phys. stat. sol. (b) 112, K111 (1982)

Subject classification: 1.3 and 1.4; 21.1

Zentralinstitut für Kernforschung der Akademie der Wissenschaften der DDR, Rossendorf[1]

On the Reproduction of the Orientation Distribution Function of Texturized Samples from Reduced Pole Figures Using the Conception of a Conditional Ghost Correction

By

S. MATTHIES and G.W. VINEL

As it is well understood now from the reduced pole figures $\tilde{P}_{\vec{h}_i}(\vec{y})$ measured in common diffraction experiments, only the reduced part $\tilde{f}(g)$ of the ODF $f(g) = \tilde{f}(g) + \tilde{\tilde{f}}(g)$ can unambiguously be reproduced containing, however, ghost phenomena /1, 2/.

For the reconstruction of $\tilde{\tilde{f}}(g)$ only the condition $f(g) \geq 0$ is an exact point of contact. This leads for a nonzero underground ("phon" - P) in $\tilde{P}_{\vec{h}_i}(\vec{y})$ to a variation width of the "ghost corrected" ODF's, i.e. there exists an infinite number of $f^M(g) \geqq 0$ all explaining the I experimental $\tilde{P}_{\vec{h}_i}(\vec{y})$ with the same quality /2 to 4/. Moreover, as it was shown in /5/ the exact intensity of the constant underground F of the ODF is of interest for the first question of a true quantitative texture analysis: which part of all crystallites in a polycrystalline sample is randomly distributed and which part prefers special orientations, i.e. is texturized?

An expedient from this situation is given by a "conditional" ghost correction, i.e. by the formulation of a physically ingenious principle of selection practically admitting only one result. The best would be a single mathematical extreme principle whose formulation seems, however, to be a nontrivial question. On the other hand, a conditional correction will automatically be realized by a reproduction method converging only to one result. All known iterative methods /2/ yielding a $f^M(g) \geqq 0$ contain arbitrary degrees of freedom injuring the unambiguity or "extremity" of the result.

The most important components of the reproduction method sketched below are at first the zero approximation of the ODF already performing the condition $\geqq 0$ and possessing all properties of symmetry of the ODF. Secondly the used

1) Postschließfach 19, DDR-8051 Dresden, GDR.

iterative procedure automatically maintains these properties. In the third place the "principle of the maximum phon F" is used selecting such a $f^M(g)$ whose phon ($F \leqq P$) is the highest one in comparison with F of other possible results. Additionally a result with a minimum number of intensive peaks in the ODF is preferred.

The starting point of our consideration in order to construct a good zero approximation of the ODF was the function /3, 6/

$$ {}^{s}\tilde{f}_1(\vec{h}_i, g) = \sum_{j=1}^{N_B} \tilde{f}_1(g_{B_j} \cdot \vec{h}_i, g)/N_B, \qquad \tilde{f}_1(\vec{h}_i, g) = \tilde{P}_{\vec{h}_i}(g^{-1} \cdot \vec{h}_i) \geqq 0 \quad , \tag{1} $$

whose linear superposition about all possible $\vec{h}_i$ leads to the function $\tilde{f}_1(g)$:

$$ \lim_{I \to \infty} \sum_{i=1}^{I} {}^{s}\tilde{f}_1(\vec{h}_i, g)/I \to \tilde{f}_1(g) = f_{\Omega'}(g) + f_{\pi}(g) \geqq 0 \quad , \tag{2} $$

containing, however, ghosts because $\tilde{f}_1(g)$ remains in the class of functions $\tilde{f}$. If the sums in (1) and (2) are changed by products this is no more valid. Representing such a (product) function by series of spherical functions there will arise terms with odd l, too, just necessary for the asked reconstruction of $\tilde{\tilde{f}}(g)$.

Our method is given by the following general relations: n step number of an inner iteration (n = 0, 1, 2, ..., N); m step number of the outer (phon-) iteration (m = 0, 1, 2, ..., M); $\tilde{P}_{\vec{h}_i}(\vec{y}_j)$ experimental values; i = 1, 2, ..., I; j = 1, 2, ..., J;

$$ {}^{m}f^{n+1}(g) = {}^{m}\hat{N} \left[{}^{m}f^{n}(g)\, {}^{m}f^{o}(g) \Big/ \left[\prod_{i=1}^{I} \left\{ \prod_{m_i=1}^{M_i} \left({}^{m}\tilde{P}^{n}_{\vec{h}_i}(g^{-1} \cdot \vec{h}_{m_i}) \right)^{1/M_i} \right\}^{r/I} \right] \right] ; \tag{3} $$

$$ {}^{m}\hat{N}\, W(g) = {}^{m}N \cdot W(g) \;, \qquad {}^{m}N = 8\pi^2 (1 - {}^{m}F) \int_G W(g)\, dg \;; \tag{4} $$

