X-ray study of the paracrystalline nature of crystallized 70S ribosome lamellae

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Appendix I: Paracrystalline distortions $g_k$ of the macrolattice

The lattice cell of a tetragonal paracrystal is expanded by three vectors $a_k$ ($k = 1, 2, 3$) which can be found in the lattice with a frequency $H_k(x)$ for $a_k = x$. The mean values $\bar{a}_k$ and relatively statistical variances $g_{ik}$ are defined as

$$\bar{a}_k = \int x H_k(x) \, dx$$

$$g_{ik} = \Delta_{ik}/a_k^2; \quad \Delta_{ik}^2 = \frac{1}{a_k^2} \int (x - \bar{a}_k)^2 H_k(x) \, dx$$  \hspace{1cm} (18)

The well known Laue-conditions

$$b \cdot \bar{a}_k = h_k \quad (k = 1, 2, 3 \text{ integers}) ; \quad b = 2 \sin \varphi / a$$ \hspace{1cm} (19)

define the centres of gravity of the paracrystalline reflections.

The integers $h_k$ are the Miller-indices. The reflections $(h, 0, 0)$ lie for instance at $b_1 = h_1/a_1$. Their relative integral widths $\delta b_1/b_1$ can be calculated from the theory of paracrystals (Hosemann & Bagchi, 1962) and are given in a good first approximation by

$$\delta b_1/b_1 = 1/N_1 + (\frac{g_{11} h_1}{a_1 b_1})^2 \quad : \quad a_1 b_1 = 1$$ \hspace{1cm} (20)

As discussed above, one finds from Fig. 7: $N_1 \sim 15$. From the slope of the straight line using point A one finds with the help of Eqs. (19) and (20)

$$a_1 \delta b_{11} = 42 \times 1.5 \times 10^{-2} = (\frac{g_{11} h_1}{a_1 b_1})^2 20 \times 10^{-2}$$

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hence $g_{11} = 1.5 \%$.

Neighboured reflections $(0, h, 0)$ emerge into each other, if

$$\delta b_{11} / b_1 \gg 1$$. From Eq. (20) follows $(\frac{x}{0.015} \times b_1 / 42) \gg 1$, hence

$$b_1 \geq 0.1 \times 10^{-1}$$. In the three-dimensional case of $(h, k, l)$ reflections this boundary for discrete reflections $h, k, l$ is much smaller. From Fig. 4 it follows $b_1 \approx 0.1 \times 10^{-1}$.
Appendix II: Paracrystalline distortions $\varepsilon_{vw}$, $\varepsilon_{v'}$, $\varepsilon_{vv}$ and $\varepsilon_{ww}$ of the sublattice

A tetragonal cell of a reciprocal lattice is expanded by three axes of the length $b_k^* (k = 1, 2, 3)$. The reflection $\mathbf{b}_k^*$ has in the direction of the $b_\ell^*$-axis the integral width $\sigma_{b_{k\ell}}$. Then it follows from the theory of paracrystals that

$$\frac{\sigma_{b_{k\ell}}}{b_{k\ell}} = \frac{1}{N_{\ell}^2} + (\mathcal{X}_k \varepsilon_{\ell k})^2 \quad \text{if} \quad h_k = 1. \quad (21)$$

In Appendix I the special case $\ell = k$ is treated. From Fig. 6 one can recognize, for instance, that the integral width of the screened reflection at $\ell = 12$ in $v$-direction $\sigma_{b_{vw}}$ divided through $b_{v}$ is in the order of $2/6$, hence

$$\varepsilon_{vw} \sim \frac{1}{2} \frac{1}{6} = 15 \%,$$

whilst $\sigma_{b_{vw}}/b_{v} \sim \frac{1}{12}$, hence $\varepsilon_{vw} = \sqrt{0.15/\mathcal{X}} \sim 12 \%$.

In the same manner one finds from Fig. 6 that

$$\sigma_{b_{vw}}/b_{v} \sim \sigma_{b_{ww}}/b_{w} \sim \frac{1}{15},$$

hence

$$\varepsilon_{ww} \sim \varepsilon_{vv} \frac{1}{\mathcal{X} \sqrt{15}} \sim 7 \%$$
Appendix III: Q-function as the convolution square of the density function $\varrho$

The Fourier-transform $R(b)$ of the electron density distribution $\varrho(x)$ is proportional to the amplitude of the scattered X-rays

$$R(b) = \int \varrho(x) = \int \varrho(x) e^{-2\pi ibx} dx^3$$ (22)

The Fourier-transformation of the Q-function easily can be calculated by substituting $bx = B(x + y - y)$. Then according to Eq. (2) follows

$$I(b) = \int Q(x) = \int \varrho(x) e^{+2\pi iby} \varrho(y+x)e^{-2\pi ib(x+y)} dx^3 dy^3$$ (23)

The integration over $x$ firstly can be carried out because a shift of the integrand by a vector $y$ does not change its integral value. One obtains

$$\int \varrho(x) e^{2\pi iby} R(b) dy^3 = R(b) \int \varrho(-x) = R^2 = I(b)$$ (24)

The convolution product of $\varrho$ is given by

$$\hat{\varrho \varrho} = \int \varrho(x) \varrho(x-y) dy^3 ; \int \hat{\varrho \varrho} = R^2(b)$$ (25)

