Comparison of several methods for the reproduction of the orientation distribution function from pole figures in medium to strong textured materials

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Abstract. A quantitative comparison of the errors introduced by several methods for the reproduction of the crystallographic orientation distribution function from poles figures is presented. The harmonic, ADC, WIMV and component methods have been employed in the characterization of the deformation and recrystallization textures of a Fe-50% Ni alloy in order to investigate the accuracy associated with each one of these methods. To carry out this study, experimental and synthetic pole figures have been used as input data. The strong and weak points of each method are examined showing that the iterative discrete methods (ADC and WIMV) are better suited for the reproduction of the texture function in the present case. In comparing these two discrete methods, it is evidenced that the ADC method reproduces more accurately both the experimental and synthetic texture functions over the entire range of texture sharpness considered.

PACS. 81.40.Ef Cold working, work hardening; annealing, post-deformation annealing, quenching, tempering recovery, and crystallization

1 Introduction

Crystallographic textures weight the anisotropy of many physical properties of polycrystalline materials [1, 2]. They are strongly modified by metallurgical processes such as phase transformation, deformation, recovery and recrystallization [3]. In most cases, a quantitative characterization of the texture developed by the material is carried out during these processes in order to control a given physical property. In the Fe-36% Ni (Invar) alloy, for example, the strong {001}⟨100⟩ cube texture commonly present after large strain and primary recrystallization, leads to highly rectangular hysteresis loops (a property required for magnetic amplifiers making) and greatly contributes to produce regular and equally shaped holes during the “chemical machining” of shadow masks for color television tubes [4].

The crystallographic texture of a material is completely described by the crystallite orientation distribution function (ODF) $f(g)$ [1]. This function is generally determined from X-rays or neutron diffraction pole figures (PFs). The two-dimensional PFs are connected with

the three-dimensional ODF by an integral equation [1]:

$$P_h(y) = \frac{1}{2\pi} \int_{\pm h \parallel y} f(g) d\gamma. \quad (1)$$

Accordingly, the pole density $P_h(y)$ of the diffracting planes $\pm h$ in the direction y of the sample coordinate reference system is given by the normalized sum of the texture function ODF, *i.e.* $f(g)$, along a projection path defined by all those orientations g for which $\pm h \parallel y$ [5]. This path corresponds to a rotation of 2π about the axis $\pm h \parallel y$, the angle γ being the integration parameter.

At present, the reproduction of the ODF from PFs can be achieved by several mathematical methods which, according to the approach used to solve equation (1), can be grouped into the following three categories: (i) continuous (or harmonic) methods [1, 6–9], (ii) discrete (or direct) methods [10–21], and (iii) component methods [22–30]. Comparative analysis of the errors associated with practical implementations of the above mentioned methods have been carried out (in most cases by their creators) on textures with weak to moderate sharpness [31–34]. However, the errors introduced by these methods in the reproduction of the texture function, as well as the benefits or shortcomings resulting from their use, remain somewhat

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unexplored for various texture types and texture sharpness ranges.

In this study, practical implementations of the harmonic method [9], the arbitrary defined cell method (ADC) [17], the Williams-Imhof-Matthies-Vinel method (WIMV) [15] and the component method [27] are employed to characterize the texture of a cold rolled and a partially recrystallized Fe-50% Ni alloy which show deformation and recrystallization textures very similar to those of the Invar alloy [3]. To carry out this investigation, experimental PFs determined by neutron diffraction are used as input data to reproduce the ODFs of these samples and the errors introduced by the compared methods are computed. In order to extend the comparison to a wider range of texture sharpness, synthetic PFs are created and used for the calculation of the corresponding ODFs. The performance of the four mentioned methods is assessed and several aspects concerning the benefits and shortcomings of each method are emphasized.

It should be mentioned that the aim of this work is to test the validity, advantages and drawbacks of these ODF reproduction methods in the characterization of the rolling and recrystallization textures of materials with medium-to-high stacking fault energy, *e.g.* the Fe-Ni alloys. This study has neither the purpose of comparing in details the physical and mathematical foundations of these methods, nor to explore the domains of applications of each one of them for different crystal symmetries or other texture types.

2 ODF calculation principles

In normal diffraction experiments, the crystallographic directions $+h$ and $-h$ are indistinguishable because of the centrosymmetry of crystals or the additional inversion center induced in the PFs according to the Friedel law [7,35,36]. As a result, the “complete” or “true” ODF $f(g)$ can be decomposed into a sum of two components: $f(g) = \tilde{f}(g) + \tilde{\tilde{f}}(g)$. In this expression, $\tilde{f}(g)$ represents the part of the ODF which is directly determinable from the experimental PFs (called “reduced” ODF), whereas $\tilde{\tilde{f}}(g)$ denotes the non directly determinable part of the ODF. This latter part is mapped onto zero in the experimental PFs because it corresponds to the kernel of the operator that projects the three-dimensional ODF into the two-dimensional PFs [31,36]. In addition, the errors caused by the experimental conditions (*e.g.* the finite number of available PFs and systematic and statistical errors) and by the mathematical process used (*e.g.* truncation, ambiguity and integration errors) are also responsible for the non determination of the true (error free) texture function [1,26].