$$ {}^{m}f^{o}(g) = {}^{m}\hat{N} \left[\prod_{i=1}^{I} \left\{ \prod_{m_i=1}^{M_i} \left({}^{m}\tilde{P}'_{\vec{h}_i}(g^{-1} \cdot \vec{h}_{m_i}) \right)^{1/M_i} \right\}^{r/I} \right] ; \tag{5} $$

$$ {}^{m}P^{n}_{\vec{h}_i}(\vec{y}) = \frac{1}{2\pi} \int_0^{2\pi} {}^{m}f^{n}\left(\{\vec{h}_i, \tilde{\varphi}\}^{-1} \cdot \{\vec{y}, 0\} \right) d\tilde{\varphi} \quad , $$

$$ {}^{m}\tilde{P}^{n}_{\vec{h}_i}(\vec{y}) = \left[{}^{m}P^{n}_{\vec{h}_i}(\vec{y}) + {}^{m}P^{n}_{-\vec{h}_i}(\vec{y}) \right] \Big/ 2 \quad , \tag{6} $$

$$ {}^{m}\tilde{P}'_{\vec{h}_i}(\vec{y}) = \tilde{P}_{\vec{h}_i}(\vec{y}) - {}^{m}F , \quad {}^{o}F = 0 , \quad {}^{m+1}F = \min\left\{{}^{m}f(g)\right\} , $$

$$ {}^{m}f(g) = {}^{m}f^{N}(g) + {}^{m}F . \tag{7} $$

N is the number of the last step in the inner iteration if for $n = N$ the following condition (v velocity of convergence; e.g. $V = 0.3\%$) is performed:

$$ {}^{m}v^{n} = 100\% \cdot \sum_{i=1}^{I} \sum_{j=1}^{J} \left| \left[{}^{m}\tilde{P}^{\,n}_{\vec{h}_i}(\vec{y}_j) - {}^{m}\tilde{P}^{\,n-1}_{\vec{h}_i}(\vec{y}_j) \right] \Big/ \left[{}^{m}\tilde{P}^{\,n}_{\vec{h}_i}(\vec{y}_j) \cdot I \cdot J \right] \right| \leqq V . \tag{8} $$

After that the m+1-th step of the outer iteration will be started with $n = 0$. M_i is the number of the different equivalent (crystal symmetry G_B) projective directions $\vec{h}^*_i = g_{B_k} \cdot \vec{h}_i$ $(k = 1, 2, \ldots, N_B)$ of the sort i with $\vec{h}^*_i \equiv (\vartheta^*_i, \varphi^*_i)$: $0 \leqq \vartheta^*_i < \frac{\pi}{2}$ or $\vartheta^*_i = \frac{\pi}{2}$, $0 \leqq \varphi^*_i < \pi$. E.g. for cubic crystal symmetry ($G_B = O$, $N_B = 24$) we have $(i = 1)$ $\vec{h}_1 \equiv (1, 0, 0)$, $M_1 = 3$ with $\vec{h}_{m_1=1} = (1, 0, 0)$, $\vec{h}_{m_1=2} = (0, 1, 0)$, and $\vec{h}_{m_1=3} = (0, 0, 1)$.

$$ {}^{m}\tilde{P}_{\vec{h}_i}(\vec{y}) = {}^{m}\tilde{P}^{N}_{\vec{h}_i}(\vec{y}) + {}^{m}F ; $$

$$ {}^{m}R = 100\% \cdot \sum_{i=1}^{I} \sum_{j=1}^{J} \left| \left(\tilde{P}_{\vec{h}_i}(\vec{y}_j) - {}^{m}\tilde{P}_{\vec{h}_i}(\vec{y}_j) \right) \Big/ \left[\tilde{P}_{\vec{h}_i}(\vec{y}_j) \cdot I \cdot J \right] \right| . \tag{9} $$

$R = {}^{M}R$; M is the number of the last step in the outer iteration for a fixed $m = M$ or if one of the conditions ${}^{m}R > {}^{m-1}R$ or ${}^{m+1}F \geqq P \equiv \min\left\{\tilde{P}_{\vec{h}_i}(\vec{y}_j)\right\}$ is performed. The end result is given by $f^{M}(g) \equiv {}^{M}f(g)$.

The ratio of the height of the "true" peaks to the height of the "ghost peaks" can be controlled in the zero approximation with the help of the parameter r. In dependence on the "sharpness" of the texture or the phon value P in the pole figures an optimum velocity of convergence or ($r > 1$) a better "oppression of ghost peaks" than for $r = 1$ can be realized, what is important for a great P and narrow peaks.

