17 Finite crystal lattice and its Fourier transform. Lattice amplitude and shape amplitude

A finite lattice $f(\vec{x})$ — a regularly distributed motif $f_U(\vec{x})$ (unit cell) over a finite region V of the N–dimensional space — can be mathematically described in two formally different ways:

$$f(\vec{x}) = f_U(\vec{x}) * \sum_{\vec{n}\in V} \delta(\vec{x} - \vec{x}_{\vec{n}}) \ , \tag{1a}$$

$$f(\vec{x}) = f_U(\vec{x}) * \sum_{\vec{n}\in \inf} \delta(\vec{x} - \vec{x}_{\vec{n}})\, s(\vec{x}) \ . \tag{1b}$$

The expression (1a) seems to be more natural because the sum has a finite number of terms (the symbol $\vec{n} \in V$ means that the sum involves the terms in which the ending point of the lattice vector $\vec{x}_{\vec{n}}$ 16(2) lies in the region V). On the other hand, in expression (1b) the sum has infinite number of terms (the summation goes over all values of the multiindex $\vec{n}$) and the finite region V is demarcated by the so–called shape function $s(\vec{x})$ (characteristic function of the region V):

$$\begin{aligned} s(\vec{x}) &= 1, \ \text{if} \ \vec{x} \in V \ , \\ s(\vec{x}) &= 0, \ \text{if} \ \vec{x} \notin V \ . \end{aligned} \tag{2}$$

If the finite lattice is formed entirely by complete unit cells, the expression (1b) does not depend on the order in which the convolution and multiplication are performed and the expressions (1a) and (1b) are equivalent.

The Fourier transforms of the two expressions (1) are, of course, also equivalent. They are, however, expressed by different functions.

The Fourier transform of expression (1a) is — according to 7.3(1) and 1.3(2) — the product

$$F(\vec{X}) = F_U(\vec{X})G(\vec{X}), \tag{3}$$

in which the function

$$G(\vec{X}) = \sum_{\vec{n}\in V} \exp\bigl(-\mathrm{i}k\vec{X}\cdot\vec{x}_{\vec{n}}\bigr) \tag{4}$$

is the sum of finite number of phasors. M. v. Laue [1] named the sum $G(\vec{X})$ the lattice amplitude. It is evidently a periodic function with the $\frac{2\pi}{k}$–multiple periodicity of the reciprocal lattice periodicity and as $\vec{X}_{\vec{h}}\cdot\vec{x}_{\vec{n}}$ is an integer, it is

$$\max\left|G(\vec{X})\right| = G\left(\frac{2\pi}{k}\vec{X}_{\vec{h}}\right) = \frac{V}{V_U}. \tag{5}$$

The ratio $\frac{V}{V_U}$ is the number of unit cells forming the finite lattice.

The Fourier transform of expression (1b) has — by the use of 7.3(1), 7.3(3), and 4.3(17) — the form

$$F(\vec{X}) = \frac{1}{A^N V_U} F_U(\vec{X}) \sum_{\vec{h}\in\inf} \delta\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right) * S(\vec{X}), \tag{6}$$

where

$$S(\vec{X}) = \mathrm{FT}\left\{s(\vec{x})\right\} = A^N \int_V \dots \int \exp\bigl(-\mathrm{i}k\vec{X}\cdot\vec{x}\bigr)\mathrm{d}^N\vec{x}. \tag{7}$$

The function $S(\vec{X})$ was named the shape amplitude by P. Ewald [2]. The same name is also used for quantities proportional to the Fourier transform of the shape function, namely for dimensionless quantities

$$S_1(\vec{X}) = \frac{1}{A^N V}\, S(\vec{X}) \qquad \text{and} \qquad G_1(\vec{X}) = \frac{1}{A^N V_U}\, S(\vec{X}). \tag{8}$$

It is evident that the absolute values of these quantities assume their maximum value at $\vec{X} = \vec{0}$:

$$S(\vec{0}) = A^N V, \qquad S_1(\vec{0}) = 1, \qquad G_1(\vec{0}) = \frac{V}{V_U}. \tag{9}$$