All mathematical methods intended for the reproduction of the ODF from PFs must provide, in principle, the same reduced ODF [31]. In each method, however, the feasible approximation to the true ODF is directly related to the mathematical approach used to solve equation (1) by taking into account the positivity condition $f(g) \geq 0$ [1].

2.1 The harmonic method

In the so called conventional or Bunge-Roe harmonic method, the texture function $f(g)$ is represented by a series of generalized spherical harmonics functions $T_\ell^{mn}(g)$ with coefficients C_ℓ^{mn} [1]:

$$f(g) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} C_\ell^{mn} T_\ell^{mn}(g). \quad (2)$$

Similarly, the PFs are expressed by continuous functions and expanded as a series of surface spherical harmonics whose coefficients are mathematically related to those of the ODF through equation (1). The coefficients C_ℓ^{mn} can be obtained by solving a least squares problem as has been described elsewhere [1,6,7]. In practice, for a given crystal symmetry, the texture function $f(g)$ is expanded up to a finite order $\ell_{\max}$ based on the number of available PFs. The errors connected with the reproduction of $f(g)$ are estimated through the TRC parameter which is defined (for the i th-PF) according to [8,9,37]:

$$TRC_i = 100(\%) \sqrt{\frac{\int [P_i^{\text{exp}}(y) - P_i^{\text{cal}}(y)]^2 dy}{\int [P_i^{\text{exp}}(y)]^2 dy}} \quad (3)$$

where $P_i^{\text{exp}}(y)$ and $P_i^{\text{cal}}(y)$ are, respectively, the experimental and calculated pole densities in the direction y of the i th-PF. The integration in equation (3) is performed over the complete hemisphere of the PF.

As a result of the physical impossibility to access to the true ODF from normal X-ray or neutron diffraction experiments, only the even ($\ell = 0, 2, 4, \dots$) C_ℓ^{mn} coefficients can be directly determined in the framework of the harmonic method so that, only the reduced ODF $\tilde{f}(g)$ can be unambiguously calculated in this case. Furthermore, this indetermination leads to physically impossible fluctuations in the ODF which are texture dependent and include both negative values and wrong maxima commonly known as “ghosts” [5,15,26].

Once the reduced ODF has been determined by the conventional harmonic method, the complete texture function can be approximated by imposing the only general physical constraint associated with this probability density function, namely, the positivity condition $f(g) \geq 0$. Nowadays, several approaches are available to impose the positivity condition in the series expansion method, *e.g.* the zero-range method [35,36], the use of model functions [22–26], the quadratic and exponential methods [38,39] and the generalized positivity method [40,41]. The present work deals with the conventional harmonic method only.

2.2 Discrete methods

In reproducing the ODF from PFs, the discrete methods divide both the orientation space and the hemisphere of

the PFs in discrete elements. A discrete form of equation (1) is then obtained [42,43]:

$$P_k = \sum_j Q_{jk} f_j \quad (4)$$

where P_k represents the pole density at the k th point (with area Δy_k) in the discrete hemisphere of the PF, f_j is the ODF value assigned to the j th cell (with volume Δg_j) in the discretized orientation space, and Q_{jk} represents a projection matrix whose elements are defined by the geometry of the interception of the ODF cells with the integration paths defined by equation (1). Relation (4) represents a system of equations which is solved for f_j not directly but by iteration.

At present, the WIMV, the ADC and the Vector (not included in this study) methods are the most widely employed discrete methods for the reproduction of the texture function from experimental PFs. The approximation to the true ODF is achieved in these methods by iteration, according to mathematical algorithms that have been described elsewhere [12–18,33]. In these algorithms, the positivity condition, the assumption that random PFs correspond to a random ODF, and the fact that any zero domain in the PFs leads to zeros in all corresponding ODF cells, are directly taken into account during the iteration process [33,42,43]. Accordingly, the interval of ambiguity in the approximation of the true ODF can be greatly reduced.