The subdivision of the Y-space into cells with the angular extent Δy is given by the experiment. The G-space is also subdivided into cells ($\Delta g \leqq \Delta y$) independently of the cell structure of the Y-space. However, the attainable real resolution power of $f^{M}(g)$ itself depends on I and the sharpness of the texture (see /4/).

Mathematically pure zeros in the experimental pole figures which do practically not occur in reality determine the "zero range" G_0 of the G-space with the help of ${}^{0}f^{0}(g') = 0$ (see (5) for m = 0). All $g' \in G_0$ with the exact result $f^{M}(g') = 0$ will be stored and will not be dealt with in the next iteration steps. I.e. there will not arise zeros in the denominator of (3). Analogically expressions (8) and (9) are to be managed.

Our approach can in principle be modified for incomplete pole figures, too. The sketched method was realized in a computer program for the case of cubic-orthorhombic symmetry. Already the first methodical tests have yielded impressively good results (R-values, degree of ghost correction, and velocity of convergence). An example demonstrating the efficiency of the method will be given in a second note.

At the end for completeness we have to add that a "product variant" for a zero approximation of the ODF was firstly utilized by Williams /7/ and that the inner iteration contains an element of the "self-consistent approach" suggested by Imhof /2/.

The authors would like to thank Dr. M. Betzl, K. Helming, Prof. Dr. K. Hennig, and Dr. A. Mücklich for their support and interest in the present subject as well as the staff of the computer centre of the ZfK whose manysided help made it possible to realize the method in the relatively short time of some months.

References

/1/ S. MATTHIES, phys. stat. sol. (b) 92, K135 (1979).
/2/ Proc. of the VI. Internat. Conf. Textures of Materials, Tokyo 1981, Iron and Steel Inst. of Japan.
/3/ S. MATTHIES, Aktuelle Probleme der quantitativen Texturanalyse, ZfK-Institutspublikation, to be published 1982.
/4/ S. MATTHIES, Kristall und Technik 16, 1061 (1981).
/5/ S. MATTHIES, phys. stat. sol. (b) 112, 705 (1982).
/6/ S. MATTHIES, Kristall und Technik 15, 1323 (1980).
/7/ R.O. WILLIAMS, J. appl. Phys. 39, 4329 (1968).

(Received June 18, 1982)

phys. stat. sol. (b) 112, K115 (1982)

Subject classification: 1.3 and 1.4; 21.1

Zentralinstitut für Kernforschung der Akademie der Wissenschaften der DDR, Rossendorf[1]

An Example Demonstrating a New Reproduction Method of the ODF of Texturized Samples from Reduced Pole Figures

By

S. MATTHIES and G.W. VINEL

The general structure of the reproduction method suggested by the authors was described in /1/. The following example using the denotations of /1/ has to demonstrate the efficiency of this method. Regarding the mentioned CPU time it should be remarked that in the current methodical phase no activities were yet attempted to optimize the program.

In Fig. 1a[2] a "true" ODF f(g) (unknown for the reproduction) is given, constructed with the help of standard functions of Gauss-like (G)/2/ and Lorentz-like (L) /3/ form yielding exact numerical values. The same concerns the pole figures of Fig. 2a[2] following from f(g) and which are to be considered as "experimental" pole figures.

The parameters of the model ODF are (cubic-orthorhombic symmetry):

$$f(g) = 0.315\ P_I(L) + 0.315\ P_{II}(L) + 0.0605\ P_{III}(G) + 0.3095\ ;$$

$$P_I = \{011\}\langle 2\bar{1}\bar{1}\rangle\ ,\quad P_{II} = \{132\}\langle 6\bar{4}3\rangle\ ,\quad P_{III} = \{121\}\langle 1\bar{1}1\rangle\ ,$$

with a full width at half maximum b = 17° for all three components.

In Fig. 1b[2] the ODF $f^M(g)$ is given resulting from our method. Here the case is shown using only the three pole figures (100), (110), and (111) of Fig. 2a for the reproduction. Fig. 2b[2] contains the pole figures derived from $f^M(g)$. In Fig. 3[2] the reduced ODF $\tilde{f}(g)$ (calculated by standard functions) is given, which would be the result of the common Bunge-Roe method in the ideal case ($I \gg 1$).

Characteristic parameters of the calculation: $\Delta y = \Delta g = 5^\circ$, I = 3, V = 0.3%, r = 1; m = 0 (N = 11, ${}^0R = 1.29\%$, ${}^0F = 0$); m = 1 (N = 13, ${}^1R = 1.09\%$, ${}^1F = 0.43$); m = 2 = M (N = 14, ${}^2R = 1.077\%$, ${}^2F = 0.53$); ${}^3F = 0.55$. Effective phon in f(g): 0.54; P = 0.55. CPU time: 42 min (ES-1040); necessary memory space: 400 K. Using I = 4 we got M = 2, ${}^2R = 1.018\%$.

