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Effects of Terms with Odd *l* on the Surface Texture of Primary-Recrystallized Silicon-Iron Sheet

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A procedure is described for determining the linearly independent coefficients of the generalized spherical harmonic expansion (GSHE) of the crystallite orientation distribution (COD) for idealized textures with Gaussian spread functions. An attempt was made to synthesize an experimentally determined COD from such functions. Coefficients with l even and l odd were then determined from the aggregate of such functions, and the resultant GSHE of the COD was calculated. The approach used is similar to that employed by Pospiech and his co-workers.

INTRODUCTION

Methods for obtaining a generalized spherical harmonic expansion (GSHE) for the crystallite orientation distribution (COD) from spherical surface harmonic expansions (SSHE) of pole figures were first proposed by Bunge (1965) and by Roe (1965, 1966). These two methods are similar, differing principally with respect to normalization and the means of imposing cubic crystal symmetry. In both methods simultaneous linear equations relate coefficients of the GSHE of the COD to coefficients of the SSHE of pole figures.

The intensity diffracted from one side of a diffracting plane is in general equal to that diffracted from the opposite side of the same plane. This effect, known as Friedel's law (1913), assures that the measured pole figure is centrosymmetric, and that coefficients of the SSHE of the pole figure with odd l are zero. For this reason, it is not generally possible to determine coefficients with odd l of the GSHE of the COD directly from measured pole figure data. It had been tacitly assumed that such coefficients were identically zero.

Representation of the COD by idealized orientations with Gaussian "spread" functions was suggested by Bunge (1969), who also provided the requisite mathematical expression for obtaining coefficients of the GSHE of the COD for such functions. Bunge's suggestion was implemented by Pospiech and his co-workers (1973, 1978). In the course of this work, Pospiech observed the appearance of "ghost phenomena" present in the GSHE but not in the original spread functions. He suggested investigation of this problem to Matthies (1979), who demonstrated that ghost phenomena were the result of omission of terms with odd l in the GSHE. Lucke, Pospiech, Virnich and Jura (1981) used Gaussian spread functions to estimate coefficients of odd l terms for recrystallized aluminum and copper sheet. An alternative method for estimating such coefficients has been proposed by Bunge and Esling (1979). The present analysis is similar to that employed by Lucke *et al.* (1981), but uses Roe's formalism (1965, 1966) rather than that of Bunge (1965, 1969) used by those authors.

THEORETICAL DISCUSSION

We first require the augmented Jacobi Polynomials, Z_{lmn}, for odd l. Programs for calculation of these functions and the closely related P^l_{mn} have been published by Morris (1975) and by Pospiech and Jura (1975). In the present work, a modification of Pospiech and Jura's program was used to calculate these functions. In order to enforce cubic crystal symmetry for odd l, we follow the procedure used by Roe (1966) for even l, obtaining nontrivial solutions for $l = 9$, 13, 15, ---. The relations between linearly dependent and linearly independent W_{lmn} for odd l have been published by Morris (1982).

DETERMINATION OF W_{lmn} FOR IDEALIZED TEXTURES

If, from Roe (1966) Table I, we set $d_1 = 0.59761430$, ---, $d_7 = 0.81491514$, ---, $d_9 = 1.4423922$, ---, $d_{41} = 1.3774637$, and, from Morris (1982) Table I, $e_1 = -0.64168895$, ---, $e_{12} = 1.1297868$, ---, $e_{15} = -1.5862311$, $e_{21} = 1.3143848$, the GSHE of the COD has the form

$$w(\psi, \xi, \phi) = \frac{1}{8\pi^2} + W_{400}[Z_{400}(\xi) + 2\,d_1\,Z_{404}(\xi)\cos 4\phi] +$$

$$+ 2W_{420}\langle Z_{420}(\xi)\cos 2\psi + d_1\{[Z_{424}(-\xi) + Z_{424}(\xi)]\cos 2\psi \cos 4\phi +$$

$$+ [Z_{424}(-\xi) - Z_{424}(\xi)]\sin 2\psi \sin 4\phi\}\rangle + --- +$$

$$+ W_{23,22,4}\langle[Z_{23,22,4}(-\xi) + Z_{23,22,4}(\xi)]\cos 22\psi \cos 4\phi +$$