Both the WIMV and the ADC methods are based on the iterative procedures early developed by Williams and Imhof [10,14]. Nevertheless, important differences exist between these two methods. The WIMV method uses projection lines along which the cells of the discrete ODF contribute to the discrete hemisphere of the PF according to the length of the projection line within each ODF cell. The ADC, by contrast, use projection tubes which are adjusted according to the area of the discrete cells in the PF and cover more uniformly the orientation space. In this latter method, the contribution of the cells intercepted in the discrete ODF to the discrete hemisphere of the PF is proportional to the volume occupied by the projection tubes in these cells. The differences between the mathematical algorithms used by the WIMV and ADC methods have been explained elsewhere [33,43].

The convergence of the iteration process is mainly controlled in both methods (with some minor variations, see [16–18]) by means of the $RP\alpha$ parameters, with $0 \leq \alpha \leq P_{\max}^{\exp}$. For the i th-PF, the $RP\alpha_i$ are defined as [32,34]:

$$RP\alpha_i = 100(\%) \frac{1}{NY} \sum_{k=1}^{NY} \left[\frac{P_{ki}^{\exp} - P_{ki}^{\text{cal}}}{P_{ki}^{\exp}} \right] \text{ for all } P_{ki}^{\exp} > \alpha \quad (5)$$

where NY is the number of points in the discrete hemisphere of the i th-PF, and $P_{ki}^{\exp}$ and P_{ki}^{cal} are the experimental and calculated pole densities at the k th point of the i th-PF, respectively.

2.3 The component method

In the component method developed by Helming and coworkers [27,30], the ODF is approximated by the superimposition of NC Gauss-type scattering functions. Each model function represents a texture component $F^c = I^c f(g^c, b^c)$ characterized by the volume fraction I^c of all crystallites with orientation within the spread b^c , called the half-width of the component hereafter, around the ideal orientation g^c

$$f(g) = F^0 + \sum_{c=1}^{NC} I^c f(g^c, b^c) \quad (6)$$

where $F^0 + \sum I^c = 1$ and F^0 represents the volume fraction of all randomly oriented crystallites.

In this method, the ODF is approximated by introducing several components according to the distribution of intensities in the measured PFs. Then, the best fit of the experimental PFs to those calculated from the component model is searched. The parameters I^c , g^c , and b^c of each component are determined by solving a non-linear algorithm as has been described elsewhere [27–30]. The quality of the fit procedure is controlled using the so-called difference PFs ($P_{ki}^{\exp} - P_{ki}^{\text{cal}}$) and the $RP0$ parameter.

Obviously, the component description allows to reduce the amount of information required to describe a given texture. The components resulting from the fitting process can be used to obtain a version of the ODF in Euler space if they are used as input data for the program FF-SGL33 [26], which enables to calculate both the reduced $\tilde{f}(g)$ and the complete $f(g)$ texture functions from the model components.

3 Experimental techniques

Experimental and synthetic complete PFs have been used as input data for comparing the ODF reproduction methods under consideration. The texture of a commercial 90% cold rolled Fe-50% Ni sample and of a partially recrystallized sample of this material (recrystallized fraction close to 50%) was determined by measuring four complete PFs by neutron diffraction. The $\{111\}$, $\{200\}$, $\{220\}$ and $\{311\}$ PFs were measured in steps of 2.5° (for the azimuthal and polar coordinates) using the 6T1 texture goniometer at the Léon Brillouin Laboratory, CEA-CNRS ($\lambda = 0.1159$ nm, (111) Cu monochromator). The measured PFs were corrected for background effects, normalized, and finally interpolated to a 5° grid (the resolution commonly used for input PFs in quantitative texture analysis).

From these data, the ODFs of the two investigated samples were determined in steps of 5° in Euler space. No assumption was made about the statistical (sample) symmetry of the texture. Thus, the ODFs were treated in the cubic-triclinic domain ($0 \leq \varphi_1 < 2\pi, 0 \leq \phi < \pi/2$, and $0 \leq \varphi_2 < \pi/2$) of Euler space. The ODFs were reproduced from the experimental PFs by employing: (i) the

Table 1. The results of the application of the component method for determining the texture of the cold rolled and partially recrystallized Fe-50%Ni samples.

Component	Euler angles ($^{\circ}$) ($\varphi 1, \phi, \varphi 2$) ^a	Volume fraction (%)		Component half-width ^b ($^{\circ}$)	
		Sample		Sample	
		Cold rolled	P. Recrystall.	Cold rolled	P. Recrystall.
Cube (W)	{0, 0, 0}	1.5	28.5	11	7
Cube Twin (WT)	{45, 70, 45}	---	13.2	----	13
Rotate Cube (WR)	{0, 21, 0}	5.1	6.4	18	14
Copper (C)	{90, 35, 45}	17.5	6.5	10	12
Brass (B)	{35, 45, 0}	18.7	7.3	10	7
Aluminum (S)	{59, 37, 63}	43.9	20.2	10	12
Random (RAN) ^c	-----	13.3	17.9	----	-----

^a In {hkl}<uvw> notation: W = {001}<100>; WT = {221}<122>; WR = {025}<100>; C = {112}<111>; B = {011}<211> and S = {123}<634>.