---

1) Postschließfach 19, DDR-8051 Dresden, GDR.

2) Figures see on the following pages.

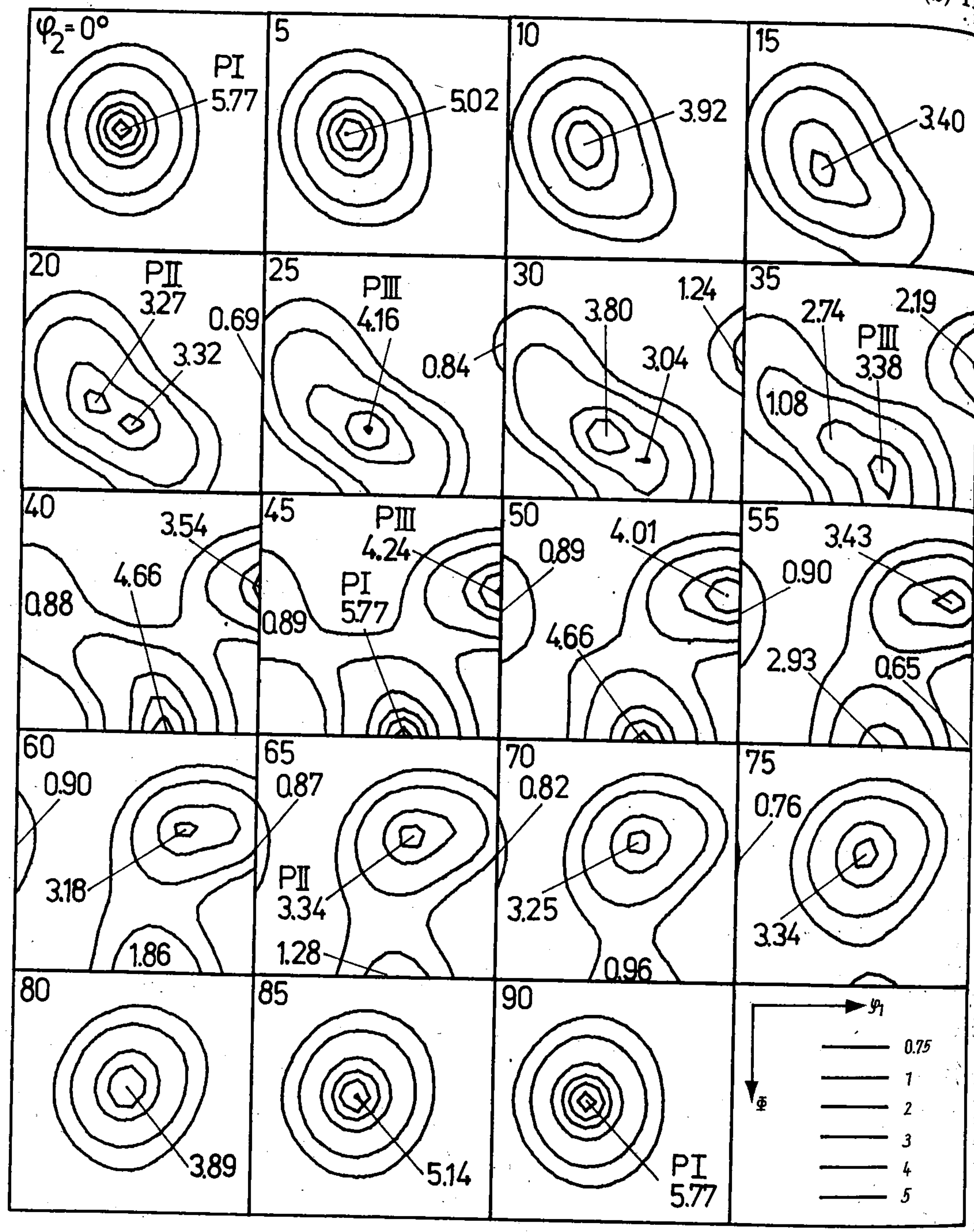


Fig. 1a. The model ODF f(g) unknown for the reproduction problem

Numerical material concerning Fig. 1, 2, or 5 is available from the authors for interested specialists who would like to test their own reproduction programs or procedures of ghost correction.

