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The Location and Magnitude of Probability Density Maxima from Higher-Order Cumulants

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A study of the Edgeworth expansion of a probability density function shows how an atom position may be refined so that it coincides with a position of maximum probability rather than the mean of the probability density function.

Introduction

An atom in a crystal moves about a mean position but not necessarily in such a way that the mean position is the most probable position. Johnson (1970) has discussed the use of cumulants in crystal-structure refinements. He defines a quantity he calls the vector of skew divergence from the third-order cumulant and notes that it lies approximately in the direction of maximum projected asymmetry. However, positions of maximum probability are obtained from probability density maps from the Edgeworth expansion of the probability density function. This procedure can be avoided. Further investigation of the Edgeworth expansion reveals that it is possible to locate simultaneously the positions of mean and maximum probability.

Theory

A probability density function $\Psi(\mathbf{u})$ of dimension n can be expanded about a zero-order approximation to obtain a better approximation. The characteristic function $\psi(\mathbf{t})$ is the Fourier transform of the probability density function and may be expressed as

$$\psi(\mathbf{t})=\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\exp(i\mathbf{t}\,.\,\mathbf{u})\Psi(\mathbf{u})\mathrm{d}u^1\mathrm{d}u^2\ldots\mathrm{d}u^n$$

where

$$\mathbf{u}=\sum_j\mathbf{u}^j,\ \mathbf{t}=\sum_j\mathbf{t}_j \text{ and } \mathbf{t}\,.\,\mathbf{u}=\sum_j t_j u^i.$$

This makes

$$\Psi(\mathbf{u})=\frac{1}{(2\pi)^n}\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\exp(-i\mathbf{t}\,.\,\mathbf{u})\psi(\mathbf{t})\mathrm{d}t_1\mathrm{d}t_2\ldots\mathrm{d}t_n\,.$$

If we have a normal distribution function $\Psi_0(\mathbf{u})$ then we can relate the variable vector $\mathbf{u}$ to the variable vector $\mathbf{U}=\sum_l\mathbf{U}^l$ by the transformation $\mathbf{U}^l=\sum_l(\mathbf{u}^j-\mathbf{x}^j)R_{jl}$ where

$$\sum_l R_{jl}R_{kl}=p_{jk}=p_{kj}.$$

$$\Psi_0(\mathbf{u})\mathrm{d}u^1\mathrm{d}u^2\ldots\mathrm{d}u^n=\hat{\psi}_0(\mathbf{U})\mathrm{d}U^1\mathrm{d}U^2\ldots\mathrm{d}U^n$$

where we choose $\mathbf{U}$ such that $\hat{\psi}_0(\mathbf{U})=1/(2\pi)^{n/2}\times\exp(-\frac{1}{2}\mathbf{U}\,.\,\mathbf{U})$ and $\mathbf{U}\,.\,\mathbf{U}=\sum_l U^l U^l$.

Thus

$$\Psi_0(\mathbf{u})=\frac{(\det|p|)^{1/2}}{(2\pi)^{n/2}}\times\exp\{-\tfrac{1}{2}\sum_{jk}p_{jk}(u^j-x^j)(u^k-x^k)\}\,. \quad (1)$$

The Fourier transform of $\Psi_0(\mathbf{u})$ is given by

$$\psi_0(\mathbf{t})=\frac{\exp(i\mathbf{t}\,.\,\mathbf{x})}{(2\pi)^{n/2}}\times\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\exp(i\mathbf{t}\,.\,\mathbf{U}-\tfrac{1}{2}\mathbf{U}\,.\,\mathbf{U})\mathrm{d}U^1\mathrm{d}U^2\ldots\mathrm{d}U^n$$

where

$$\mathbf{t}\,.\,\mathbf{U}=\sum_l T_l U^l \text{ and } T_l=\sum_j(R^{-1})_{lj}t_j\,.$$

Thus

$$\psi_0(\mathbf{t})=\exp(i\mathbf{t}\,.\,\mathbf{x})\exp(-\tfrac{1}{2}\sum_l T_l T_l)=\exp(i\sum_j x^j t_j-\tfrac{1}{2}\sum_{jk}\sigma^{jk}t_j t_k) \quad (2)$$

where

$$\sigma^{jk}=\sum_l(R^{-1})_{lj}(R^{-1})_{lk} \text{ so that } \sum_j p_{kj}\sigma^{jl}=\delta_{kl}\,.$$