^b Average values calculated by taking into account all the components included in the class.

^c Includes the non classified components and the true isotropic component.

Table 2. Description of the experimental texture components used to create the synthetic texture functions.

Experimental components		Classified as	Distance ($^{\circ}$) ^a	V. fraction (%)	Half-width ($^{\circ}$) ^b
No.	($\varphi 1, \phi, \varphi 2$) ($^{\circ}$)				
1	(0, 0, 0)	W	0	2	5 - 35
2	(36, 44, 87)	B	3.1	18	idem
3	(83, 32, 49)	C	5	21	idem
4	(47, 38, 74)	S	7.4	35	idem
5	Random ^c	RAN	----	24	-----

^a Angular distance between the experimental component and the ideal orientation used to define the corresponding orientation class (see Tab. 1).

^b The half-width of the components were set to be 5°, 6°, 7°, 8°, 10°, 12°, 15°, 18°, 25° and 35° to obtain synthetic ODFs with texture indices of 51, 39, 26, 19, 12, 8, 5, 4, 2 and 1, respectively.

^c Includes the non classified components and the true isotropic component.

harmonic method with $\ell_{\max} = 34$, (ii) the ADC method implemented in the TEXTURES software package, and (iii) the WIMV method implemented in the BearTEX software package [44].

The component method implemented in the MULTEX software package [30] was also used with these experimental PFs in order to estimate the principal components of the texture of the cold rolled and partially recrystallized samples. In this case, the orthorhombic statistical symmetry observed in the experimental PFs was rigorously imposed in order to simplify the calculations.

The principal texture components (see Tabs. 1 and 2) frequently found in cold rolled and annealed *fcc* materials with medium-to-high stacking fault energy [45], were used to classify the texture components found in both samples by means of the component method. The angular distance between the ideal and experimentally determined orientations was used as the classification parameter. Next, the corresponding ODFs were approximated from these components using the FFSGL33 program.

Synthetic PFs were created by superimposing several Gauss shaped texture functions. The parameters describing these components, *i.e.* their volume fraction, position and half-width, are given in Table 2. They correspond to the parameters of the principal texture components found by means of the component method for the experimental textures. In order to expand the range of texture sharpness, the half-width of these components was adjusted. Different sets of synthetic PFs, corresponding to different texture sharpness, were thereby obtained. This allowed to compare the performance of the tested ODF reproduction methods for textures weaker and stronger than those of the deformed and partially recrystallized samples.

The errors associated with the computed ODFs (for both the experimental and the synthetic ODFs) were estimated with independence of the errors reported by the tested methods in order to use an unique quality index to compare them. The *RP0* and *RP1* errors were computed by comparing the normalized input PFs and the PFs calculated from the reproduced ODFs and used as the main criterion for the present comparison.

Fig. 1. The texture of the investigated Fe-50% Ni samples represented by their $\{111\}$ and $\{200\}$ pole figures (measured by neutron diffraction), and by the $\varphi_2 = 20^\circ$ and $\varphi_2 = 45^\circ$ sections of their cubic-triclinic texture function in Euler space. (a) Cold rolled sample. (b) Partially recrystallized sample.

4 Results

4.1 Experimental pole figures

The experimental $\{111\}$ and $\{200\}$ PFs of the cold rolled and partially recrystallized Fe-50% Ni samples are shown in Figures 1a and 1b, respectively. The results of the application of the component method using the measured PFs of both samples are given in Table 1. In these calculations,

the components found during the fitting process (called experimental components hereafter) were classified into the ideal orientation classes given in the first column of Table 1. The unclassified components were ascribed to a random class (RAN). With the aid of the FFSGL33 program, the ODFs of the investigated samples were computed from the texture components found by employing the component method. The $\varphi_2 = 20^\circ$ and $\varphi_2 = 45^\circ$ sections of the computed ODFs are also shown in Figure 1.

The texture of the cold rolled sample consists mainly of the β -fibre [45] running from the copper $\{112\}\langle 111 \rangle$ orientation, through the aluminum $\{123\}\langle 634 \rangle$ orientation to the brass $\{011\}\langle 211 \rangle$ orientation. The sharpness of this texture is characterized by a texture index [1] of 13 whereas the ODF maximum reaches 42 m.r.d. The texture of the partially recrystallized sample is characterized by the presence of the cube $\{001\}\langle 100 \rangle$ orientation. The cube twin $\{221\}\langle 122 \rangle$ orientation and the orientations typical of the cold rolled state are also present in this sample where the texture index and the ODF maximum are 25 and 180 m.r.d., respectively. It is important to emphasize that the texture of both samples are much stronger than those which have been previously used (see [31–34]) to carry out comparisons between the ODF reproduction methods considered in this work.