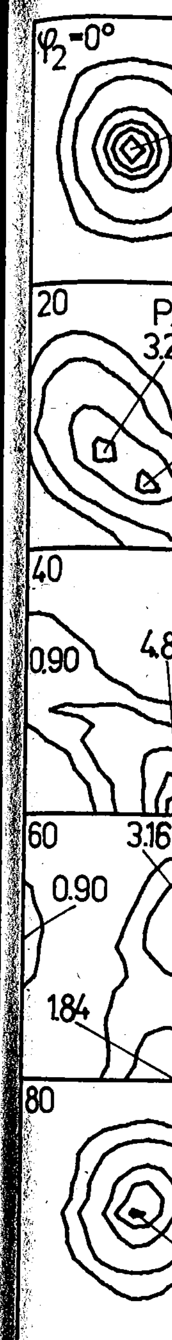


Fig. 1b. The

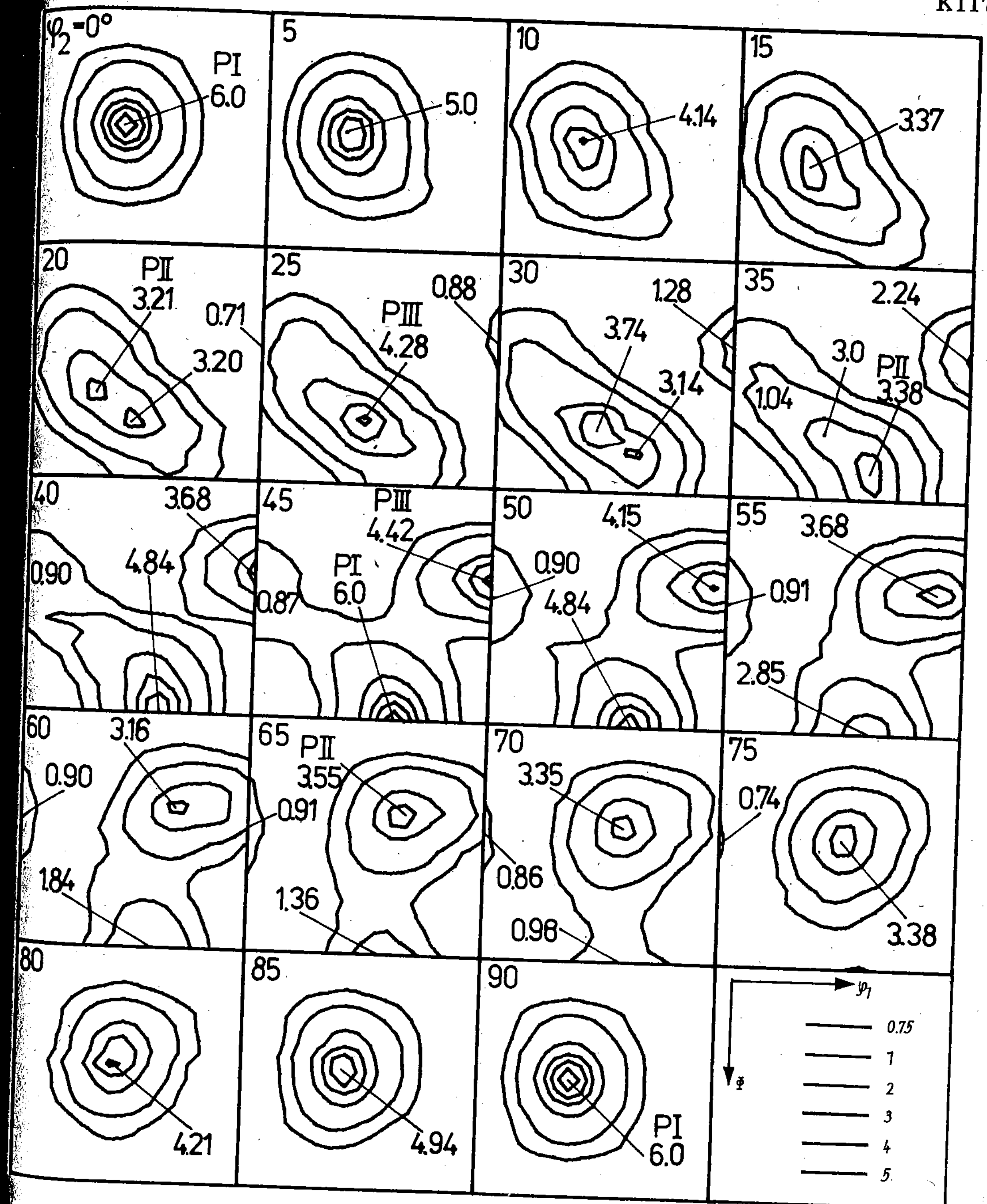


Fig. 1b. The reproduced and ghost corrected ODF $f^M(g)$ for I = 3

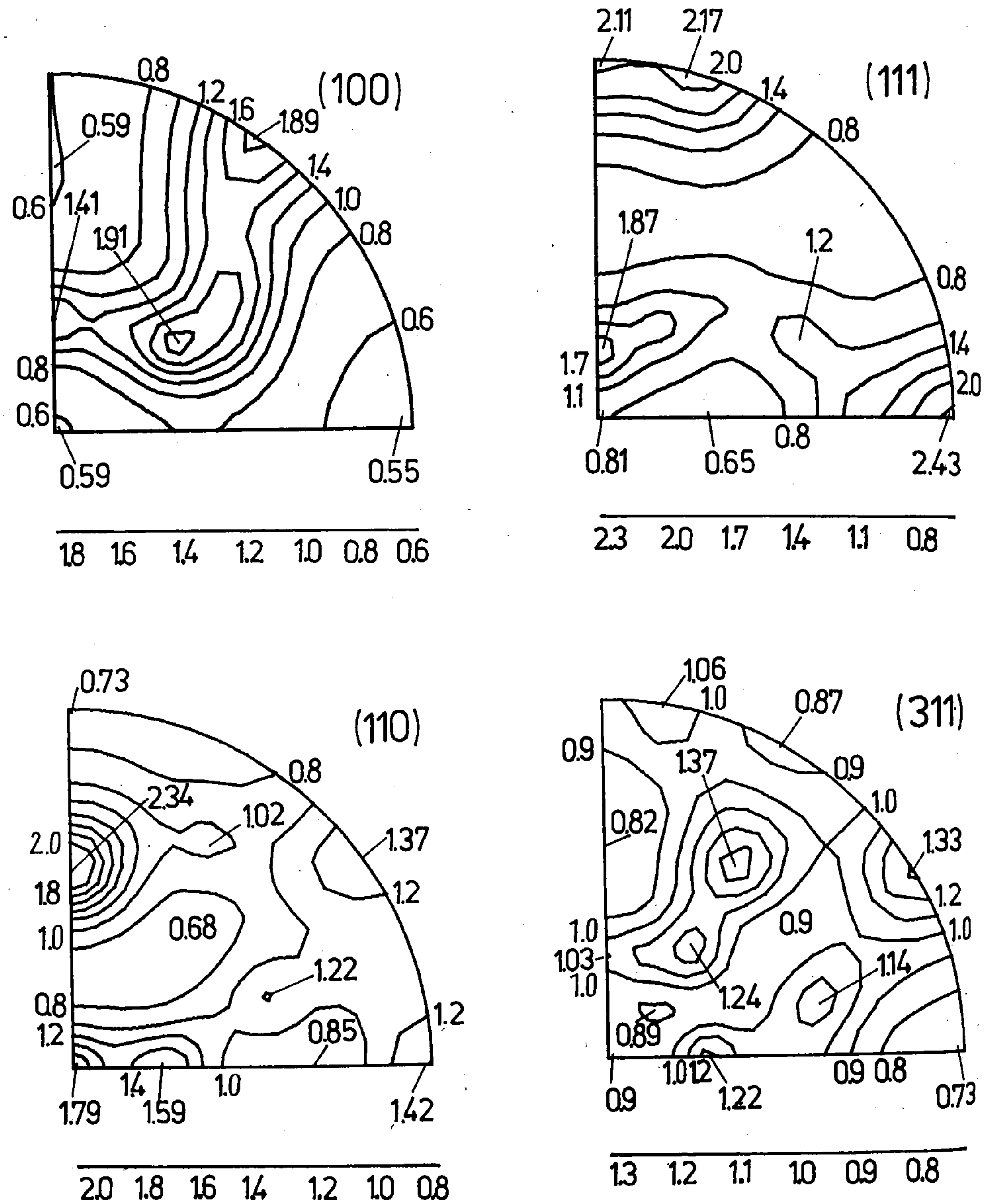


Fig.2a. The "experimental" pole figures $\tilde{P}_{\vec{h}_i}(\vec{y})$ derived from f(g)

References

/1/ S. MATTHIES and G.W. VINEL, phys. stat. sol. (b) 112, K111 (1982).

/2/ S. MATTHIES, phys. stat. sol. (b) 101, K111 (1980).

