JOURNAL OF MATERIALS SCIENCE 25 (1990) 2846–2850

Determination of the orientation distribution function from arbitrary pole figure regions

J. A. SZPUNAR, D. C. HINZ
Department of Metallurgical Engineering, McGill University, Montreal, Canada

A full pole figure is required to calculate the series expansion coefficients of the pole figure, by integration. The orientation distribution function (ODF) is then calculated by solving a system of linear equations relating the coefficients of the pole figures and those of the ODF. Using a method proposed by Bunge which does not require integration at all, but assuming a fit between the theoretical ODF and the isolated experimental points, we calculated the ODF from various arbitrary chosen regions of the pole figures. This technique was applied to analyse the experimental data obtained from the measurement of three, two and one pole figures. Various tests described in this paper allow us to suggest an empirical rule indicating that the number of experimental data points should be three times higher than the number of required series expansion coefficients of the ODF.

1. Introduction

Pole figures for various crystallographic planes $\{h\,k\,l\}$ provide a useful representation for the experimental texture data obtained from X-ray and neutron diffraction measurements. The X-ray methods commonly used in industrial research laboratories require two independent texture measurements, using the reflection and transmission techniques. Unification of the results of these two techniques always introduces a considerable error. Nevertheless full pole figures are required to calculate by integration the series expansion coefficients of the pole figures. Accordingly, for the calculation of the crystal orientation distribution function, (ODF) one can use a system of equations relating the coefficients of expansion of the pole figure and the ODF coefficients [1]. It has already been demonstrated by Morris [2] and also Jura and Pospiech [3], that the back reflection part of the pole figure alone can be used to determine the ODFs coefficients by integration over an angular interval of the pole figure. In this case, the orthogonality relations of the surface spherical harmonics will not hold and thus the solution of $C_l^{\mu\nu}$ results in a large system of equations containing all pole figure coefficients. The method therefore, offers a simpler experimental procedure at the expense of more complex computation. Bunge [4] has further relaxed the experimental requirements in response to the energy dispersive X-ray and neutron diffraction methods of ODF determination [5]. More than three pole figures are examined using this method allowing one to reduce the number of data points measured on each pole figure. However for a small number of points we would be unable to perform the integration with a sufficient accuracy. The procedure, therefore, suggested by Bunge does not require integration at all but requires a least squares fit between the theoretical ODF and the isolated experimental points as described by [4]

$$\sum_i \sum_j [P_{ij} N_j - P_j^{\mathrm{th}}] W_{ij} = \min \qquad (1)$$

where P_{ij} is measured at point i (having angular coordinates α, β) of the pole figure j, N_j is a normalizing factor used to express the pole density value in units corresponding to random density, and W_{ij} is a weight factor.

A theoretical pole figure is expressed by the following formula

$$P_{ij}^{\mathrm{th}} = 1 + \sum_{l=2}^{L} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} \frac{4\pi}{2l+1} C_l^{\mu\nu} \dot{k}_l^{\mu}(j) \dot{k}_l^{\nu}(i, j) \qquad (2)$$

where $C_l^{\mu\nu}$ are the series expansion coefficients of the ODF and $\dot{k}_l^{\mu}(j)$ and $\dot{k}_l^{\nu}(i, j)$ are the surface spherical harmonics invariant with respect to crystal and specimen symmetry. Minimization of Equation 1 is carried out with respect to variables N_j and $C_l^{\mu\nu}$ and yields previously presented relations [4].

2. Application of the method

Using the presented theoretical method, we have freedom in selecting the experimental points in pole figure orientation space; however, such selection will affect the accuracy of the obtained results.

In order to test the method we will compare the ODF results obtained using three complete pole figures with the ODF obtained using the partial pole figures. This comparison will be based on three parameters: (1) the number of data points, (2) the measured area of the pole figure and, (3) the maximum value of the series expansion number. The texture of Fe–Si transformer steel will be analysed restricting gradually the amount of data available for ODF calculation.