The errors associated with the reproduction of the ODFs from the experimental PFs of the cold rolled and partially recrystallized samples are shown in Figure 2. In Figure 2a, the errors reported by the harmonic, ADC, WIMV and component methods are given. The $RP0$ and $RP1$ errors computed by comparing the experimental (normalized) input PFs and the PFs calculated from the reproduced ODFs are presented in Figures 2b and 2c, respectively.

According to the results shown in Figure 2a, the reproduction of the texture functions of the investigated samples from the experimental PFs is accomplished with comparable accuracy when the tested methods are employed. Quantitatively, the errors given in this figure approach in all cases the value commonly accepted as representative of a good reproduction process, *i.e.* about 10% [31, 32, 34, 37]. By contrast, the $RP0$ values given in Figure 2b evidence some important differences in the accuracy attained by the tested method for the reproduction of the experimental texture functions considered. The $RP0$ of the associated with the ADC are smaller than those related to the other methods. The WIMV method follows the ADC with respect to accuracy, showing $RP0$ values that double those of the ADC. The $RP0$ values related to these two methods remain relatively unchanged for both samples. The $RP0$ errors of the harmonic and the component methods are considerably higher than those of the discrete methods and decrease with the sharpness of the texture.

On the other hand, the $RP1$ values presented in Figure 2c indicate that the quality of the reproduction of the main peaks of the texture functions is similar for the four methods. The ADC shows the smallest $RP1$ values ($\sim 2\%$) which approach the quality index for an almost perfect reproduction [32]. The $RP1$ values for this method, and

(a)

(b)

(c)

Fig. 2. Errors associated with the reproduction of the texture function from the experimental pole figures. (a) Errors reported by the methods under comparison. (b) *RP0* errors and (c) *RP1* errors computed by comparing the normalized input and recalculated poles figures.

those related to WIMV, remain rather unaltered for both samples.

4.2 Synthetic pole figures

The synthetic PFs used to evaluate the validity of the methods investigated here were created from the

(a)

(b)

Fig. 3. (a) The $\{111\}$ and $\{200\}$ synthetic pole figures obtained by superimposing the texture components described in Table 2 with half-width of 10° . (b) $\varphi_2 = 20^\circ$ and $\varphi_2 = 45^\circ$ sections of the corresponding synthetic texture function in Euler space.

orientation classes described in Table 1. However, the parameters of each component were taken from the principal experimental component included in each orientation class. Next, the half-width of these components were varied between 5° and 35° in order to obtain ten sets of synthetic PFs which have associated textures qualitatively similar to those described in Table 1 but with texture indices ranging from 1 to 51.

The parameters of the components used to create these sets of synthetic PFs are listed in Table 2, where the angular distance of these components to the ideal orientations that define each orientation class are given as well. Figure 3 presents the $\{111\}$ and $\{200\}$ PFs of the set created by setting the half-width equal to 10° . The $\varphi_2 = 20^\circ$ and $\varphi_2 = 45^\circ$ sections of the corresponding cubic-triclinic ODF in Euler space is also presented in this figure. This set of synthetic PFs is that which better describes the experimental texture of the cold rolled sample (compare Figs. 1a and 3).

The errors reported by the compared methods (the component method was excluded in this case) for the reproduction of the synthetic ODFs are presented in Figure 4a. The *RP0* and *RP1* errors calculated by comparing

Fig. 4. Errors related to the reproduction of the texture functions from the synthetic pole figures. (a) Errors reported by the methods under comparison. (b) $RP0$ errors and (c) $RP1$ errors computed by comparing the normalized input and calculated poles figures.

the synthetic input PFs and the PFs calculated from the synthetic ODFs reproduced by these methods are shown in Figures 4b and 4c, respectively. In Figure 4a one can see that the accuracy of the reproduction of the synthetic ODFs, as reported by the methods, is of the same order for the WIMV and the harmonic methods and results excellent for the ADC. In all cases, the errors increase with the texture index of the reproduced ODF. For the harmonic and the WIMV methods, the synthetic ODFs seem to be reproduced within the limit of errors commonly considered for a good reproduction, *i.e.* 10%, up to a texture index of 5. In the case of the ADC this condition is fulfilled for the complete range of texture sharpness under consideration.