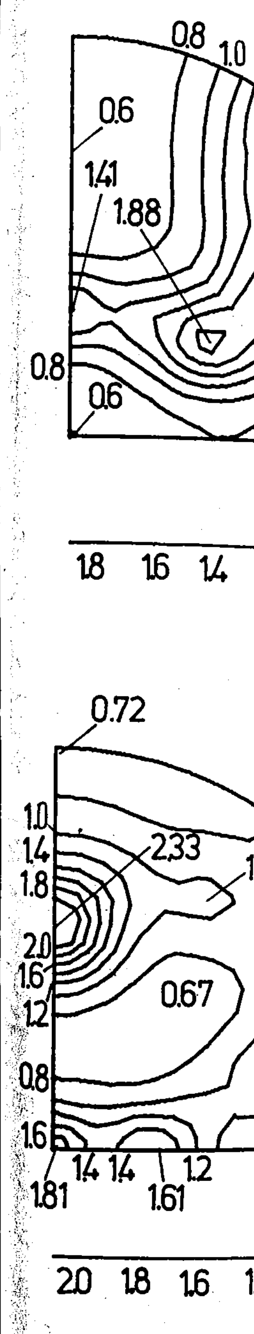
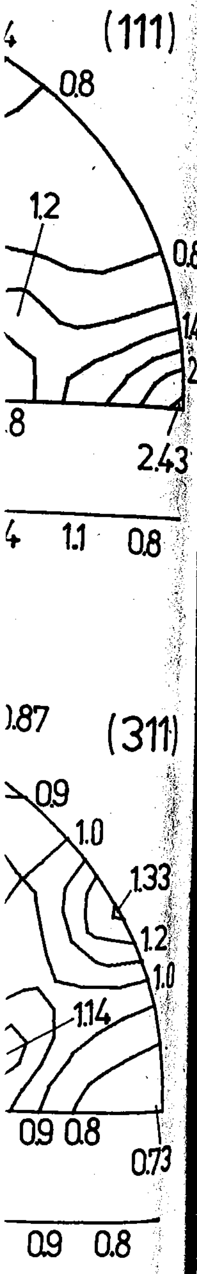


Fig.2b. The "theore



(1982).

