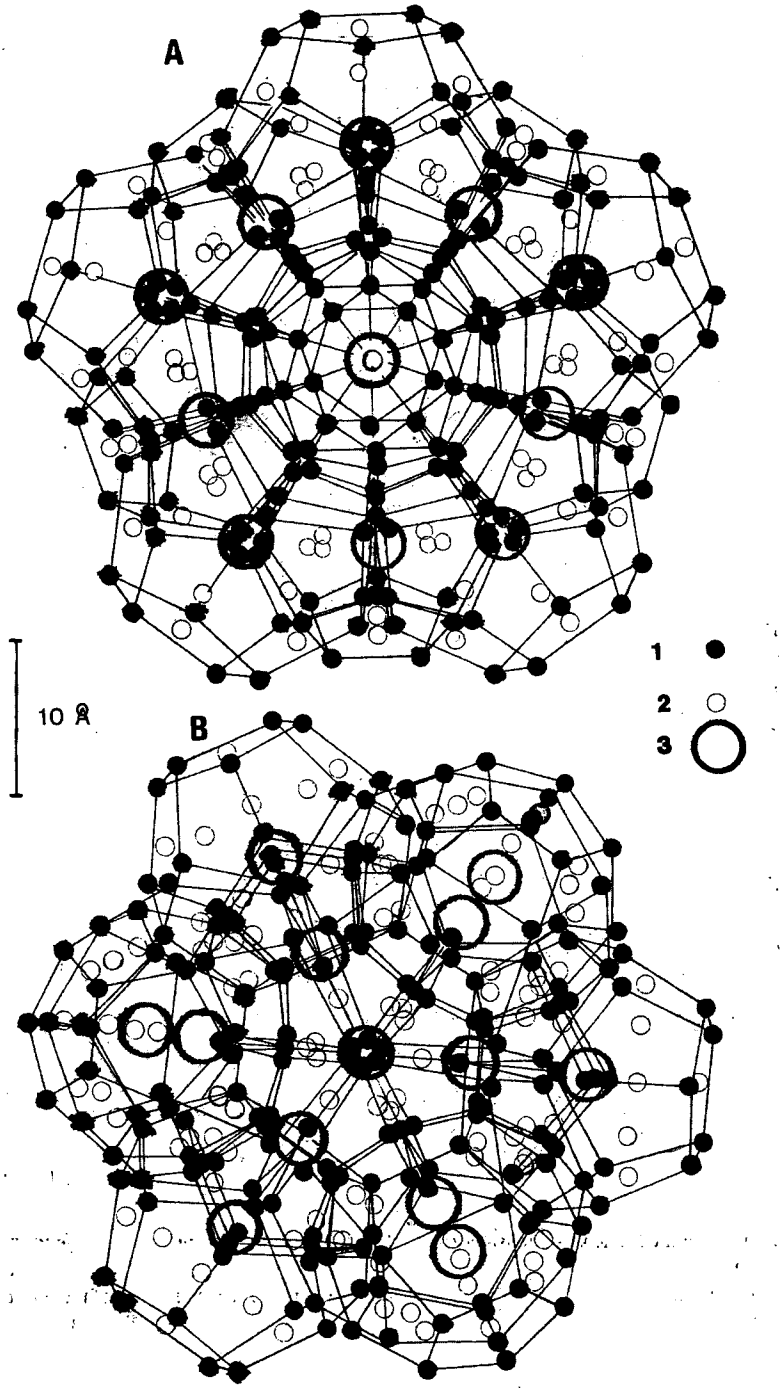
2.1. One is linear until the point of symmetry of the inner central unit of the surrounding dodecahedron.

2.2. The linear arrangement is broken with clusters of four points of symmetry of the edges.



Text–fig. 6.1. ▸

Computer model of the PENROSE–I quasi–crystalloid skeleton in two basic views; A = The PENROSE–I type skeleton is placed on one plane of one dodecahedron. On the basis there are five points of symmetry (edges) of the same dodecahedron unit. B = The PENROSE–I skeleton is placed on three sides of three dodecahedron units. On the basis there are three times two points of symmetry (edges of three dodecahedron units).
Legends:
1 - points of symmetry of the edges of the pentagon dodecahedron unit,
2 - the centres of the regular pentagon planes,
3 - the centrum of the pentagon dodecahedron unit.