With the use of the shape amplitude G_1 the Fourier transform (6) of a finite lattice may be rewritten into the form

$$F(\vec{X}) = F_U(\vec{X}) \sum_{\vec{h}\in\inf} \delta\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right) * G_1(\vec{X}), \tag{10}$$

which has exactly the same structure as expression (1b) characterizing the finite lattice. Therefore, the Fourier transform of finite lattice is formed by shape amplitudes $G_1(\vec{X})$ situated at points $\frac{2\pi}{k}\vec{X}_{\vec{h}}$ of the reciprocal lattice and multiplied by the Fourier transform $F_U(\vec{X})$ of the unit cell. This analogy between the finite lattice and its Fourier transform may even be more evident from expressions that are obtained from (1b) and (10) by carrying out the first the multiplication and then the convolution:

$$f(\vec{x}) = \sum_{\vec{n}\in\inf} s\left(\vec{x}_{\vec{n}}\right) f_U\left(\vec{x} - \vec{x}_{\vec{n}}\right), \tag{11}$$

$$F(\vec{X}) = \sum_{\vec{h}\in\inf} F_U\left(\frac{2\pi}{k}\vec{X}_{\vec{h}}\right) G_1\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right). \tag{12}$$

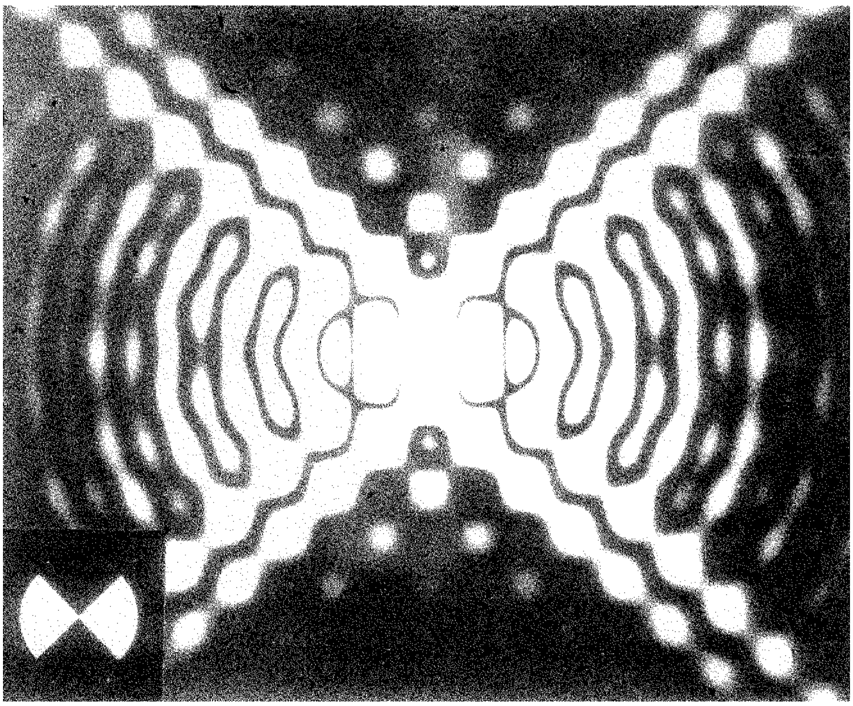

Figure 1: The Fraunhofer diffraction from the sector star with two–fold symmetry. The star is shown in the left lower corner of the figure. The arms of the diffraction pattern are perpendicular to the straight–line parts of the boundary of the star. The two–fold sector star serves as the motif by the repetition of which the lattices in Figure 2 arisen.

In other words and formally viewed, the Fourier transform of a finite lattice is again a finite lattice with shape amplitudes G_1 in the role of unit cells and with the Fourier transfrom F_U of the unit cell in the role of the shape function s limiting the region of the finite lattice in the space of the Fourier transform (cf. Figures 2, 3 and 4). We may recognize in it the feature of reciprocity: What is large in the space of the variable $\vec{x}$ is small in the Fourier space of the variable $\vec{X}$ and vice versa. In reality the analogy between the finite lattice and its Fourier transform in not so perfect as in symbols. The reason is that the finite lattice is spatially limited by the shape function $s(\vec{x})$ which takes its zero value abruptly (cf. (2)), whereas the Fourier transform of the finite lattice is a finite lattice only in the sense that is limited by the Fourier transform $F_U(\vec{X})$ of the unit cell, which goes to zero only asymptotically as $X \to \infty$.