The cumulants appear when the characteristic function is expressed in the form

$$\psi(\mathbf{t})=\exp(i\sum_j{}^1K^j t_j+\frac{i^2}{2!}\sum_{jk}{}^2K^{jk}t_j t_k+\frac{i^3}{3!}\sum_{jkl}{}^3K^{jkl}t_j t_k t_l+\frac{i^4}{4!}\sum_{jklm}{}^4K^{jklm}t_j t_k t_l t_m+\ldots)\,. \quad (3)$$

This may be abbreviated to

$$\ln\psi(\mathbf{t})=\sum_{s=1}^{r}\frac{{}^sK}{s!}(it)^s+O(t^s)\,.$$

The characteristic function may also be expressed in the form

$$\psi(\mathbf{t})=1+\sum_{s=1}^{r}\frac{{}^s\mu}{s!}(it)^s+O(t^s)$$

where

$$\lim_{t\to0}O(t^s)/t^s=0\,.$$

Any cumulant ${}^sK$ is a polynomial in the moments ${}^1\mu$ to ${}^s\mu$ and any moment ${}^s\mu$ is a polynomial in the cumulants ${}^1K$ to ${}^sK$.

The Edgeworth expansion is obtained by making use of the central limit theorem (see *e.g.* Cramer, 1946). The sum of n values belonging to the probability density function $\psi(\mathbf{u})$ whose characteristic function is $\psi(\mathbf{t})$ has a probability density function which is asymptotically a normal distribution with a characteristic function $\varphi(t/\sqrt{n})=[\psi(t)]^n$. Now

$$\ln\varphi\left(\frac{t}{\sqrt{n}}\right)=n\sum_{s=1}^{r}\frac{{}^sK}{s!}(it)^s+O(t^s)$$
$$=n\sum_{s=1}^{r}\frac{{}^s\hat{K}}{s!}\left(\frac{it}{\sqrt{n}}\right)^s+O(t^s)$$

where ${}^s\hat{K}=n^{(1-s/2)s}K$ so that ${}^2K={}^2\hat{K}$. Since ${}^s\hat{K}$ decreases with increase of n for $s>2$, $\varphi(t/\sqrt{n})$ approaches the characteristic function for a normal distribution.

We can express $\ln\psi(\mathbf{t})$ as $\ln\psi_0(\mathbf{t})+\ln\psi_1(\mathbf{t})$ where $\psi_0(\mathbf{t})$ is given by (2) so that

$$\ln\psi_1(\mathbf{t})=i\sum{}^1\lambda^j t_j+\frac{i^2}{2!}\sum_{jk}{}^2\lambda^{jk}t_jt_k+\frac{i^3}{3!}\sum_{jkl}{}^3K^{jkl}t_jt_kt_l$$
$$+\frac{i^4}{4!}\sum_{jklm}{}^4K^{jklm}t_jt_kt_lt_m+\ldots. \quad (4)$$

where

$${}^1\lambda^j={}^1K^j-x^j \text{ and } {}^2\lambda^{jk}={}^2K^{jk}-\sigma^{jk}.$$

Thus

$$\ln\varphi\left(\frac{t}{\sqrt{n}}\right)=n\ln\psi_0(t)+\ln\varphi_1\left(\frac{t}{\sqrt{n}}\right)$$

where

$$\ln\varphi_1\left(\frac{t}{\sqrt{n}}\right)=n\ln\psi_1(t)={}^1\hat{\lambda}\left(\frac{it}{\sqrt{n}}\right)+\frac{{}^2\hat{\lambda}}{2!}\left(\frac{it}{\sqrt{n}}\right)^2$$
$$+n\sum_{s=3}^{r}\frac{{}^s\hat{K}}{s!}\left(\frac{it}{\sqrt{n}}\right)^s. \quad (5)$$

Since ${}^2K$ is independent of n we can assume that ${}^1\hat{\lambda}$ and ${}^2\hat{\lambda}$ are also independent of n. Arranged in powers of $n^{-1/2}$, (5) becomes

$$\ln\varphi_1\left(\frac{t}{\sqrt{n}}\right)=\left[{}^1\hat{\lambda}(it)+\frac{{}^3\hat{K}}{3!}(it)^3\right]/\sqrt{n}$$
$$+\left[\frac{{}^2\hat{\lambda}}{2!}(it)^2+\frac{{}^4\hat{K}}{4!}(it)^4\right]/n+n\sum_{s=5}^{r}\frac{{}^s\hat{K}}{s!}\left(\frac{it}{\sqrt{n}}\right)^s$$

so that

$$\varphi_1\left(\frac{t}{\sqrt{n}}\right)=1+\left\{{}^1\hat{\lambda}(it)+\frac{{}^3\hat{K}}{3!}(it)^3\right\}/\sqrt{n}+\left\{\frac{{}^2\hat{\lambda}}{2!}(it)^2\right.$$
$$\left.+\frac{{}^4\hat{K}}{4!}(it)^4+\frac{1}{2!}\left[{}^1\hat{\lambda}(it)+\frac{{}^3\hat{K}}{3!}(it)^3\right]^2\right\}/n+\ldots. \quad (6)$$