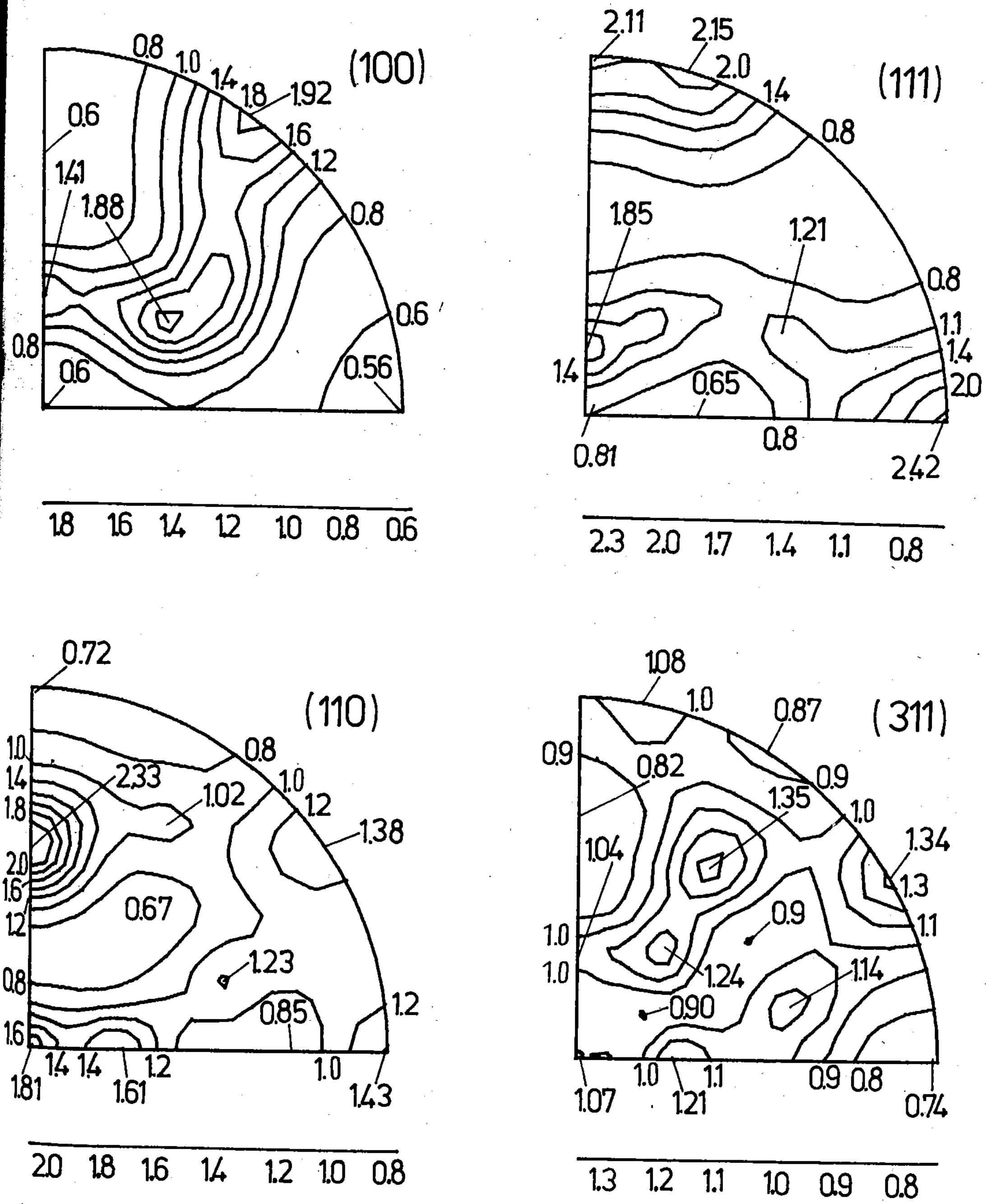


Fig. 2b. The "theoretical" pole figures derived from $f^M(g)$

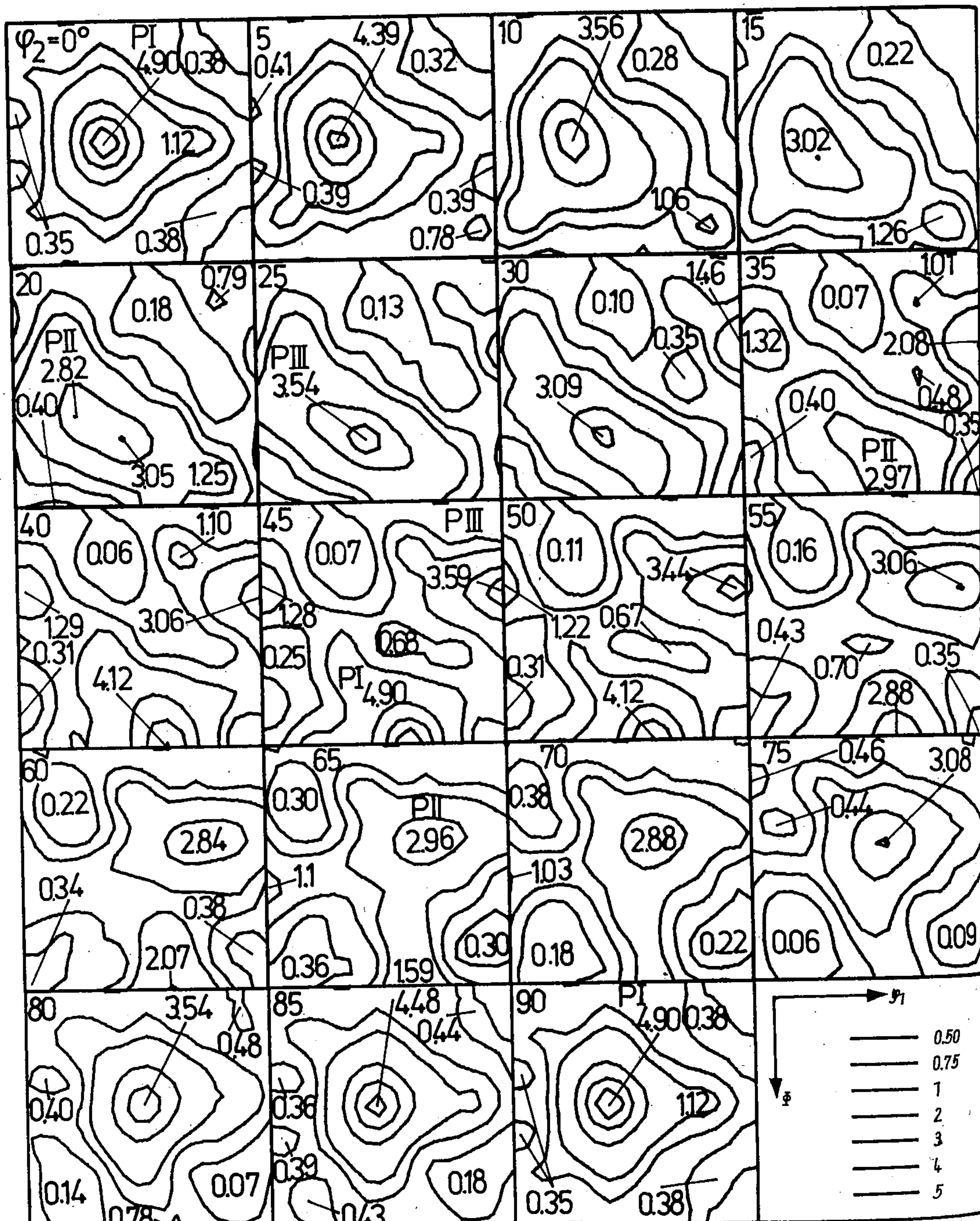


Fig. 3. The reduced ODF $\tilde{f}(g)$ containing ghost phenomena

/3/ S. MATTHIES, phys. stat. sol. (b) 112, 705 (1982).

(Received June 18, 1982)