As we have seen the Fourier transform of a finite lattice can be expressed in two formally different ways: On the one hand by expression (3) in terms of the lattice amplitude (4), and on the other hand by expression (10) and (12), respectively, in terms of the shape amplitude (8). One may think that it is always advantageous to use expression (3) which is the product of two simple functions rather than expression (10) or (12) which represent the N–multiple infinite series. There are, however, at least three reasons to make it cleare that just the opposite is usually true:

(i) Usually it is not at all easy to calculate the lattice amplitude $G(\vec{X})$ according to its definition (4). If the boundaries of the lattice are complicated it is quite difficult to specify the limits of the sum (4). Therefore, the relation obtained by comparing (3) and (10) may be useful:

$$G(\vec{X}) = \sum_{\vec{h}\in\inf} G_1(\vec{X}) * \delta\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right) = \sum_{\vec{h}\in\inf} G_1\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right). \tag{13}$$

It expresses the lattice amplitude $G(\vec{X})$ (a periodic function) by superposition of shape amplitudes $G_1(\vec{X})$ (non–periodic functions).

(ii) If the finite lattice is formed by a large number of unit cells in any direction the modulus of the shape amplitude $\left|G_1(\vec{X})\right|$ has a sharp maximum at the origin, i.e. the function $G_1(\vec{X})\frac{V_U}{V} = S_1(\vec{X})$ is essentially different from zero only in the vicinity of the origin. Consequently, in the vicinity of the points $\vec{X} = \frac{2\pi}{k}\vec{X}_{\vec{h}}$ it holds that

$$G(\vec{X}) \doteq G_1\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right), \qquad \text{if} \quad \left|\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right| \ll \frac{2\pi}{|k|}\left|\vec{a}_r^{\,+}\right|, \tag{14}$$

because the contributions of all other terms of the series (13) are negligible. Hence, the shape amplitude $G_1\left(\vec{X} - \frac{2\pi}{k}\vec{X}_{\vec{h}}\right)$ may be used as a local approximation of the lattice amplitude $G(\vec{X})$ within the vicinity of points $\vec{X} = \frac{2\pi}{k}\vec{X}_{\vec{h}}$. This was, in fact, the initial motivation for the study of the shape amplitude when M. v. Laue [3] approximated the sum (4) by the integral expressing the shape amplitude G_1.

Good local approximation of the lattice amplitude G by the shape amplitude G_1 in the vicinity of the points $\frac{2\pi}{k}\vec{X}_{\vec{h}}$ may be illustrated by the one dimensional lattice formed by $(2n+1)$ points: $f(x) = \sum_{j=-n}^{n}\delta(x - ja)$. The lattice amplitude of such a lattice is

$$G(X) = \sum_{j=-n}^{n}\exp\left(-\mathrm{i}kXja\right) = \frac{\sin\left[kX(2n+1)a/2\right]}{\sin\left(kXa/2\right)} \tag{15}$$

and the shape amplitude

$$G_1(X) = \int_{-(2n+1)a/2}^{(2n+1)a/2}\exp\left(-\mathrm{i}kXa\right)\mathrm{d}x = \frac{\sin\left[kX(2n+1)a/2\right]}{kXa/2}. \tag{16}$$

Efficient local approximation of the lattice amplitude (15) by the shape amplitude (16) in the vicinity of the lattice point $X = 0$ is obvious from the algebraic expressions of the two functions. Figure 5 illustrates it for the case of the lattice formed by nine points.