$$
\begin{aligned}
&+[Z_{23,22,4}(-\xi)-Z_{23,22,4}(\xi)]\sin 22\psi \sin 4\phi + e_{18}\{[Z_{23,22,8}(-\xi)+\\
&+Z_{23,22,8}(\xi)]\cos 22\psi \cos 8\phi + [Z_{23,22,8}(-\xi)-\\
&-Z_{23,22,8}(\xi)]\sin 22\psi \sin 8\phi\} + e_{19}\{[Z_{23,22,12}(-\xi)+\\
&+Z_{23,22,12}(\xi)]\cos 22\psi \cos 12\phi + [Z_{23,22,12}(-\xi)-\\
&-Z_{23,22,12}(\xi)]\sin 22\psi \sin 12\phi\} + e_{20}\{[Z_{23,22,16}(-\xi)+\\
&+Z_{23,22,16}(\xi)]\cos 22\psi \cos 16\phi + [Z_{23,22,16}(-\xi)-\\
&-Z_{23,22,16}(\xi)]\sin 22\psi \sin 16\phi\} + e_{21}\{[Z_{23,22,20}(-\xi)+\\
&+Z_{23,22,20}(\xi)]\cos 22\psi \cos 20\phi + [Z_{23,22,20}(-\xi)-\\
&-Z_{23,22,20}(\xi)]\sin 22\psi \sin 20\phi\}\rangle. \qquad (1)
\end{aligned}
$$

We now allow $w(\psi, \xi, \phi)$ to take on the character of a Dirac delta-function, centered about ψ_0, ξ_0, ϕ_0, i.e., w is allowed to become infinite at ψ_0, ξ_0, ϕ_0 and zero elsewhere, in a manner such that the integral of $w(\psi, \xi, \phi)\, d\psi\, d\xi\, d\phi$ is equal to unity if the integral includes the point ψ_0, ξ_0, ϕ_0, and to zero if it does not. We then multiply both sides of Eq. (1) by $[Z_{400}(\xi) + 2d_1 Z_{404}(\xi)\cos 4\phi]\, d\psi\, d\xi\, d\phi$ and integrate over $0 \leqslant \psi \leqslant 2\pi$, $-1 \leqslant \xi \leqslant 1$, $0 \leqslant \phi \leqslant 2\pi$. In this way we obtain

$$
Z_{400}(\xi_0) + 2d_1 Z_{404}(\xi_0)\cos 4\phi_0 = 4\pi^2 W_{400}(1 + 2d_1^2). \qquad (2)
$$

Similarly, multiplication of both sides of Eq. (1) by $\langle Z_{420}(\xi)\cos 2\psi + d_1 \{[Z_{424}(-\xi) + Z_{424}(\xi)]\cos 2\psi \cos 4\phi + [Z_{424}(-\xi) - Z_{424}(\xi)]\sin 2\psi \sin 4\phi\}\rangle\, d\psi\, d\xi\, d\phi$ and integration with respect to ψ, ξ, ϕ yields

$$
\begin{aligned}
&Z_{420}(\xi_0)\cos 2\psi_0 + d_1\{[Z_{424}(-\xi_0) + Z_{424}(\xi_0)]\cos 2\psi_0 \cos 4\phi_0 +\\
&\quad + [Z_{424}(-\xi_0) - Z_{424}(\xi_0)]\sin 2\psi_0 \sin 4\phi_0\} = 4\pi^2 (1 + 2d_1^2) W_{420}. \qquad (3)
\end{aligned}
$$

In like manner, we obtain

$$
\begin{aligned}
&[Z_{924}(-\xi_0) + Z_{924}(\xi_0)]\cos 2\psi_0 \cos 4\phi_0 + [Z_{924}(-\xi_0) - Z_{924}(\xi_0)]\\
&\quad \sin 2\psi_0 \sin 4\phi_0 + e_1\{[Z_{928}(-\xi_0) + Z_{928}(\xi_0)]\cos 2\psi_0 \cos 8\phi_0 +\\
&\qquad + [Z_{928}(-\xi_0) - Z_{928}(\xi_0)]\sin 2\psi_0 \sin 8\phi_0\} = 8\pi^2 (1 + e_1^2) W_{924} \qquad (4)
\end{aligned}
$$