A
B
10 Å
1
2
3

Further, outer points of symmetry of the edges are more or less on the axis of the central units of the surrounding dodecahedrons. On the basis of this arrangement, two kinds may also be distinguished:

1. Five points of symmetry are "inside" of the central unit, or better say near the perpendicular axis of the PENROSE-I type skeleton.
2. Three points of symmetry of the edges are in this kind of arrangement.

The modelled biopolymer system bordered with the ten central units of the surrounding pentagon dodecahedron, forming a not so characteristic TICOS polyhedra, represents another large biopolymer system. The outest region forms another peculiar TICOS polyhedra, but these units can be characterized only with the points of symmetry of the edges and/or with the centres of the pentagon planes.

Aspect "B" (Text-fig. 6.1., B) is quite different, which can be characterized by three or hexaradiate symmetries. The triangles of the hexaradiate system are also heterogeneous on the basis of the disposition of all kinds of points of symmetry.

It is also interesting, that the more or less concentric areas are not so characteristic in contrast to the previous aspect. This view may be characterized with the accumulation of the points of symmetry of the edges and planes of the surrounding dodecahedrons. From this point of view, three of them are extremely characteristic.

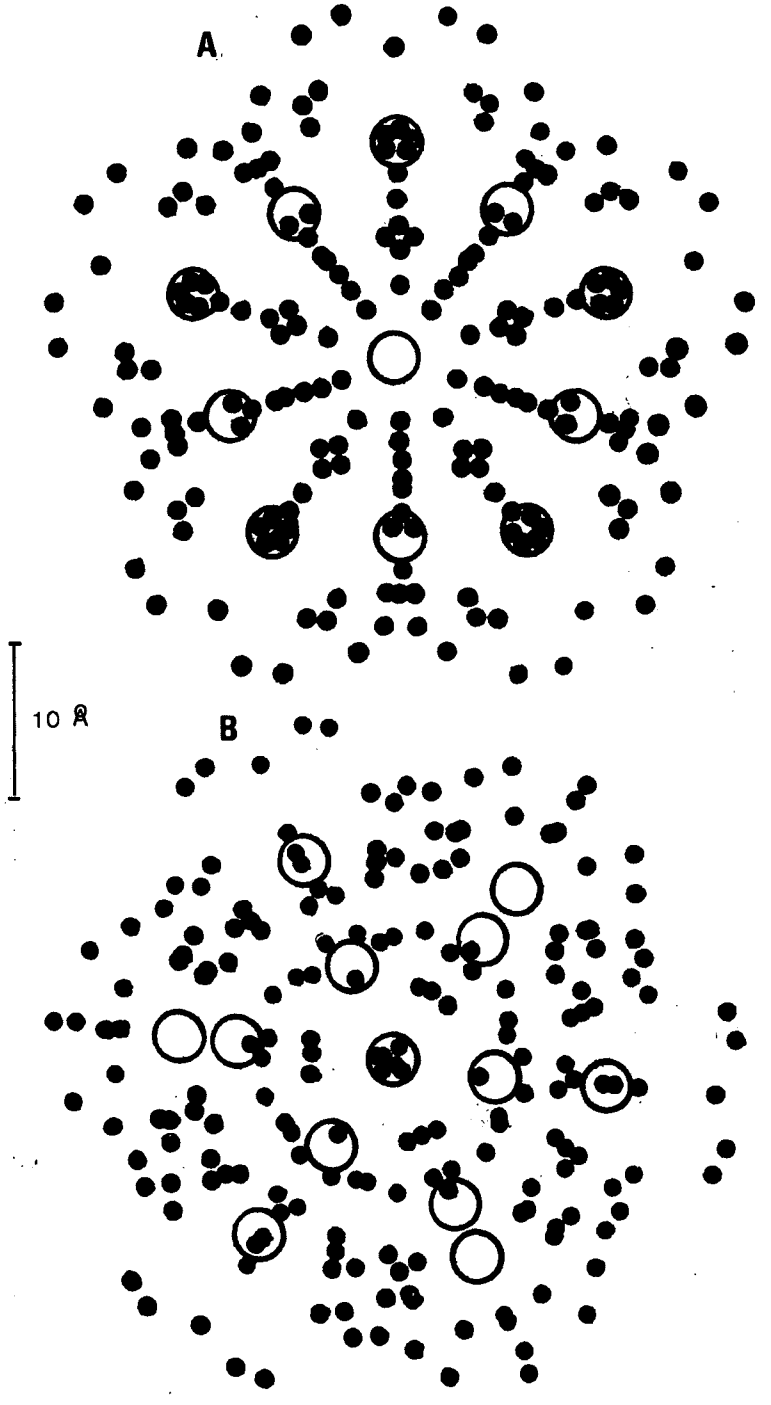
COMPUTER MODELLING OF TWO KINDS OF POINTS OF SYMMETRY OF THE PENROSE-I UNIT WITHOUT THE NETWORK OF THE SKELETON (Text-fig. 6.2., A, B)