In Figure 4b, however, only the $RP0$ values associated with the ADC and the WIMV methods are of the same order for all the synthetic ODFs (those related to the ADC are smaller as in Figs. 4a and 4c). The harmonic method shows $RP0$ values that result comparable to those of the discrete methods up to a texture index of 5. For texture indices greater than this value, the harmonic method has associated $RP0$ values considerably greater than those of the discrete methods. According to the results given in this figure, the reproduction of the synthetic ODFs has been carried out with a rather good accuracy (with errors less than 10%) up to a texture index of 5.

In the case of the errors related to the main peaks, given in Figure 4c by means of the $RP1$ values, all the methods considered show similar results. Thus, the main features of the synthetic ODFs seem to be reproduced with a rather good accuracy by all the methods in the complete range of texture sharpness under evaluation. Surprisingly, the harmonic method has associated $RP1$ values slightly smaller than those related to the discrete methods.

5 Discussion

5.1 On the quality of the input pole figures

Neutron diffraction allowed us to measure complete PFs with reduced experimental errors, *e.g.* by averaging the possible texture gradients in the cold rolled and recrystallized Fe-50% Ni sheets. Analysis of Figures 2 and 4 permits to compare the errors associated with the reproduction of the experimental and synthetic textures in the range of texture index (~ 13) of the experimental ODFs for the cold rolled sample. In the cases of the ADC and the WIMV methods, the $RP0$ and $RP1$ values are of the same order for the experimental and synthetic texture functions (the ADC method shows better results for both type of textures). In addition, the relative deviation of the RP values related to individual PFs from the mean RP value in each sample (given in Fig. 2a) were small in all case. These facts indicate, in principle, that the experimental PFs are all of good quality and compatible.

As has been mentioned, the experimental and synthetic PFs used in this work were given in 5° steps. The texture functions were similarly computed in 5° steps in Euler space. Let b_0 be the half-width of the narrowest peak

in the texture function. In the harmonic method, a good reproduction is obtained if [32]: (i) the series in equation (2) is expanded to an order $\ell_{\max}$ based on a sufficient number of PFs such as $2\pi < b_0\ell_{\max}$, and (ii) the measuring distance Δy in the PF grid is less than $b_0/2$. Hence, if $\ell_{\max} = 34$ and the measuring step Δy for the PFs equals 5° , then the peaks in the texture function will be satisfactorily well reproduced if their half-width are greater than 10° or approach this value.

In the case of the discrete methods, the optimum relation between the resolution of the PFs and that of the ODF has been established by Pospiech [42,43] as: $(\delta y)^{1/2} \approx (\delta g)^{1/3}$. In this relation, $\delta g(\delta y)$ represents the volume (area) element of the equivolume (equiareal) division of the orientation space (PF hemisphere). In terms of the orientation distance Δg and measuring distance Δy , this relation acquires the form: $\Delta g \approx \Delta y$. Thus, the peaks in the texture function with half-width less than 10° will be reproduced with poor accuracy if Δy equals 5° .

Correspondingly, for a measuring distance $\Delta y = 5^\circ$ in the PFs, the feasible resolution in reproducing the texture function by discrete methods is similar to that found when the harmonic method is used with $\ell_{\max} = 34$. In the case of the discrete methods, however, the resolution is less dependent on the number of input PFs and the series-truncation related errors do not occur.

In the sense just depicted, the data in the fifth and sixth columns of Table 1, and those in the sixth column of Table 2, indicate that the experimental PFs are within the limit (mean component half-width of 10°) of the resolution required for an accurate reproduction of the respective texture functions. The results shown in Figure 2 indicate that the resolution of the experimental PFs does not affect notably the reproduction of the texture functions related to these PFs. If it were the case, the errors given in Figure 2 should be greater for the cold rolled sample than for the partially recrystallized one. Except for the $RP1$ values related to the harmonic method, the errors given in Figure 2 remains unaltered or decrease with the sharpening of the texture.

On the other hand, the 5° step used to create the synthetic PFs seem to be insufficient for reproducing with good quality those synthetic ODFs with texture indices greater than 12 (component half-widths smaller than 10° , see footnote b in Tab. 2). The fact that errors increase notably with texture index in Figure 4, is most likely connected with the absence of the adequate resolution for those synthetic PFs describing textures with indices greater than 12. On the assumption that most of the narrowest peaks in the texture functions are those with the highest intensities, *i.e.* $f(g) \geq 1$, the evolution of the $RP1$ values with texture index in Figure 4c could be used to state that the harmonic, ADC and WIMV methods react similarly to the reduction of the resolution of the input PFs. The anomalous increase in the $RP0$ errors in Figure 4b for the harmonic method is most likely due to the bad reproduction of those zones in the texture function where $f(g) \in [0, 1]$.