In the method used by Roe (1966) to enforce cubic crystal symmetry, where, for specified l and m, more than one linearly independent W_{lmn} exists, the resulting symmetry generalized spherical harmonics are not orthogonal, e.g., $Z_{12,0,0}(\xi) + 2d_7 Z_{12,0,8}(\xi)\cos 8\phi + 2d_8 Z_{12,0,12}(\xi)\cos 12\phi$ and $Z_{12,0,4}(\xi)\cos 4\phi + d_9 Z_{12,0,8}(\xi)\cos 8\phi + d_{10} Z_{12,0,12}(\xi)\cos 12\phi$ are not orthogonal to one another. Multiplication of both sides of Eq. (1) by the first of these and integration with respect to ψ, ξ, ϕ yields

$$Z_{12,0,0}(\xi_0) + 2d_7\, Z_{12,0,8}(\xi_0)\cos 8\phi_0 + 2d_8\, Z_{12,0,12}(\xi_0)\cos 12\phi_0 =$$
$$= 4\pi^2 \left[W_{12,0,0}(1 + 2d_7^2 + 2d_8^2) + 2W_{12,0,4}(d_7 d_9 + d_8 d_{10})\right]. \quad (5)$$

Multiplication of both sides of Eq. (1) by the second expression and integration with respect to ψ, ξ, ϕ yields

$$Z_{12,0,4}(\xi_0)\cos 4\phi_0 + d_9\, Z_{12,0,8}(\xi_0)\cos 8\phi_0 +$$
$$+ d_{10}\, Z_{12,0,12}(\xi_0)\cos 12\phi_0 = 8\pi^2[W_{12,0,0}(d_7 d_9 + d_8 d_{10}) + W_{12,0,4}$$
$$(d_9^2 + d_{10}^2)]. \quad (6)$$

It is then necessary to solve Eqs. (5) and (6) in order to obtain $W_{12,0,0}$ and $W_{12,0,4}$.

SPREAD FUNCTIONS

Equations (2) to (6) indicate the procedure used to obtain the coefficients of the GSHE of the COD for idealized texture components, i.e., a single crystal in the orientation ψ_0, ξ_0, ϕ_0 and in crystallographically and physically equivalent orientations. Such textures are seldom encountered. Instead, it is common to encounter textures which can be described in terms of the location of maxima, and "spread" about the maxima. For this purpose, it is mathematically convenient to suppose that all orientations which result from the orientation corresponding to the maximum, by rotations through the same angle ω (about an arbitrary axis) are equally populated, and that this population decreases monotonically with increasing rotation. Functions which satisfy these criteria have been called "spread functions." Lucke *et al.* (1981) have used spread functions of the form

$$S(\omega) = S_0 \exp(-\omega^2/\omega_0^2). \quad (7)$$

According to Bunge (1969), this may be expanded in a Fourier series

$$S(\omega) = \sum_{n=-\infty}^{\infty} c_n e^{in\omega}, \quad (8)$$

where

$$c_n = \frac{S_0 \cdot \omega_0}{(4\pi)^{1/2}} e^{-n^2\omega_0^2/4} \quad (9)$$

In Bunge's notation, the coefficients of the symmetric GSHE of the COD for an ideal orientation, g_0, are given by

$$C_l^{\mu\nu} = (2l+1)\,\dot{\dot{T}}{}_l^{\mu\nu}(g_0) \quad (10)$$

For an ideal orientation with spread function, they are given by

$$C_l^{\mu\nu} = Z\ a_l\ \dot{\dot{T}}_l^{\mu\nu}(g_0), \tag{11}$$

where

$$a_l = c_l - c_{l+1} \tag{12}$$

That is,

$$C_l^{\mu\nu} \text{ spread} = \frac{Z\ a_l}{2l+1}\ C_l^{\mu\nu} \text{ ideal}. \tag{13}$$

In Roe's notation, this may be written

$$W_{lmn} \text{ spread} = \frac{Z\ a_l}{2l+1}\ W_{lmn} \text{ ideal}. \tag{14}$$

In Eqs. (11), (13) and(14), Z denotes the multiplicity of the texture, i.e., 96 for general (hkl) $[uvw]$ with no crystal symmetry operations.