At this modelling an attempt was made for the better understanding of the points of symmetry of our TEM pictures of the biopolymer systems after partial degradation and the modified MARKHAM rotation method. Taking the previous results into consideration, the quasi-crystalloid skeleton was omitted, and the arrangement of the points of symmetry of the centre of the dodecahedrons and those of the edges were illustrated from the two usual views.

Text-fig. 6.2., A. – Around the central units, ten points of symmetry of the edges are forming a pentagon. To this cf. the picture of Plate 4.1., fig. 3, C.P.5.A.5.5. of the biopolymer no V (M. KEDVES, TÓTH and VÉR, 1995, in this number). The pentagon mentioned above is followed by another larger one, in the same direction. The peculiarity of this pentagon is that on the edges there are clusters of points of symmetry composed of four points of edges. The outest pentagon together with the previous one forms a peculiar TICOS polyhedra. At the edges there are the points of symmetry of the centres of the surrounding polyhedrons, with five points of

Text–fig. 6.2. ▸

Computer model of two kinds of points of symmetry of the PENROSE–I type quasi–crystalloid biopolymer unit, without network. The points of symmetry of the centrums and the edges of the dodecahedron units are illustrated here.


A
10 Å
B

symmetry of the edges. The opposite pentagon is "connected" with 2+1 points of symmetry of the edges.

Regarding the outest areas, they are as it was discussed previously.

Text-fig. 6.2., B. – This view is interesting from the point of view of the investigated points of symmetry. A well defined area of a shape of a triangle with convex sides is well illustrated. The peculiarity of this view is the clusters of three points of symmetry of the edges, in 2+1+2 arrangement. In this position they are nearly extra-areal.

SURFACE MODELLING OF THE PENROSE-I TYPE BIOPOLYMER UNIT (Text-fig. 6.3., A, B)

The superficial elements are modelled only, in this way without inner points of symmetry, namely without the centres of the dodecahedron.

From the point of view of Text-fig. 6.3., A, the following is well illustrated:

1. The frustrations between the central and the surrounding dodecahedron units.
2. Interesting clusters composed of three points of symmetry of the edges are characteristic, forming further pentagons. The edges of the outest, third pentagon are composed of two points of symmetry of edges, and one point of the centrum of the plane.
3. The outest areas are identical with the previous ones, cf. Text-fig. 6.1., A.

View "B" (Text-fig. 6.3., B) illustrates the shape of the frustrations between the dodecahedron units in the first place. The triangular "central" hole system is connected to three "V" shape holes.