The convolution square of $\varrho$ is given by

$$\hat{\varrho \varrho} = \varrho(x) \varrho(-x) = \int \varrho(y) \varrho(y-x) dy^3 = \int \varrho(-x) \varrho(y-x) dy^3$$ (26)
Appendix IV: The functions $\xi(u,v)$ and $\xi(v)$

The Fourier inverse transform of $I(0,k,l)$ is given by

$$
\sum_{k,l} I(0,k,l) e^{2\pi i (kV+lW)} = \int Q(u,v,w) \, du = \xi(v,w),
$$

(27)

because the two-dimensional Fourier-transform of $\xi(v,w)$ is given by

$$
\int e^{-2\pi i (kV+lW)} \, dv \, dw \int Q(u,v,w) \, du
$$

We can add $e^{-2\pi i (u,0)}$ in the integrand without changing its value

and have a three-dimensional transform for the reciprocal lattice

points $0,k,l$. $\xi(u,w)$ itself is nothing else than

$$
\xi(v,w) = \iiint S(\xi + u, \eta + v, \zeta + w) \xi(\xi, \eta, \zeta) \, d\xi \, d\eta \, d\zeta du
$$

The $u$-integration can be carried out: With $\int S \, du = \tilde{S}$ one obtains

$$
\iiint \tilde{S}(\eta + v, \zeta + w) \xi(\xi, \eta, \zeta) \, d\xi \, d\eta \, d\zeta
$$

The $\xi$ integration then leads to

$$
\tilde{Q}(u,w) = \int \xi(v,w) \, dv = \int Q(u,v,w) \, du \, dw
$$

(28)

If one integrates $\tilde{Q}(v,w)$ over $w$,

$$
\tilde{Q}(v) = \int \tilde{Q}(v,w) \, dw = \int Q(u,v,w) \, du \, dw
$$

one finds in the same manner

$$
\tilde{\xi}(v) = \sum_{k,l} I(0,k,l) e^{2\pi i kV}.
$$
Appendix V: Radius of Gyration of a Folding Product

The second moment \( \Delta \) (radius of gyration) of the convolution product of two functions \( g(x) \) and \( h(x) \) with

\[
\int g \, dx = \int h \, dx = 1 \quad ; \quad \int x \, g(x) \, dx = \int x \, h(x) \, dx = 0
\]

\[
\Delta_g^2 = \int x^2 \, g(x) \, dx \quad ; \quad \Delta_h^2 = \int x^2 \, h(x) \, dx \quad (29)
\]

easily can be calculated:

\[
\Delta_2 = \int \int x^2g(y) \ h(x - y) \, dx \, dy
\]

Substituting

\[
x^2 = (x - y)^2 + 2y(x - y) + y^2
\]

one can perform the integration independent from the value of \( y \) and obtains

\[
\Delta_2 = \int \left( \Delta_h^2 + 2y \cdot 0 + y^2 \right) g(y) dy = \Delta_h^2 + \Delta_g^2 \quad (30).
\]
Appendix VI : Volume of a tetramer approximated by a three-axial ellipsoid

The radius of gyration $\Delta$ for a three-dimensional density distribution according to Appendix V is given in orthogonal coordinates $x_1, x_2, x_3$ of $\mathbf{X}$ by

$$\Delta^2 = \Delta_1^2 + \Delta_2^2 + \Delta_3^2$$

$$\Delta_2 = \int x_2^2 g(\mathbf{x}) \, dx^3$$

(31)

The $N_q$-values of Table 3, IV can be used directly to calculate $\Delta_2$ in $b$-direction. Here $\int g(\mathbf{x}) dx^3$ is not normalized to unity, but has a value $\sum N_q = 136$. We obtain

$$\Delta_2 = \left[ \sum_{q} N_q (q-3)^2 / 136 \right]^{1/2} = 1.84 \times 5.3 = 9.7 \text{ nm}$$

Let us assume that the distribution of the subcells in each $q$-cross-section is for convenience as symmetric as possible. Hence, in each cross section exist $\sqrt{N_q}$ fibrils with $\sqrt{N_q}$ subcells each, over all $\sum \sqrt{N_q} = 33$ fibrils. The $\Delta^2$-value of a rod of the length $L$ is given by

$$\Delta^2 = L^2 / 12 = N_q / 12$$

We obtain herefrom for $\Delta_1$ in $a$-direction

$$\Delta_1 = \left[ \sum_{q} \sqrt{N_q} \cdot N_q / 12 \cdot 33 \right]^{1/2} = 1.23 \times 7.1 = 8.7 \text{ nm}$$

and $\Delta_3 = 1.23 \times 4.2 = 5.2 \text{ nm}$. The rayon of gyration is therefore in fine agreement with values reported in the introduction according to Eq. (31):

$$\Delta = \left( \sum (95 + 76 + 27) \right)^{1/2} = 14.1 \text{ nm}$$

One can obtain from the three $\Delta_k$-values the approximated value of the volume of one tetramer, if one multiplies them with $\sqrt{12}$ and takes their product $3^4 \times 30 \times 18 = 18,300 \text{ nm}^3$. 