If we approximate $\Psi(\mathbf{u})$ by the normal distribution $\Psi_0(\mathbf{u})$, see (1), we may describe $\Psi(\mathbf{u})$ by the expression

$$\Psi(\mathbf{u})=\Psi_0(\mathbf{u})-\sum_j{}^1c^jD_j\Psi_0(\mathbf{u})+\frac{1}{2!}\sum_{jk}{}^2c^{jk}D_jD_k\Psi_0(\mathbf{u})$$
$$-\frac{1}{3!}\sum_{jkl}{}^3c^{jkl}D_jD_kD_l\Psi_0(\mathbf{u})\ldots \quad (7)$$

where the mth term is abbreviated to $(-1)^m/m!{}^mc\Psi_0^{(m)}(\mathbf{u})$. D_j is the operator $\partial/\partial u^j=\sum_l R_{jl}\partial/\partial U^l$ where $U^l=\sum_j(u^j-x^j)R_{jl}$ (see above).

The Fourier transform of $D_jD_k\Psi_0(\mathbf{u})$ is given by

$$F(\mathbf{t})=\int_{-\infty}^{\infty}\ldots$$
$$\ldots\int_{-\infty}^{\infty}\exp(i\mathbf{t}.\mathbf{u})D_j\sum_l R_{kl}\frac{\partial}{\partial U^l}\hat{\psi}_0(\mathbf{U})\mathrm{d}U^1\mathrm{d}U^2\ldots\mathrm{d}U^n.$$

Integration by parts gives

$$F(\mathbf{t})=(-it_k)\int_{-\infty}^{\infty}\ldots$$
$$\ldots\int_{-\infty}^{\infty}\exp(i\mathbf{t}.\mathbf{u})D_j\hat{\psi}_0(\mathbf{U})\mathrm{d}U^1\mathrm{d}U^2\ldots\mathrm{d}U^n$$

since

$$T_l=\sum_j(R^{-1})_{lj}t_j.$$

Thus the Fourier transform of $\Psi(u)$ given in (7) is

$$\psi(\mathbf{t})=\left[1+i\sum_j{}^1c^jt_j+\frac{i^2}{2!}\sum_{jk}{}^2c^{jk}t_jt_k+\ldots\right]\psi_0(\mathbf{t}), \quad (8)$$

where the mth term may be abbreviated to $(i)^m/m!{}^mc\times t^m\psi_0(\mathbf{t})$.

From (6) and (8) we see that we can define an expansion of

$$\Psi(\mathbf{u})\cong[1+\sum_{j=1}^{m}Q_j(\mathbf{u})]\Psi_0(\mathbf{u}) \text{ so that } [1+\sum_{j=1}^{m}Q_j(\mathbf{u})]\Psi_0(\mathbf{u})$$

is the best possible approximation to $\Psi(\mathbf{u})$ using all cumulants up to the $(m+2)$th. This is known as the Edgeworth expansion and the $Q_j(\mathbf{u})$ operators are evaluated with successive powers of $n^{-1/2}$ in (6). Thus

$$Q_1(\mathbf{u})=-\sum_j{}^1\lambda^jD_j-\frac{1}{3!}\sum_{jkl}{}^3K^{jkl}D_jD_kD_l$$

and

$$Q_2(\mathbf{u})=\frac{1}{2!}\sum_{jk}{}^2\lambda^{jk}D_jD_k+\frac{1}{4!}\sum_{jklm}{}^4K^{jklm}D_jD_kD_lD_m$$
$$+\frac{1}{2!}[Q_1(\mathbf{u})]^2. \quad (9)$$

$\Psi_0(\mathbf{u})$ is given in (1) so that

$D_j\Psi_0(\mathbf{u})=-Z_j\Psi_0(\mathbf{u})$ where $Z_j=\sum_k p_{jk}(u^k-x^k)$,