Accordingly, the ODF is calculated at first from three full pole figures, each having 200 data points

0022-2461/90 $03.00 + .12

TABLE I The normalization constants N_{hkl} calculated from pole figures

$l_{\max}$	Number of points	N_{200}	N_{110}	N_{112}
Calculated using three complete pole figures				
12	3 × 100	0.725	0.855	0.848
16	3 × 100	0.849	0.933	0.922
20	3 × 100	0.953	0.998	0.974
22	3 × 100	0.988	1.017	0.990
20	3 × 200	0.898	0.848	0.848
22	3 × 200	0.956	0.956	0.956
Calculated using data obtained from the reflection technique $\alpha_{\max} = 40°$				
8	3 × 37	0.534	0.783	0.767
10	3 × 37	0.611	0.813	0.817
12	3 × 37	0.850	0.948	0.911
14	3 × 37	0.938	0.950	0.938
Calculated using data obtained from the reflection technique $\alpha_{\max} = 50°$				
8	3 × 39	0.404	0.627	0.729
10	3 × 39	0.466	0.679	0.753
12	3 × 39	0.680	0.866	0.873
14	3 × 39	0.712	0.902	0.911
16	3 × 39	0.947	0.994	0.964
Calculated using data obtained from the transmission technique only $\alpha(60–90)°$				
8	3 × 40	0.451	0.697	0.657
10	3 × 40	0.607	0.736	0.778
12	3 × 40	0.835	0.862	0.910
14	3 × 40	0.865	0.891	0.954
16	3 × 40	0.956	0.952	0.987
18	3 × 40	0.962	0.971	0.995
Calculated using data obtained from the angular interval $\alpha(0–90)°$, $\beta(0–45)°$				
8	3 × 37	0.422	0.621	0.720
10	3 × 37	0.583	0.660	0.808
12	3 × 37	0.839	0.860	0.911
14	3 × 37	0.877	0.872	0.927

selected at equal angular intervals. Calculations are carried out for various orders of series expansion coefficients giving the normalization constants listed in Table I. The {2 0 0} pole figure obtained from the $C_l^{\mu\nu}$ coefficients having l less than 22 is presented in Fig. 1; it compares favourably with the experimental pole figure. Differences are observed only between values calculated for various $l_{\max}$. The smaller calculated N_j for lower the $l_{\max}$ is an indication that the calculated series expansion underestimates the existing texture maxima. This fact is also illustrated by a decrease in the amplitude of the $C_l^{\mu\nu}$ coefficients (see Table II).

The results obtained for 3 × 200 points were also calculated using one normalization constant. There is only a small difference between the value of one normalization constant and value of constants obtained for different pole figures. This is justified, because the experimental pole figures used in this calculation, were already normalized and the density of poles was expressed in multiples of random units (where the random unit characterizes the specimen without texture). In conclusion we observe that direct fitting of theoretical ODF to available experimental points is an accurate and reliable method of ODF calculation.

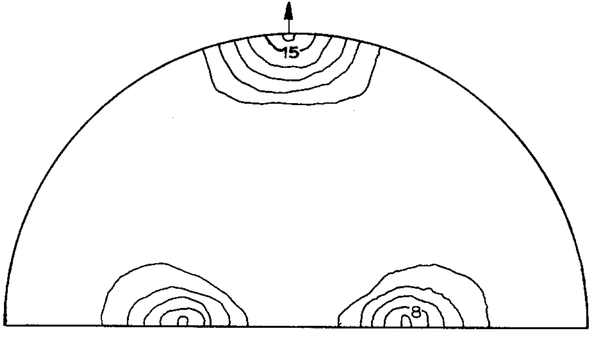

Figure 1 {2 0 0} pole figure calculated from the ODF (experimental data from three pole figures were used).

We will now describe another test where the results were obtained using the reflection part of the pole figure only. Three pole figures are used in this calculation with 37 points on each pole figure. The experimental data are taken from the angular interval $0° < \alpha < 40°$ (where α is an angle between the crystallographic plane normal and the normal to the sheet surface).

In another example (Table I) the maximum value of $\alpha = 50°$ is used. Both these examples demonstrate that a minimum of $l_{\max} = 14$ is usually needed for a realistic description of the ODF. For $l_{\max}$ lower than 14, the normalization constant N is low, and therefore the sharpness of texture is underestimated. The required value of $l_{\max}$, depends not only on the complexity of texture but also on the research problem which is studied. Studies of the texture related anisotropy of properties [1], usually require only a few texture series expansion coefficients. These coefficients can be, however, considerably changed if the chosen value of $l_{\max}$ is too low.