5.2 On the error criteria

The most striking result in Figures 2 and 4 is the notable difference between the errors given by the methods investigated here and those computed by comparing directly the input and calculated PFs. This obviously indicates that the calculation of errors in these methods does not follow a standard procedure and that minor differences in such calculations give rise to important variations in the accuracy criteria reported by them. In the case of the harmonic method, the TRC parameter does not reveal the accuracy actually attained by this method (compare Figs. 2a and 2b, and Figs. 4a and 4b). Comparison of relations (3) and (5) shows that the RP parameter are more sensitive to differences between the input and calculated PFs than the TRC (see also [32]).

As has been suggested previously [31,32], in those cases where the RP values are greater than 10%, difference PFs should be plotted in order to evaluate the relative contribution of the different domains of the texture function (and PFs) to the RP values. In Figure 5, the distribution of errors (error PFs) computed using two different error functions are presented. To carry out these computations, the set of synthetic PFs created by setting the half-width of the components equal to 10° was used. Besides the $RP0$ function, the difference pole figures, *i.e.* $DPF = |P_i^{\exp} - P_i^{\text{cal}}|$, are presented in this figure.

In the case of the $RP0$ function (Fig. 5a), the errors are distributed quite similarly for the case of the ADC and WIMV. In these methods, the error function reaches their maximum values in the neighborhood (in most cases in PFs locations where $P_{\exp} \sim 1$) of the primary and secondary maxima of the input PFs. For the harmonic method, nevertheless, the positions of the $RP0$ maxima are shifted to the zones where the input PFs show low density values. The three methods show significant values of $RP0$ errors for those zones of the input PFs where $P_{\exp} < 1$.

On the other hand, the DPF errors in Figure 5b show their maxima at the same locations (or in the close neighborhood) than the principal maxima of the input PFs for the three methods. However, a significant dispersion is observed for the DPF related to the harmonic method. The evolution of the average DPF errors with the texture index is shown in Figure 6a. The three methods show similar accuracy up to texture indices of 20. For greater texture indices, the ADC method attains the best accuracy. A similar result is obtained if the $RP\alpha$ error function is selected with α close but greater than the minimum value of each input PF ($P_{\min}^{\exp}$). In Figure 6b, this error function is plotted when α is greater than $P_{\min}^{\exp}$ in 5% (relative to $P_{\min}^{\exp}$). The results depicted in Figure 6 indicate that up to a texture index of 20 the reproduction of the reduced texture function is achieved with the same accuracy for the three methods considered. Beyond this texture index important differences are noted, the ADC and the harmonic methods being those which show the best and the worse accuracy, respectively. Obviously, in the case of the harmonic method, this result can not be extended to

Fig. 5. Distribution of errors computed by using the *RP0* and difference pole figures (*DPF*) error functions for the synthetic $\{111\}$ pole figures created by setting the half-width of the components equal to 10° .

Fig. 6. (a) Average difference pole figure (*PDF*) errors related to the reproduction of the texture functions from the synthetic pole figures. (b) Average *RP α* errors with α greater (in 5%) than the minimum values of the synthetic pole figures.

Fig. 7. Evolution of the ODF maxima with texture index for the synthetic texture functions computed using the investigated ODF reproduction methods.

the analysis of the accuracy attained in the reproduction of the complete texture function.

On the other hand, the $RP1$ values give information only about the quality of the reproduction of the main peaks of the texture function. If Figures 2c and 4c are analyzed, no conclusions can be drawn with respect to the global quality of the reproduction of the complete texture function. In Figure 7, for example, the evolution of the maxima of the synthetic true ODFs with texture index is plotted. The texture functions computed from the model components given in Table 2 (using the FFSGL33 program) can be used as reference to explore how the principal peaks of the texture functions are reproduced. The results in Figure 7 indicate that the ADC and the WIMV methods are capable of reproducing with good quality the maxima of the texture functions over the complete range of texture sharpness considered.

The harmonic method, however, reproduces the maxima of the complete texture function with poor quality when the texture becomes sharper and exceeds a texture index of about 8. As Figure 7 also shows, the use of the generalized positivity method with $r_{\min} = P_{\min}^{\exp}$ [40,41] for eliminating ghost errors increases this value to 12. Accordingly, the $RP1$ values associated with the harmonic method in Figures 2c and 4c become meaningless when the reproduction of the complete texture function is considered for texture index greater than 12.