DETERMINATION OF W_{lmn} WITH ODD l FOR AN EXPERIMENTALLY MEASURED TEXTURE

Methods for determination of the GSHE of the COD from incomplete pole figures have been published by Pospiech and Jura (1974), and by Morris (1975). In the present work the method of Morris was used to determine the linearly independent W_{lmn} for l even to $l = 22$. An Enraf-Nonius CAD-4 diffractometer, equipped with a sample oscillating device, was used to collect data for (110), (002) and (112) pole figures. The data collection net was composed of 1536 points ranging in colatitude angle from approximately 3.6° to 73.7°. For mathematical convenience and sampling efficiency, data points were chosen along parallels of latitude and longitude in such manner that the area of the pole sphere represented by each data point is constant. The steel specimen used in this work had the following chemical composition: 2.92 Si, 0.044 C, 0.031 Al, 0.0059 N, 0.096 Mn and 0.028 S. Processing was similar to that previously described by Flowers and Heckler (1976), including a single-stage cold reduction of 87% to 0.30 mm with no interpass aging, and a decarburization-recrystallization anneal at 830° C for 2 min.

The GSHE of the COD was first calculated on a 5° × 5° × 5° net of ψ, θ, ϕ from the set of 3 measured pole figures. A Guassian spread function was then fit to the largest maximum. (Only coefficients with l even were included in the fitting process). Coefficients of the GSHE of the spread function calculated according to Eqs. (2) and (6), (9), (12) and (14) were then accumulated in a file. The GSHE of the spread function was subtracted from

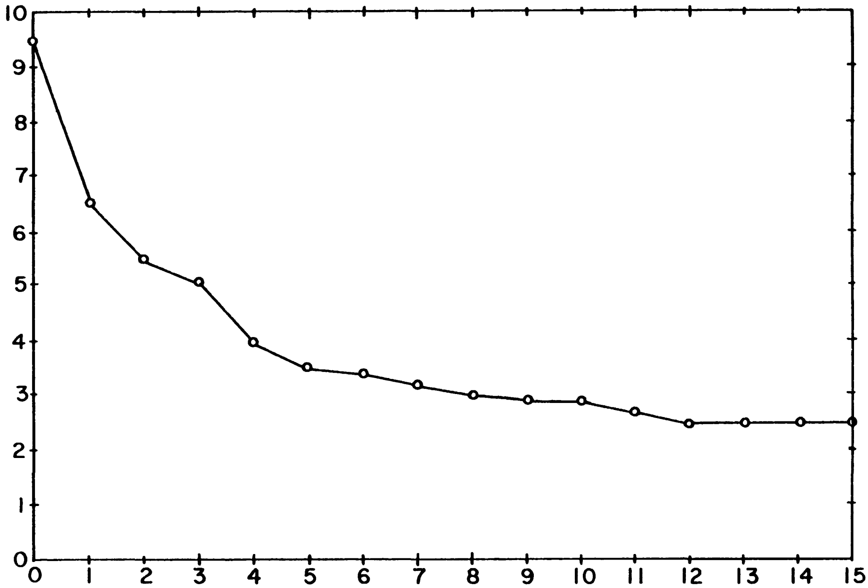

Figure 1 – |R| VERSUS PASS NUMBER

the original GSHE, and a second spread function fit to the largest remaining maximum. Coefficients of the second spread function were then added to those of the first. The absolute value of the maximum, |R|, after 0, 1, ---, 15 passes is shown in figure 1. This computational process was terminated after 15 passes.

At this time, the GSHE resulting from the sum of coefficients with l even and l odd of the 15 spread functions was calculated and examined for the largest negative value. A spread function was fit to this minimum and subtracted from the GSHE, the coefficients of this negative spread function being added to those from the previous 15 spread functions. (Both coefficients with l even and l odd were included in this fitting process). This process was terminated after 3 passes, at which point the largest remaining negative value was -0.3.

Constant ϕ sections of the GSHE of the COD determined from measured pole figures (containing only terms with even l to $l = 22$) are shown in Figure 2. Similar plots of the GSHE obtained from the coefficients of 18 spread functions (containing terms with even l and odd l to $l = 23$) are shown in Figure 3. The introduction of terms with odd l is accompanied by a dilemma, in that the results are not unique (Virnich *et al.*, 1978), and may be expected to depend upon the computation method. Figure 4 contains plots of measured pole figures and SSHE recalculated from the W_{lmn} obtained from the pole figures and from the Gaussian spread functions. While the distribution shown in Figure 3 is not unique, comparison of the third (Guass.) pole figure in Figure 4 with the measured and recalculated pole figures provides one assessment of the reasonableness of the distribution.