ATTEMPT FOR THE MODELLING OF THE STABILIZING BIOPOLYMER SYSTEM OF THE QUASI-CRYSTALLOID SKELETON (Text-fig. 6.4., A, B)

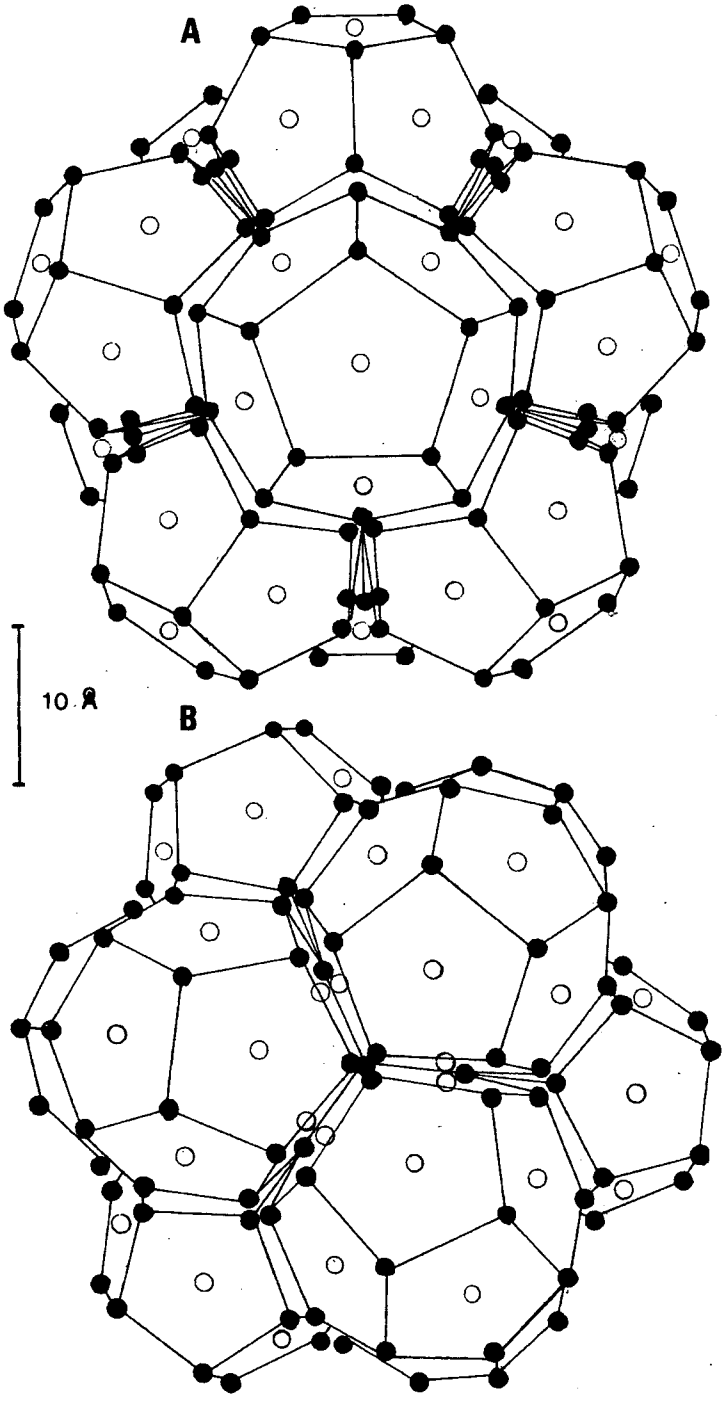
The starting points of this modelling were the frustrations and holes of the quasi-crystalloid PENROSE-I unit, and the centres of the dodecahedrons of the biopolymer skeleton.