$D_jD_k\Psi_0(\mathbf{u})=(Z_jZ_k-p_{jk})\Psi_0(\mathbf{u})$,

$D_jD_kD_l\Psi_0(\mathbf{u})=[-Z_jZ_kZ_l+(Z_jp_{kl}+Z_kp_{lj}+Z_lp_{jk})]\Psi_0(\mathbf{u})$, $D_jD_kD_lD_m\Psi_0(\mathbf{u})$

$=[Z_jZ_kZ_lZ_m-(Z_jZ_kp_{lm}+Z_jZ_lp_{mk}+Z_jZ_mp_{kl}+Z_kZ_lp_{jm}+Z_mZ_kp_{jl}+Z_lZ_mp_{jk})+(p_{jm}p_{kl}+p_{jl}p_{km}+p_{jk}p_{lm})]\Psi_0(\mathbf{u})$ *etc.*

It should be pointed out that if we choose x^j and σ^{jk} such that

$$ {}^1\lambda^j = {}^1K^j - x^j = \tfrac{1}{2}\sum_{kl} {}^3K^{jkl}p_{kl} \qquad (10) $$

and

$$ {}^2\lambda^{jk} = {}^2K^{jk} - \sigma^{jk} = \tfrac{1}{4}\sum_{lm} {}^4K^{jklm}p_{lm} \qquad (11) $$

then

$$ Q_1(\mathbf{u})\Psi_0(\mathbf{u}) = \frac{1}{3!}\sum_{jkl} {}^3K^{jkl}Z_jZ_kZ_l\Psi_0(\mathbf{u}) \qquad (12) $$

and

$$ \begin{aligned} Q_2(\mathbf{u}) = \Psi_0(\mathbf{u}) = \Big\{ & \frac{1}{4!}\sum_{jklm} {}^4K^{jklm}Z_jZ_kZ_lZ_m - \tfrac{1}{2}\sum_{jk} {}^2\lambda^{jk}Z_jZ_k \\ & + \tfrac{1}{72}\sum_{jkl}\sum_{pqr} {}^3K^{jkl}\,{}^3K^{pqr}(Z_jZ_kZ_lZ_pZ_qZ_r \\ & - 9Z_jZ_kZ_pZ_qp_{lr} + 18Z_jZ_pp_{kq}p_{lr} - 6p_{jp}p_{kq}p_{lr})\Big\}\Psi_0(\mathbf{u}) . \end{aligned} \qquad (13) $$

Then $\Psi(\mathbf{u})$ at $\mathbf{u}=\mathbf{x}$ is independent of the values of ${}^3K^{jkl}$ if we assume $Q_m(\mathbf{u})\psi_0(\mathbf{u})=0$, $m>1$ and is independent of the values of ${}^4K^{jllm}$ if we assume $Q_m(\mathbf{u})\Psi_0(\mathbf{u})=0$, $m>2$.

In both cases $\partial\Psi(\mathbf{u})/\partial u^j=0$ at $\mathbf{u}=\mathbf{x}$ so that $\mathbf{x}$ corresponds to a position of maximum probability, and σ rather than ${}^2K$ determines the probability density at $\mathbf{u}=\mathbf{x}$.

Now $\ln\psi(\mathbf{t})$ is given by (3) but from (10) and (11)

$$ \begin{aligned} \ln\psi(\mathbf{t}) = i\sum_j x^jt_j + \frac{i^2}{2!}\sum_{jk}\sigma^{jk}t_jt_k + \frac{i}{2}\sum_{jkl} {}^3K^{jkl}p_{kl}t_j \\ + \frac{i^3}{6}\sum_{jkl} {}^3K^{jkl}t_jt_kt_l + \frac{i^2}{8}\sum_{jklm} {}^4K^{jklm}p_{lm}t_jt_k \\ + \frac{i^4}{24}\sum_{jklm} {}^4K^{jklm}t_jt_kt_lt_m . \end{aligned} \qquad (14) $$

We can thus refine ${}^1K^j$, ${}^2K^{jk}$, ${}^3K^{jkl}$, ${}^4K^{jklm}$ using (3) and determine x^j and σ^{jk} using (10) and (11) or alternatively refine x^j, σ^{jk}, ${}^3K^{jkl}$, ${}^4K^{jklm}$ using (14) and determine ${}^1K^j$ and ${}^2K^{jk}$ using (10) and (11). With either procedure an estimate of $p_{lm}=(\sigma^{-1})_{lm}$ has to be made and it may be reasonably assumed to be the value from the previous cycle.