(iii) The finite lattice always has the shape of an N–dimensional polyhedron (a polygon in E_2, a polyheron in E_3). The shape amplitudes of polyhedra can easily be calculated because the integral (7) can always be evaluated analytically, as mentioned in Section 11.1. In the three–dimensional case this was pointed out by M. v. Laue [3] who recommended to use the Abbe transform for calculation of the integral (7) (cf. [5] and Appendix D of these lectures). In 1939 Patterson [4] calculated the shape amplitudes of several palyhedra in such a way that he decomposed the polyhedron into tetrahedra, calculated the shape amplitude of a general tetrahedron and expressed the shape amplitude of the polyhedron by summing up the shape amplitudes of the constituent tetrahedra. Algebraic formulae of the shape amplitudes of general polygons and polyhedra derived by the use of the Abbe transform 11.1(2) have been published

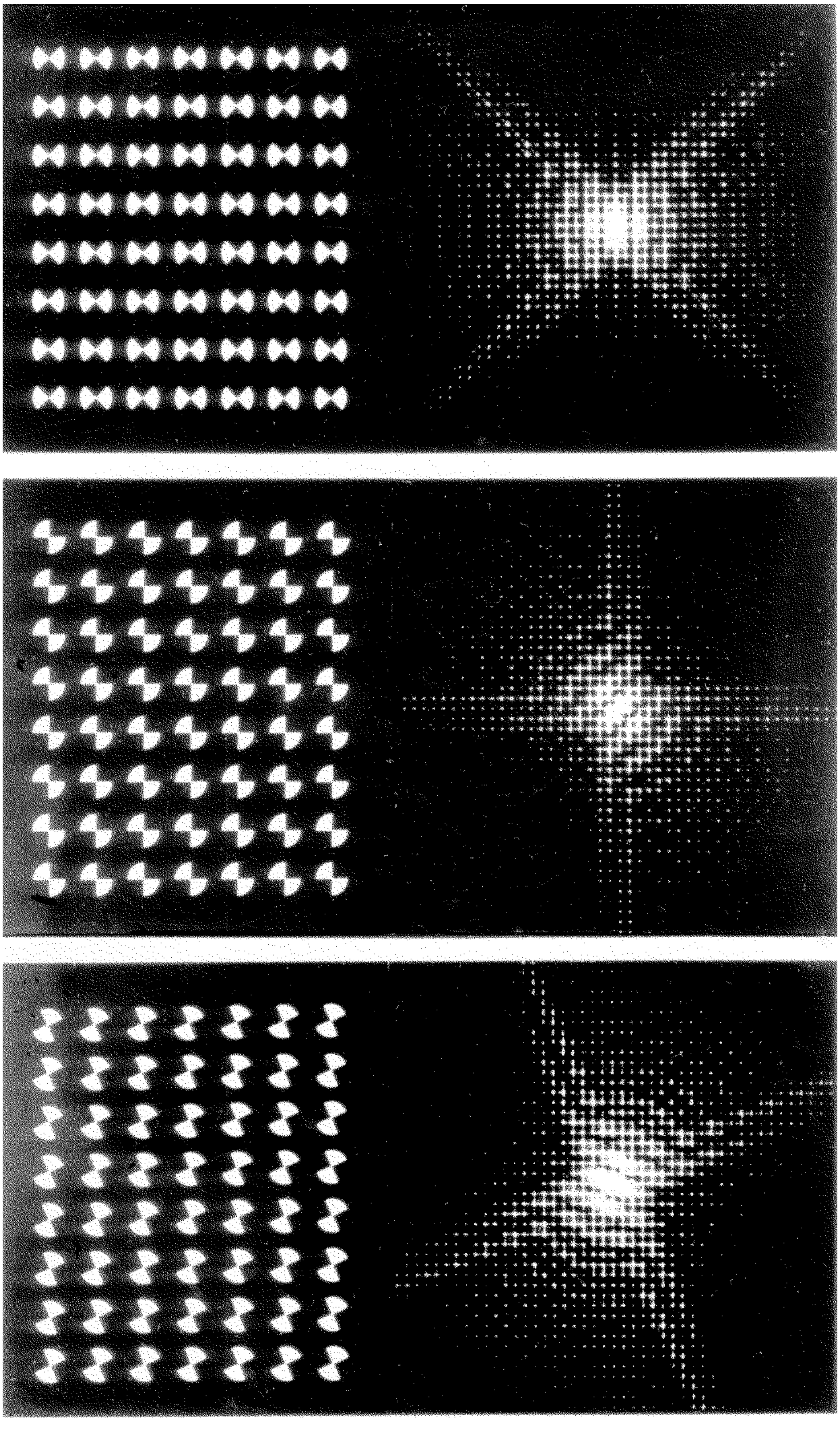

Figure 2: Two–dimensional square lattices in the left–hand column resulted from translations of sector stars with different orientation. The Fraunhofer diffraction pattern in the right–hand column illustrate that the diffraction pattern from the lattice is restricted by the diffraction from the motif. (Note that the arms of the diffraction patterns are perpendicular to the straight–line boundaries of the sector stars.)