DISCUSSION OF RESULTS

The principal differences between Figures 2 and 3 consist of a "sharpening" of the texture (in which the maximum increases from 9.5 to 12.7) and a reduction in physically meaningless negative regions (enclosed by level zero contours). As noted by Lucke *et al.* (1981), the resultant distribution (Figure 3) is much "cleaner" than the original distribution (Figure 2). While the increase in the maximum due to inclusion of terms with odd *l* in the GSHE noted above is generally consistent with that reported by Lucke *et al.* (1981) (see their Figure 8b), any technique which entails fitting spread functions to certain features of the COD may be expected to enhance such features at the expense of those not considered in the fitting process.

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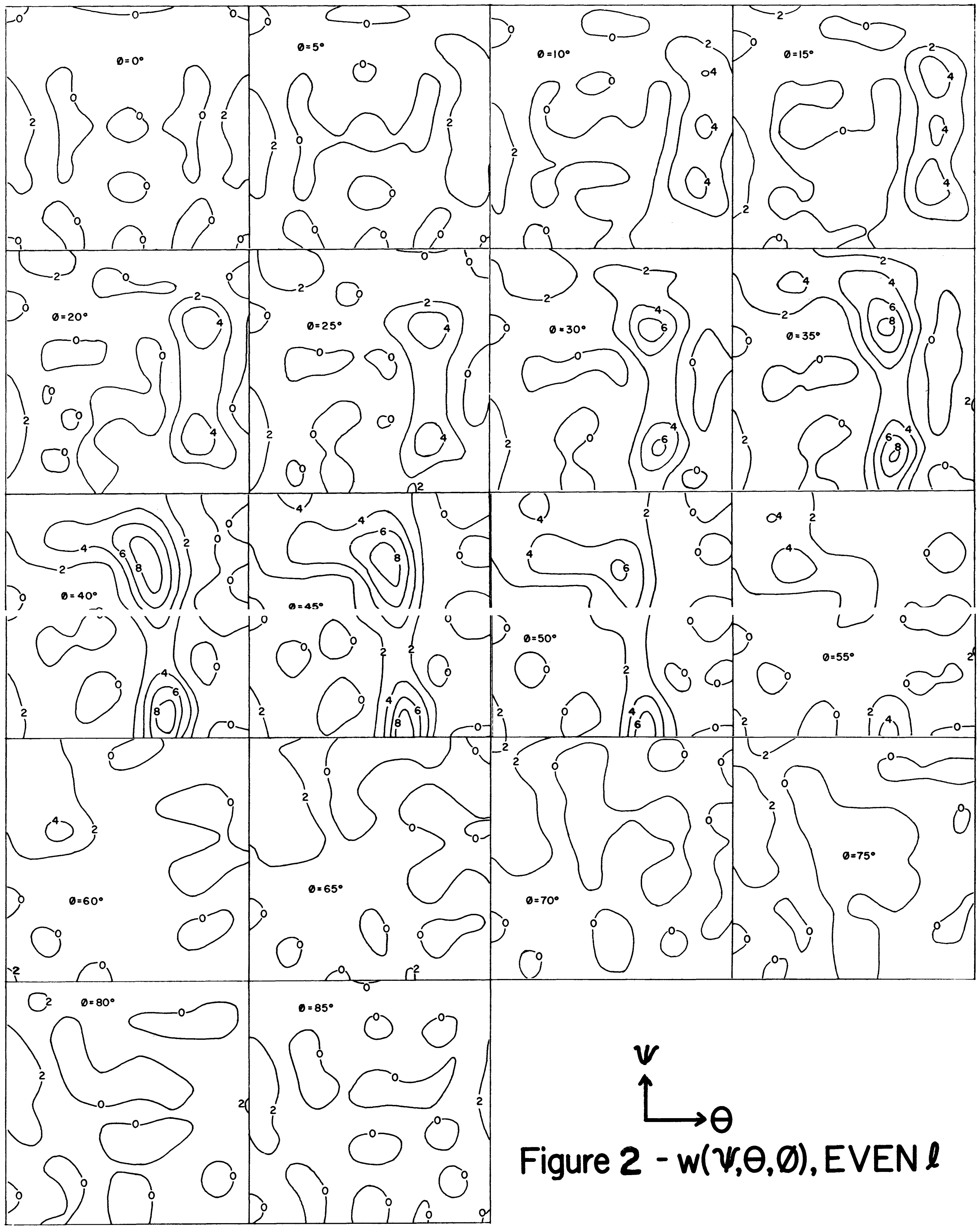