TABLE II Series expansion coefficients of the ODF calculated from various parts of the pole figures

$l_{\max}$	No. of normalization constants	No. of points	Area $\alpha(\alpha_1 - \alpha_2)$ $\beta(\beta_1 - \beta_2)$	C_4^{11}	C_4^{12}	C_4^{13}	C_6^{11}	C_6^{12}	C_6^{13}	C_6^{14}
22	3	3 × 200	0–90 0–90	0.055	−6.132	3.580	−5.600	2.062	2.618	3.679
16	3	3 × 100	0–90 0–90	−0.065	−5.425	3.083	−5.097	1.819	2.35	3.257
12	3	3 × 100	0–90 0–90	−1.04	−4.735	2.662	−4.628	1.586	2.099	2.899
22	1	3 × 200	0–90 0–90	0.183	−6.037	3.469	−5.354	1.778	2.522	3.491
14	3	3 × 37	0–90 0–45	0.092	−5.561	3.458	−4.456	2.272	2.367	3.264
16	3	3 × 37	0–90 0–45	0.140	−5.965	3.641	−5.178	2.192	2.462	3.378
12	3	3 × 12 + 1	0–40 0–80	−0.165	−5.673	3.573	−5.081	1.941	2.257	3.848
12	3		0–50 0–90	0.252	−4.418	2.471	−4.869	1.522	1.845	4.866
14	3	3 × 12 + 1	0–50 0–90	0.168	−4.691	1.373	−4.949	1.745	2.144	6.0
16	3	3 + 12 + 1	0–50 0–90	0.006	−5.908	3.076	−5.558	1.869	2.603	3.591
12	3	3 × 40	60–90 0–90	−0.744	−5.482	3.039	−5.482	1.549	1.949	3.095
16	3	3 × 40	60–90 0–90	−0.217	−5.979	3.446	−5.788	1.942	2.873	3.432
22	Polyn. fitting	3 × 400	0–90 0–90	0.08	−6.186	3.612	−4.171	2.055	2.604	3.663

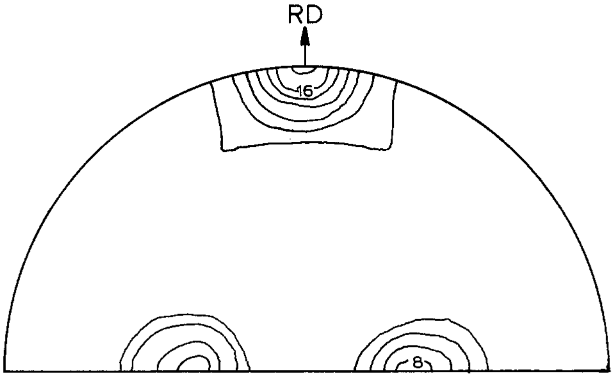

Figure 2 {2 0 0} pole figure. The expansion $C_l^{\mu\nu}$ coefficients calculated from transmission part (60° < α < 90°) of the three pole figures.

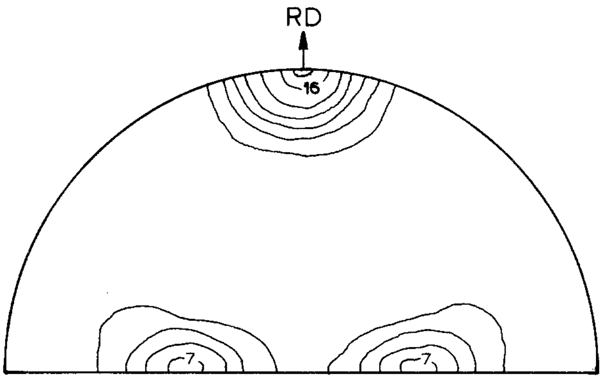

Figure 3 {2 0 0} pole figure. The $C_l^{\mu\nu}$ calculated from a part of the pole figure α(0–90)°, β(0–45)°.

Having discussed the results of calculation obtained using reflection only we will proceed to calculations of the ODF from transmission type data only. Normally the results obtained using the transmission techniques are limited to thin specimens. Transmission data are on the peripheral part of the pole figure and this technique is used together with the reflection technique to obtain the full pole figure. It has not been used alone to determine the ODF. The results obtained in this work show that the transmission technique can provide reliable series expansion coefficients of the ODF.

The normalization constants listed in Table I demonstrate that for a low number of experimental data (forty points on each pole figure) reliable texture coeffients for values of $l_{\max}$ between 12 and 18 can be obtained. The pole figure calculated from the series expansion coefficients of the ODF is presented in Fig. 2.