It should be noted that if ${}^1\lambda^j=0$ then $\sum_{kl} {}^3K^{jkl}p_{kl}=0$; $i=1,2,3$ and that if ${}^2\lambda^{jk}=0$ then $\sum_{lm} {}^4K^{jklm}p_{lm}=0$; $jk=11,12,13,22,23,33$ where we now assume three-dimensional space. The cumulants are invariant to pairwise interchange of indices and summations are made easier by using multiplicities and assuming $j\le k\le l\le m$. The appropriate multiplicities and constraints imposed on the cumulants by site symmetry have been discussed elsewhere (Johnson, 1970; Birss, 1964).

We can say ${}^3K^{jkl}={}^3K_0^{jkl}+{}^3K_1^{jkl}$ where $\sum_{kl} {}^3K_0^{jkl}p_{kl}=0$ so that for point symmetry 1 we have ${}^3K$ described by seven variables and ${}^3K$ by three (${}^3K$ is described by two variables for point symmetry m and by one for the other polar point symmetries).

In order to satisfy (10) we make

$$ {}^3K_1^{jkl} = \tfrac{2}{5}({}^1\lambda^j\sigma^{kl} + {}^1\lambda^k\sigma^{lj} + {}^1\lambda^l\sigma^{jk}) $$

and the number of independent variables is the number of independent values of ${}^1\lambda^j$. Thus if the third-order cumulant is to be used to describe the riding motion of one atom on another we can constrain the refinement so that ${}^3K_0^{jkl}={}^4K^{jklm}=0$ and say

$$ \begin{aligned} \ln{}^3\psi(\mathbf{t}) = i\sum_j (x^j + {}^1\lambda^j)t_j + \frac{i^2}{2}\sum_{jk}\sigma^{jk}t_jt_k \\ + \frac{i^3}{5}\sum_{jkl} {}^1\lambda^j\sigma^{kl}t_jt_kt_l . \end{aligned} \qquad (15) $$

This expression contains the useful quantities x^j, ${}^1\lambda^j={}^1K^j-x^j$ and σ^{jk} and is simple to program.

We may also say ${}^4K^{jklm}={}^4K_0^{jklm}+{}^4K_1^{jklm}$ where $\sum_{lm} {}^4K_0^{jklm}p_{lm}=0$ so that for point symmetry 1 ${}^4K_0$ is described by 9 variables and ${}^4K_1$ by 6. We can say

$$ \begin{aligned} {}^4K_1^{jklm} = \tfrac{4}{7}({}^2\bar{\lambda}^{jk}\sigma^{lm} + {}^2\bar{\lambda}^{lm}\sigma^{jk} + {}^2\bar{\lambda}^{jl}\sigma^{km} \\ + {}^2\bar{\lambda}^{km}\sigma^{jl} + {}^2\bar{\lambda}^{kl}\sigma^{jm} + {}^2\bar{\lambda}^{jm}\sigma^{kl} \end{aligned} \qquad (16) $$

so that from (11)

$$ {}^2\lambda^{jk} = \tfrac{1}{4}\sum_{lm} {}^4K_1^{jklm}p_{lm} = {}^2\bar{\lambda}^{jk} + \tfrac{1}{7}\sigma^{jk}\sum_{lm} {}^2\bar{\lambda}^{lm}p_{lm} . \qquad (17) $$

The number of independent values of ${}^2\bar{\lambda}^{jk}$ is not dependent on the existence of the operator $\bar{1}$ and only the 11 centrosymmetric point groups need be considered (6 values for $\bar{1}$, 4 for $2/m$, 3 for mmm, 2 for $4/m$, $4/mmm$, $6/m$, $6/mmm$, $\bar{3}$, $\bar{3}m$ and 1 for $m3$ and $m3m$).

Thus if we assume ${}^3K_0^{jkl}={}^4K_0^{jklm}=0$ we can refine $\psi(\mathbf{t})={}^3\psi(\mathbf{t})+{}^4\psi(\mathbf{t})$ where ${}^3\psi(\mathbf{t})$ is given by (15) and

$$ {}^4\psi(\mathbf{t}) = \frac{i^2}{2}\sum_{jk} {}^2\lambda^{jk}t_jt_k + \frac{i^4}{7}\sum_{jklm} {}^2\bar{\lambda}^{jk}\sigma^{lm}t_jt_kt_lt_m \qquad (18) $$

where ${}^2\lambda^{jk}$ and ${}^4K_1^{jklm}$ are described in terms of the variables ${}^2\bar{\lambda}^{jk}$ by (16) and (17).