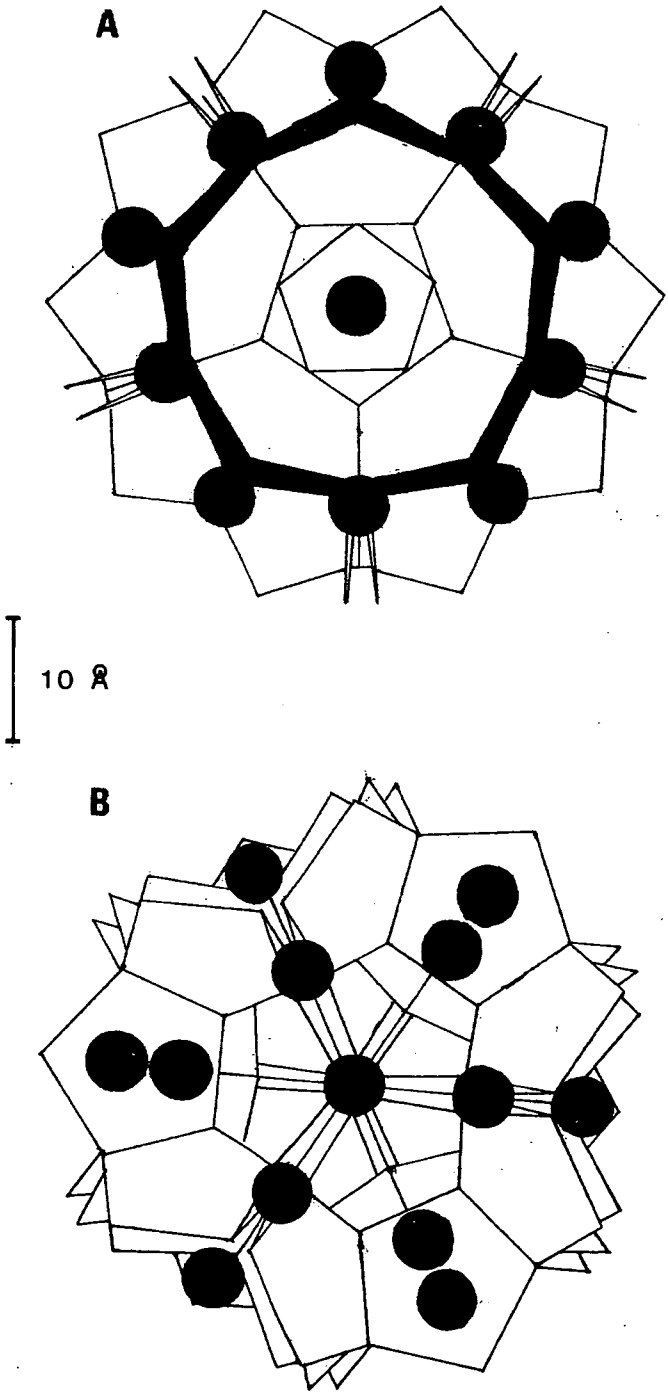
View "A" illustrates well that the central stabilizing unit is surrounded with a more or less circular ring really with a ten-edged shape in sectional view. Two times five points of symmetry of the centrums of the surrounding dodecahedrons are connected seemingly to this system. Such configurations may be seen at the TEM pictures, too.

View "B" seems to be very useful in the interpretation of our TEM pictures, because depending on the position, the settlements of the biopolymer units can be changed.

Text-fig. 6.3. ▸

Computer model of the two basic views of the PENROSE–I unit from above. The superficial networks, together with the so–called superficial points of symmetry – the edges, and the centrums of the regular pentagon planes are illustrated here.


A
10 Å
B


A
10 Å
B

Discussion and Conclusions

As it has been emphasized several times, chemistry and the biopolymer organization of the plant cell wall, particularly of the sporoderm, are much more complicated than they were believed to be some years ago. It is necessary to repeat it again and again that the sporopollenin is not a "uniform biopolymer", but extremely heterogeneous, and its composition is alternating and not constant.

The quasi-crystalloid metastable skeleton, and its stabilizing molecular system concept is one way of interpreting and trying to understand this extremely complex molecular organization.

Now we have another method, and we will use the opportunities of this method to understand and know this complex system better. Here we have presented selected basic results from our models and further ones will follow them. We hope that this contribution is a step worth mentioning in the knowledge about this problem.

Acknowledgements

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◄ Text–fig. 6.4.

Computer model of the stabilizing biopolymer system of the metastable quasi–crystalloid skeleton, PENROSE–I type unit. The centres of the dodecahedron and the so–called frustrations (sensu NELSON, 1986) are illustrated here. The more or less circular unit of view "A" has been emphasized.