NOTE ON THE THEORY OF X-RAY DIFFRACTION BY SPHERICAL SHELL STRUCTURES

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ABSTRACT An equation is derived, which connects two functions $P(r)$ and $g(x)$, the first being related to the scattering intensity by a simple transformation, the second to the elctron density distribution of a spherically symmetric structure. This relation seems to be a suitable starting point for an analysis of shell structures from diffraction patterns.

INTRODUCTION

In the following a formula is derived which seems to be useful for the interpretation of diffraction patterns from structures of spherical symmetry, especially in the case of shell structures such as vesicles (see Pape et al., 1974).

If r denotes the distance from the center, and $\rho(r)$ the electron density distribution of the structure, its scattering amplitude is given by the well known formula

$$F(s) = (2/s) \int_0^{\infty} r\rho(r) \sin (2\pi sr) \, dr, \tag{1}$$

with

$$s = 2 \sin \vartheta/\lambda. \tag{2}$$

We now introduce a function $g(x)$, defined—for mathematical reasons—on the whole real axis by the following equation:

$$g(x) = \begin{cases} r\rho(r) & \text{for } x = r \geq 0 \\ 0 & \text{for } x < 0. \end{cases} \tag{3}$$

Let $f(s)$ denote the Fourier transform of $g(x)$, we then obtain from Eq. 3

$$f(s) = \int_0^{\infty} r\rho(r) e^{-2\pi isr} \, dr, \tag{4}$$

and further from Eq. 1 the relation

$$sF(s) = -2\,Im f(s) = i(f(s) - f^*(s)). \tag{5}$$

Taking the square and performing an inverse Fourier transformation on both sides of this equation, the left-hand side yields a function

$$P(x) = 2\int_0^\infty s^2F^2(s)\cos(2\pi sx)\,ds, \tag{6}$$

which may be considered as "observable," since it is obtained from the intensity ($\sim F^2(s)$) by a unique transformation. The right-hand side, according to the convolution theorem of Fourier transformations, yields (apart from the factor i^2) the convolution product[1] of the inverse Fourier transform of $f(s) - f^*(s)$, that is (with $g_-(x) = g(-x)$)

$$\widehat{(g(x) - g_-(x))(g(x)} - g_-(x)). \tag{8}$$

Since this expression as well as $P(x)$ is an even function, the further discussion may be restricted to positive values $x = r$.

Making use of the notation ("convolution square")

$$\widehat{g}^2(r) = \widehat{gg_-} = \widehat{g_-g} = \int_{-\infty}^{\infty} g(x)g(x-r)\,dx, \tag{9}$$

and noticing, that[2]

$$\widehat{g_-g_-}(r) = 0, \tag{10}$$

we finally obtain the following relation between the functions P and g:

$$P(r) = 2\,\widehat{g}^2(r) - \widehat{gg}(r). \tag{11}$$

This relation proves to be particularly useful, if the two contributions $2\widehat{g}^2$ and $-\widehat{gg}$ do not overlap. This is the case, if the structure is confined to an interval $R_1 < r < R_2$ and the "thickness" of the shell is smaller than its inner diameter:

$$R_2 - R_1 < 2R_1. \tag{12}$$

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[1] Following the notation of Hosemann and Bagchi (1962), the convolution product of two functions $\varphi(x)$ and $\psi(x)$ is defined as $\widehat{\varphi\psi}(x) = \int_{-\infty}^{+\infty} \varphi(y)\psi(x-y)\,dy$.

[2] The term $\widehat{g_-g_-}(r) = \int_{-\infty}^{+\infty} g_-(y)g_-(r-y)\,dy = \int_{-\infty}^{+\infty} g(-y)g(y-r)\,dy$ is zero for all $r > 0$, since for $y > 0$ the first factor in the integrand, and for $y < 0$ the second one vanishes according to the definition of $g(x)$ (Eq. 3).

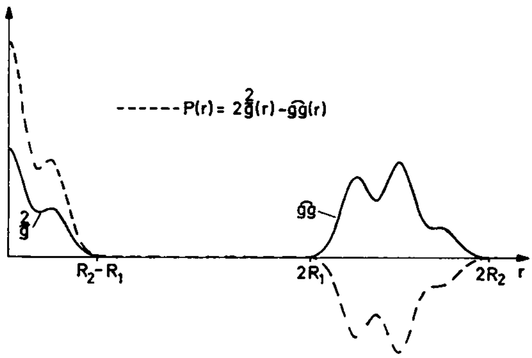

FIGURE 1 The convolution square $\tilde{g}^2(r)$ (——), convolution product $\widehat{gg}(r)$ (——), and the function $P(r) = 2\tilde{g}^2 - \widehat{gg}$ (------) for some arbitrary function $g(x)$, which was chosen to be composed of two Gaussians of different height confined to the interval $R_1 < x < R_2$.

Under this condition the function $P(r)$ provides two independent informations about the structure (see for illustration Fig. 1), a fact, which obviously enhances the reliability of the results obtained in this way.

In practical cases the determination of the structure from $P(r)$ (which in principle is possible except for a factor ± 1) may be impeded by a lack of experimental accuracy and a polydispersity of the specimen, for instance a range of vesicle radii.

However, and this seems to be a particular advantage of the method suggested in this paper, the function $P(r)$ itself, as obtained from the observed intensity data (Eq. 6), will indicate the degree of refinement, to which statements about the structure are possible.

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