The method of calculation of the ODF used here can be applied to any experimental data. The data can be, for example, chosen in a triangle of the pole figure i.e. α(0, 90) and β(45, 90). The total number of the experimental points is 3 × 37. Calculated normalization factors for various $l_{\max}$ are displayed in Table I and the series expansion coefficients are listed in Table II. Even such limited experimental data give us reliable values for series expansion coefficients up to $l_{\max}$ 12 and 14. The {2 0 0} pole figure calculated from the coefficients of C (Fig. 3) displays the same maxima as the figure calculated from three complete pole figures.

In the next test the number of pole figures used in calculation will be further limited to two. The ODF calculated from two pole figures, with 100 points each and $l_{\max} = 14$ is in good agreement with the ODF calculated using three pole figures. Various combinations of pole figures were tested (results shown in Table III) and the best agreement with the results obtained using three pole figures was obtained for {1 1 0} and {1 1 2} pole figures.

As a next step in verification of this method, the ODF was calculated only from one pole figure. Some exemplary results of these calculations are listed in Table IV. The values for $C_l^{\mu\nu}$ are satisfactory for low l value, but for $l = 12$ and 14 high values of the $C_l^{\mu\nu}$ were registered indicating the instability of the solution.

TABLE III The coefficients of C calculated from two pole figures

$l_{\max}$	Pole figures	Normalization coefficients	Coefficients						
			C_4^{11}	C_4^{12}	C_4^{13}	C_6^{11}	C_6^{12}	C_6^{13}	C_6^{14}
14	2 0 0 1 1 0	0.712 0.834	−0.147	−4.583	2.588	−4.433	1.569	2.059	2.822
14	2 0 0 1 1 2	0.746 0.882	−0.132	−4.824	2.727	−4.874	1.470	2.082	2.725
14	1 1 0 1 1 2	0.906 0.933	0.641	−5.665	3.686	−5.041	1.846	2.278	3.165

TABLE IV The coefficients of C calculated from one pole figure

$l_{\max}$	Pole figures	Normalization coefficients	Coefficients						
			C_4^{11}	C_4^{12}	C_4^{13}	C_6^{11}	C_6^{12}	C_6^{13}	C_6^{14}
10	2 0 0	0.425	−0.121	−4.357	2.380	−4.050	1.206	1.633	2.400
10	1 1 0	0.743	0.095	−5.124	3.227	−4.339	1.267	1.986	2.751
10	1 1 2	0.873	−0.378	−5.401	3.223	−4.627	1.887	2.253	3.110
12	2 0 0	0.648	−0.138	−4.218	2.288	−4.097	1.180	1.587	2.374
12	1 1 0	0.907	0.478	−5.821	3.513	−5.130	1.762	2.361	3.284
12	1 1 2	0.925	0.010	−5.921	3.421	−5.333	2.144	2.295	3.178
14	2 0 0	0.673	−0.121	−4.357	2.380	−4.050	1.206	1.633	2.400
14	1 1 0	0.919	0.437	−5.730	3.562	−5.193	1.851	2.382	3.306
14	1 1 2	0.955	0.024	−6.007	3.518	−5.697	2.186	2.413	3.456

5. Conclusions

The method used in our analysis can be applied to any experimental data registered in the pole figure or in the inverse pole figure. The normalization constants which are normally associated with measurements of the different diffraction maxima are treated as variables in our calculations. The number of significant experimental data points is a variable which determines how many expansion coefficients can be reliably calculated. The accuracy of the calculation depends, however, on other factors such as the type and sharpness of the measured texture. From various tests performed here we may suggest only an empirical rule which states that the number of experimental data points should exceed three times the number of the coefficients to be calculated.

References

1. H. J. BUNGE, "Texture Analysis in Materials Science", (Butterworths, London, 1982).
2. P. R. MORRIS, *Adv. X-ray Anal.* **18** (1975) 514.
3. J. POSPIECH and J. JURA, *Z. Metallkde* **65** (1974) 324.
4. H. J. BUNGE, *Texture of Crystalline Solids* **2** (1977) 169.
5. J. A. SZPUNAR, *Atomic Energy Rev.* **142** (1976) 199.

Received 14 December 1988
and accepted 23 August 1989