According to the previous paragraphs, the DPF and the $RP\alpha$ (with $P_{\min}^{\exp} < \alpha < 1$) errors functions are also suitable to characterize the quality of the reproduction of the texture function. They are not affected by the mathematical instabilities associated with the $RP0$ function when very low values of $P_{\min}^{\exp}$ are involved. They also contain information of both the $f(g) \in [0, 1]$ and $f(g) > 1$ zones of the ODF ($P^{\exp}(y) \in [0, 1]$ and $P^{\exp}(y) > 1$ in the PFs), and are highly sensitive to those errors connected with the first of these two complementary zones which

must be reproduced with similar accuracy for obtaining a good approximation to the true texture function [32].

5.3 On the choice of the reproduction method

The harmonic method is appropriate in reproducing the texture function considered in this work for those case where the texture index is less than 8. In order to extent this limit of applicability, three main approaches could be used: (i) to increase the resolution of the input PFs by reducing the measuring distance in the PFs, (ii) to increase the expansion order $\ell_{\max}$ beyond 34 and (iii) to use the ghost correction algorithm that better adapts to the specific reproduction problem under investigation. The harmonic method has the advantage of its mathematical simplicity. In addition, the calculation of the mean values of many anisotropic physical properties of polycrystalline solids can be easily carried out in the framework of this method [1,2,7]. For those physical properties described by functions or tensor of even order (most of the magnetic, elastic and plastic ones) this is specially true because only the even ($\ell = 0, 2, 4, \dots$) C_{ℓ}^{mn} coefficients are required [1,2]. In such cases, therefore, the conventional harmonic method can be used directly in the present texture up to texture indices of 20.

The component method has the advantage of reducing the amount of information required to describe a given texture. Additionally, this method gives directly the difference PFs which have proved useful in analyzing the errors during the reproduction process. The volume fraction of the texture components, *i.e.* the only parameter that has an explicit physical meaning in quantitative texture analysis, is also directly obtained when this method is applied. As Figures 2 and 4 show, the higher the texture index, the better is the reproduction of the texture function when the component method is used. This is obviously connected with the fact that this method produces excellent results in those cases where the texture function is composed of a reduced number of strong and clearly distinguishable components [22,26,27]. In other cases, *e.g.* textures described by several fibres with strongly overlapped components, the results obtained by employing this method must be analyzed with caution and, if possible, complemented with the computation of the texture function by other methods.

The ADC and the WIMV methods are better suited for the reproduction of texture functions similar to those used in this work. As measured by the $RP0$, $RP1$, DPF and $RP\alpha$ (with $P_{\min}^{\exp} < \alpha < 1$) values, the errors associated with these two discrete methods are similar. However, the ADC shows, in all cases (see Figs. 2, 4 and 6), errors smaller than those of the WIMV method, especially for higher texture indices.

6 Conclusions

A comparative analysis of the accuracy associated with practical implementations of the harmonic, ADC, WIMV

and component methods has been carried out with textures typical of the deformed and partially recrystallized states of a Fe-50% Ni alloy (medium-to-high stacking fault energy materials). The errors introduced by these methods in the reproduction of the complete texture function, and the benefits and shortcomings resulting from their use, have been explored for this specific type of textures over a wide range of texture sharpness by using experimental and synthetic PFs.

As has been shown, the parameters characterizing the accuracy of the methods under comparison are not appropriate in comparing them relatively so that, a unique quality index must be computed by comparing the input and calculated PFs in order to explore the relative accuracy of each method. The average DPF and $RP\alpha$ ($P_{\min}^{\exp} < \alpha < 1$) error functions seem to be as useful as the $RP0$ in describing the errors introduced by these methods. However, if some subtle aspects of the $RP0$ are considered, *e.g.* its instability when $P_{\min}^{\exp} \rightarrow 0$, the DPF and $RP\alpha$ ($P_{\min}^{\exp} < \alpha < 1$) functions could be more suitable than the $RP0$ errors in measuring the accuracy attained by a given reproduction method.

For the present textures (experimental ODFs showing components with mean half-width of 10°), a measuring distance $\Delta y = 5^\circ$ in the PF grid is mandatory for reproducing the texture functions with good accuracy, *i.e.* RP values less smaller than 10%. For this resolution, the harmonic, ADC and WIMV methods show similar accuracy in the reproduction of the complete ODF for those textures with texture indices less than 8. For the harmonic method, this limit can be extended to 12 if an available method for eliminating ghost errors is employed or to 20 in those cases where only the reduced ODF is of interest. For sharper textures, the accuracy of the harmonic method is greatly decreased whereas that of the two mentioned discrete methods is less affected. The ADC method shows a better accuracy in the reproduction of both the experimental and synthetic texture functions over the entire range of texture sharpness under investigation.

The component method, on the other hand, is useful in determining textures characterized by a reduced number of non overlapping texture components and consequently shows $RP0$ and $RP1$ errors that decrease with the sharpness of the experimental texture considered here.

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