If all the cumulants up to third order are refined it is possible to evaluate ${}^3K_0={}^3K-{}^3K_1$ and if all the cumulants up to fourth order are refined it is possible to evaluate ${}^4K_0={}^4K-{}^4K_1$.

Discussion

It should be pointed out that (10), (11), (12), (13) do not necessarily imply that $\partial\Psi(\mathbf{u})/\partial u^j\neq 0$ at any other point. Other localized maxima may occur provided the higher-order cumulants are of sufficient magnitude. For example the one-dimensional function $(1+\alpha y^4)\exp(-\beta y^2)$ has 3 maxima and 2 minima for positive

β provided $\alpha > \beta^2$. If $\alpha < \beta^2$ there is just 1 maximum at $y=0$. If the higher-order cumulants are sufficiently large the point $\mathbf{u}=\mathbf{x}$ need not be an absolute maximum and the question as to whether the probability density function may be better described as a sum of probability densities from more than one probability density function may only be resolved by comparing the results so obtained.

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Indirekte Lichtbeugungsversuche an Stäbchenaussengliedern des Frosches

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Light diffraction and image reconstruction experiments have been done with photomicrographs obtained from two different objects: one type of object was an electron micrograph taken from ultrathinly sectioned rod outer segments of the retina of the frog *Rana esculenta*. (The outer segments are the biological structures by which light is converted into electrical excitation.) The other type of object was a photo-reproduction of a model drawing. This model represents an essentially unmodified version of a working hypothesis put forward earlier as an interpretation of (the direct lattice of) electron micrographs from freeze-etched rod outer segments. The comparison of the reciprocal lattices of the two types of object leads to good agreement as far as any comparison between a biological organelle and a geometrical model allows; the same is true for the comparison between the original electron micrograph and its reconstruction by double light diffraction. Hence the working hypothesis on the fine structure of the rod outer segment is further supported.

Einführung

Die Stäbchenaussenglieder (Stäbchen) stellen diejenigen Strukturen in der Wirbeltiernetzhaut dar, in denen das einfallende Licht in elektrische Erregung umgewandelt wird. Das Stäbchen ist im Prinzip ein Zylinder aus über tausend aufeinandergestapelten Schichten von insgesamt 50 μm Länge und 6 μm im Durchmesser. Die Stäbchenquerschnittsfläche ist rosetten- oder kleeblattartig gegliedert. Jedes einzelne im Querschnitt kleeblattförmige Segment des Stäbchens kann als Parakristall angesehen werden, weil einerseits Teile der Schichten aus einem – in Grenzen – regelmässigen Fibrillengeflecht zu bestehen scheinen und andererseits die übereinander gestapelten Schichten nicht starr miteinander verbunden sind: aufgrund des hohen Wassergehaltes im Stäbchen müssen sie vielmehr als in einer Matrix schwebend vorgestellt werden. Aus diesem Grunde erfüllen die Bestimmungsstücke der Elementarzellen im Laufe der Zeit eine Statistik; das elektronenmikroskopische Bild spiegelt nur eine Momentaufnahme einer keinesfalls statischen biologischen Struktur wider.

Die Aussage, die Stäbchen des Frosches *Rana esculenta* seien im Prinzip parakristallin aufgebaut, wurde als Arbeitshypothese aufgestellt (Rosenkranz, 1970) und in weiteren Untersuchungen (Hauser & Rosenkranz, 1971; Rosenkranz & Hauser, 1972; Rosenkranz, 1973) in wesentlichen Teilen abgesichert. Eine weitere Prüfung der Arbeitshypothese stellen die Ergebnisse der Lichtbeugungsversuche dar, die an elektronenmikroskopischen Aufnahmen von Stäbchen und an Modellzeichnungen durchgeführt wurden, sowie die Rekonstruktionen der elektronenmikroskopischen Aufnahmen. Über diese Ergebnisse soll kurz berichtet werden.

Versuche

An einem umgebauten Diffraktometer der Firma Polaron Equipment (Watford, England) konnten noch Periodizitäten im Objekt mit ihrer ± 2. Ordnung nachgewiesen werden, deren Gitterkonstante $a=0{,}22$ mm betrug, entsprechend, im vorliegenden Falle, 40 Å im elektronenmikroskopischen Präparat. Mit diesem Gerät wurden zwei Reihen von Lichtbeugungsversuchen vorgenommen: einmal dienten als Objekt für die