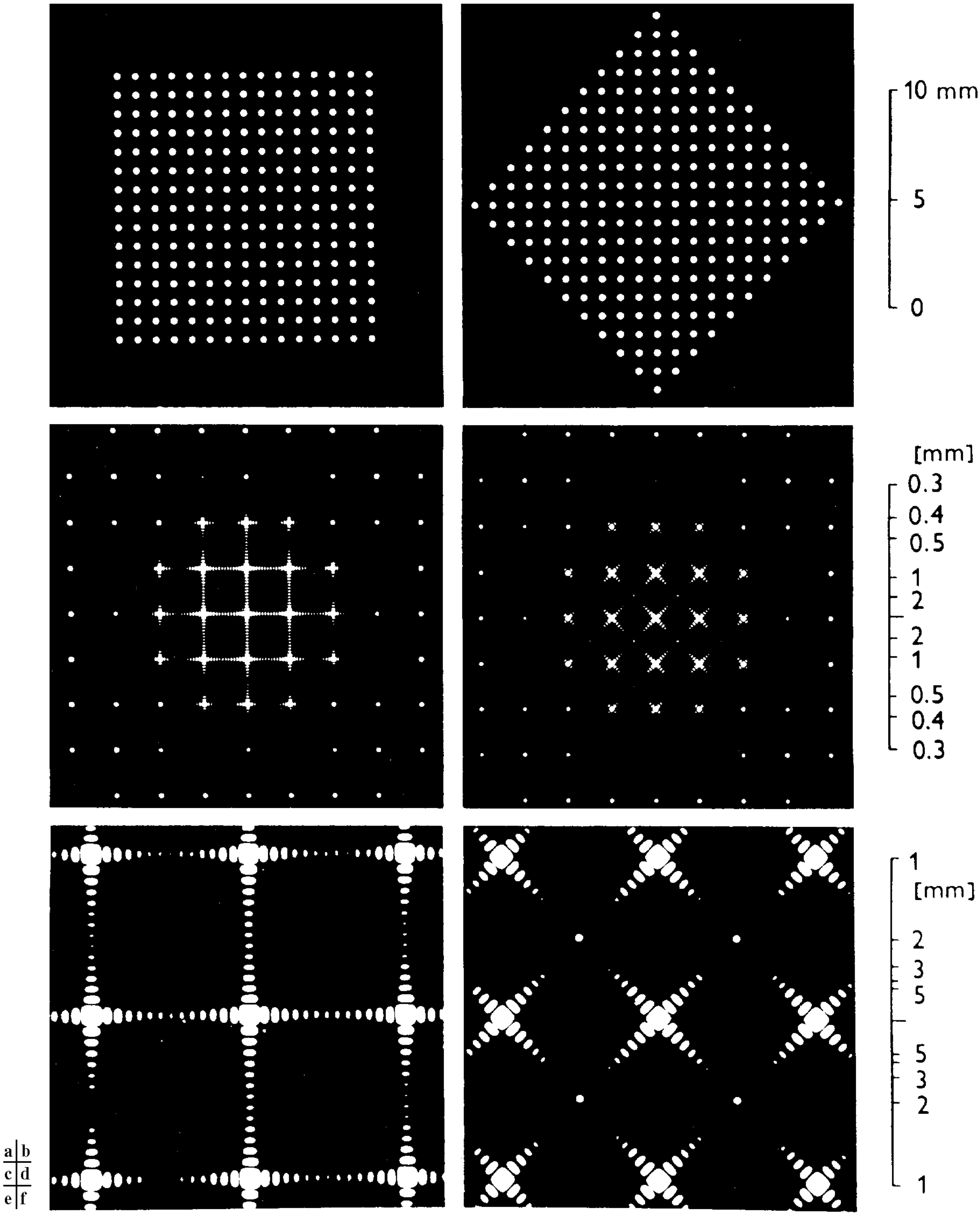

Figure 3: Influence of the external shape of the finite lattice on the shape of diffraction spots [5]. (a),(b) — two–dimensional lattices of the same structure (squared) but with different external boundaries. (c),(e) and (d),(f) — the Fraunhofer diffraction patterns from (a) and (b). (c),(d) — the whole central region of the patterns, (e),(f) — a detail showing the shape of the diffraction spots (squared modulus of the lattice amplitude $G(\vec{X})$). The subsidery maxima in the centre of the reciprocal lattice cells, clearly visible in (f), disappear with the increasing number of scattering centres. (Their intensity is proportional to the number of the scattering centres, whereas the intensity of the principal maxima is proportional to the square of the number of scattering centres.)