Figure 2 - w(ψ,θ,Ø), EVEN ℓ

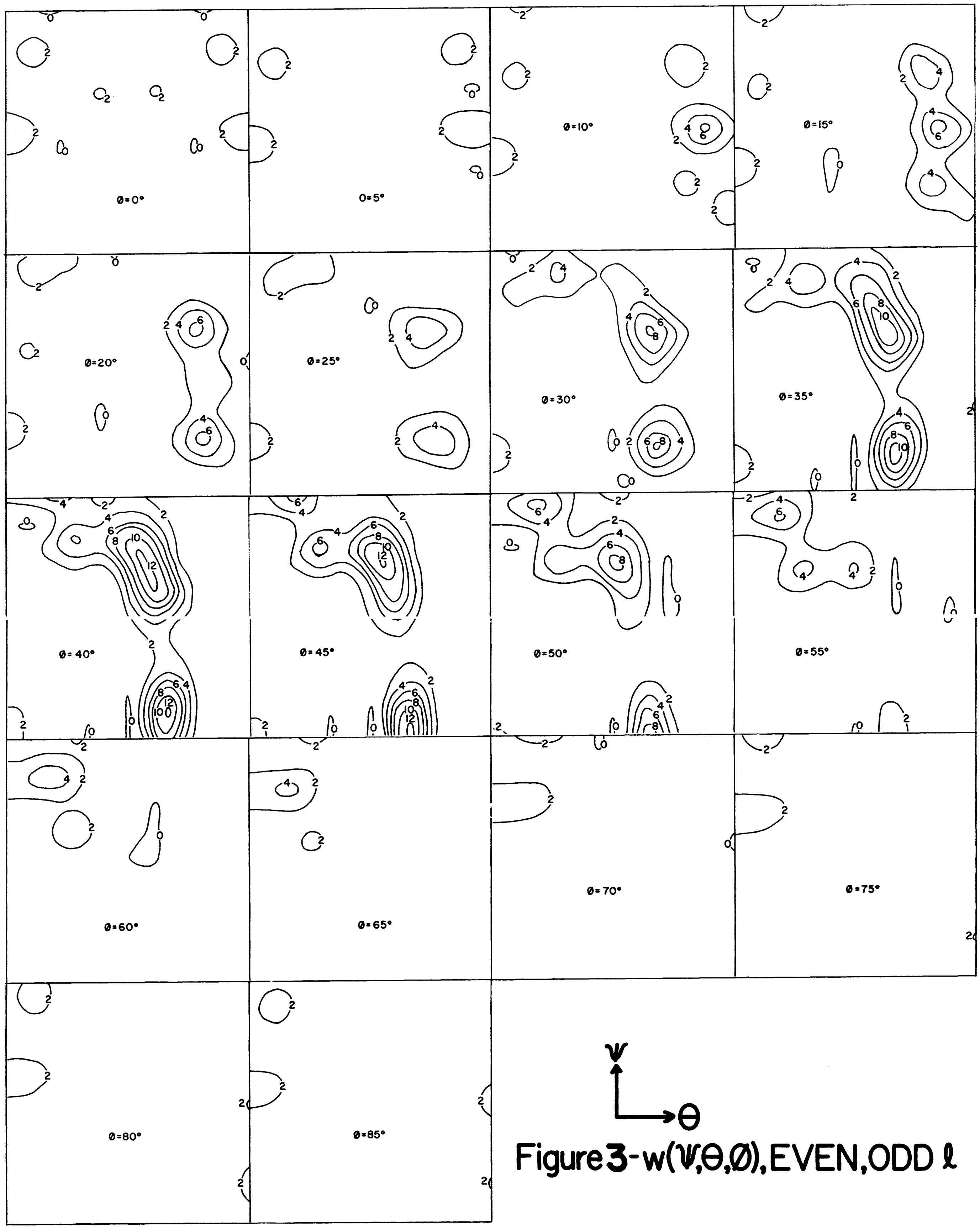

Figure 3 - w(ψ,θ,Ø), EVEN, ODD ℓ