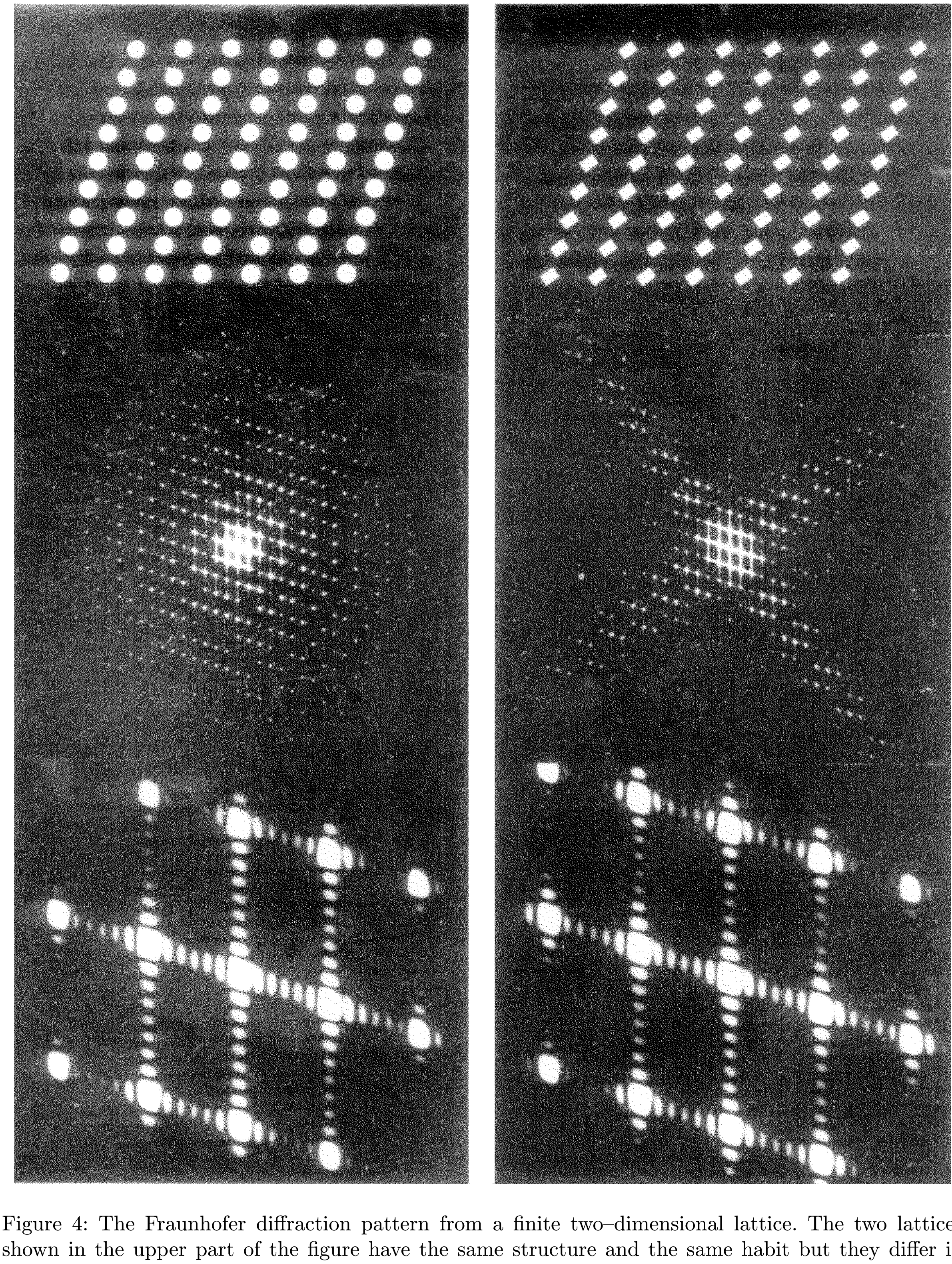

Figure 4: The Fraunhofer diffraction pattern from a finite two–dimensional lattice. The two lattices shown in the upper part of the figure have the same structure and the same habit but they differ in motif: The apertures are circular (left) or rectangular (right). The middle part of the figure shows the whole Fraunhofer diffraction patterns from the lattices. It is evident that the diffraction pattern as a whole is marked off by the diffraction from the motif (the Airy pattern with rotational symmetry corresponds to diffraction from the circular aperture, the cross with arms perpendicular to the sides corresponds to diffraction from the rectangular aperture). The lower part of the figure shows enlarged central regions of the diffraction patterns. They are almost identical because the structure of the two lattices is the same. The principal maxima form reciprocal lattice of the diffraction lattice.

Figure 5: The lattice amplitude $G(X) = \frac{\sin\left(9kXa/2\right)}{\sin\left(kXa/2\right)}$ and the shape amplitude $G_1(X) = \frac{\sin\left(9kXa/2\right)}{kXa/2}$ of the one–dimensional lattice formed by nine points. It is obvious from the graphs that the shape amplitude $G_1(X)$ well approximates the lattice amplitude $G(X)$ in the vicinity of the lattice point $X = 0$, i.e. if $|X| \ll \frac{2\pi}{ka}$.