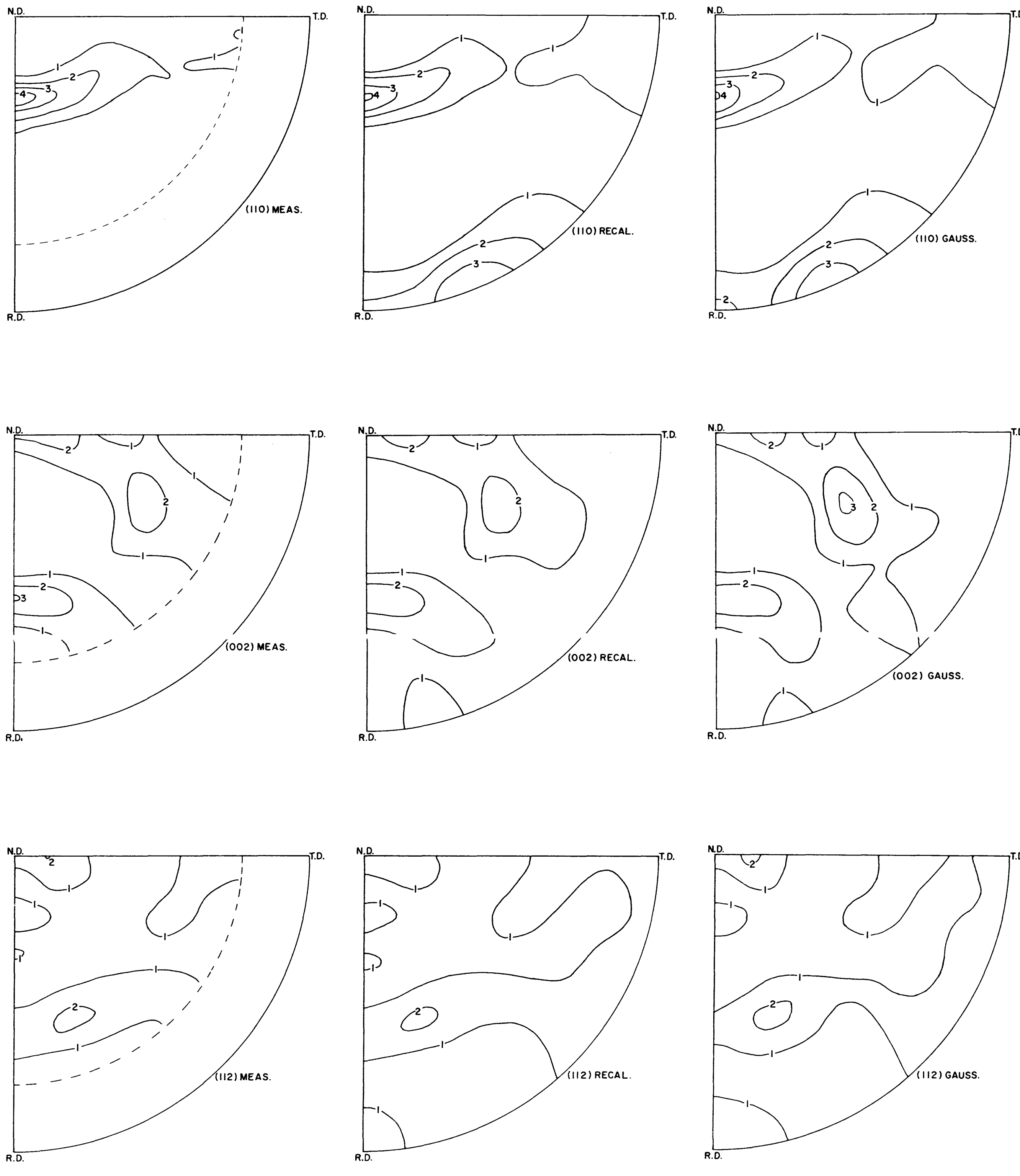

Figure 4 - MEAS., RECAL., GAUSS.
POLE FIGURES