in 1988 [5]. By means of them the shape amplitudes of polygons and polyhedra can easily be calculated (cf. Section 13.2, Appendix D and papers [6], [7]). Therefore it is advantageous to calculate the Fourier transform of finite lattice according to (12). In doing so the infinite series (12) may be replaced in the vicinity of points $\vec{X} = \frac{2\pi}{k}\,\vec{X}_{\vec{h}}$ by several its terms only, often — in fact almost always — by only the one, as indicated by (14) and illustrated in Figure 5.

References

[1] Laue M. v.: *Materiewellen und ihre Interferenzen.* 2. Auflage. Akademische Verlagsgesellschaft, Geest & Portig, Leipzig 1948.

[2] Ewald P. P.: X-ray diffraction by finite and imperfect crystal lattices. *The Proceedings of the Physical Society (London)* **52** (1940), 167–174.

[3] Laue M. v.: Die äussere Form der Kristalle in ihrem Einfluss auf die Interferenzerscheinungen an Raumgittern. *Annalen der Physik.* 5. Folge **26** (1936), 55–68.

[4] Patterson A. L.: The Diffraction of X-Rays by Small Crystalline Particles. *Phys. Rev.* **56** (1939), 972–977.

[5] Komrska J.: Algebraic expressions of shape amplitudes of polygons and polyhedra. *Optik* **80** (1988), 171–183.

[6] Komrska J., Neumann W.: Crystal Shape Amplitudes of Platonic Polyhedra. I. General Aspects and the Shape Amplitudes of the Tetrahedron, Cube and Octahedron. phys. stat. sol. (a) 150 (1995), 89–111.

[7] Neumann W., Komrska J.: Crystal Shape Amplitudes of Platonic Polyhedra. II. The Regular Pentagonal Dodecahedron and the Icosahedron. phys. stat. sol. (a) 150 (1995), 113–126.