# COMPUTER PROGRAMS

*J. Appl. Cryst.* (1998). **31**, 262–269

## *BEARTEX*: a Windows-based program system for quantitative texture analysis

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(*Received 15 November 1996; accepted 29 May 1997*)

**Abstract**

*BEARTEX* is a general PC-based Windows software package for quantitative texture analysis. The 30 programs that it contains provide corrections for experimental pole figures, orientation distribution calculations from complete or incomplete pole figures for all crystal and sample symmetries down to triclinic, graphical display of data, polycrystal tensor property determinations and various other operations.

### 1. Introduction

Over the last 30 years, texture analysis has evolved from a simple qualitative tool into a sophisticated quantitative science. It encompasses three major branches. Data acquisition relies on complicated instrumentation, including X-ray pole figure goniometers, neutron diffraction, synchrotron, transmission and scanning electron microscopes. Data analysis involves a sequence of procedures from corrections of experimental data, determination of the orientation distribution (OD), representation of orientation data in a way that is easy to visualize and obtaining texture-dependent physical properties of polycrystals. Finally, the formation of texture needs to be understood by comparing experimental data with results from simulations of deformation and growth processes. Texture analysis is pursued in such diverse fields as mechanics, physics, materials science (metals, ceramics and polymers), mineralogy, geophysics, structural geology and biomimetics, both in research institutions as well as in industrial laboratories. The methods are relatively complicated, fill several books (*e.g.* Bunge, 1982; Matthies, Vinel & Helming, 1987) and are generally beyond the expertise of most users. With 'computer program packages' quantitative texture research has now come within reach for the applied scientists. The comprehensive package *popLA* (Kallend *et al.*, 1991) has been widely distributed and other systems are available from commercial vendors.

Mainly to respond to the needs of students and outside users of the Berkeley texture laboratory, we have attempted to develop a user-friendly texture system to analyze preferred orientations in polycrystalline materials, which works in an interactive computer environment. *BEARTEX* is independent of X-ray hardware and many programs can also be used to process neutron or electron diffraction data. The basic input consists of diffraction intensities, measured on a pole figure goniometer. These intensities can be corrected, modified and used as data for the OD calculation. Data can be displayed on the CRT (cathode-ray tube) monitor or hard copies can be prepared with a laser printer.

It is assumed that the user is familiar with the basic concepts of texture analysis (see *e.g.* Wenk, 1985; Kocks, Tomé & Wenk, 1998) and such terms as pole figures (and how they are measured), orientation (defined by three Euler angles which represent rotations to bring crystal and sample coordinate systems to coincidence), orientation distribution (derived from measured pole figures) *etc.* In *BEARTEX*, the standard Euler convention is Roe/Matthies as defined in Fig. 1. Transformations to other conventions can be performed in some of the programs (for relationships see Table 1; also, bear in mind the identities $\alpha$, $\beta$, $\gamma$ and $\alpha + \pi$, $-\beta$, $\gamma + \pi$).

We are at a stage where this package can be made available to a wider group of texture researchers for a nominal cost which is used to maintain and develop the system further. For information about how to obtain this package contact beartex@seismo.berkeley.edu or consult the web site at www.seismo.berkeley.edu.

### 2. System requirements

*BEARTEX* requires a 386, 486 or Pentium processor and a Windows 3.1, Windows 95 or Windows NT operating system. A math coprocessor is a necessity as most of the programs are

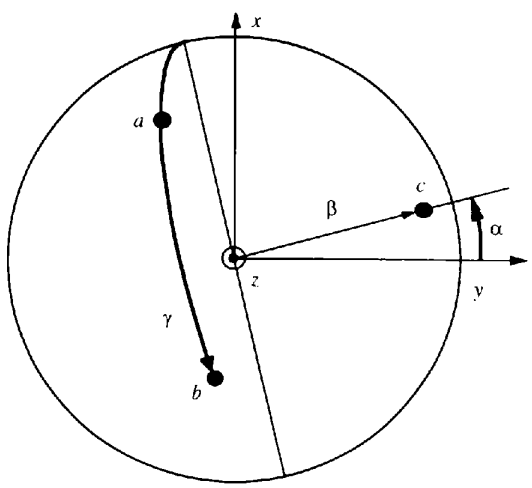


Fig. 1. Definition of Roe/Matthies Euler angles relating the crystal coordinate system {$c$ = [001], $b$ = normal to [001] and [100], pole to (010), and $a$ normal to $b$ and $c$} and the sample coordinate system ($x$, $y$, $z$). Both coordinate systems are right-handed and rectangular. Stereographic projection.

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Table 1. *Relationships between different conventions of Euler angles*

| Matthies | Roe | Bunge | Canova | Kocks |
|---|---|---|---|---|
| $\alpha$ | $\Psi$ | $\varphi_1 = \alpha + \pi/2$ | $\omega = 3\pi/2 - \alpha$ | $\Psi$ |
| $\beta$ | $\Theta$ | $\Phi$ | $-\Theta$ | $\Theta$ |
| $\gamma$ | $\Phi$ | $\varphi_2 = \gamma + 3\pi/2$ | $\varphi = \pi/2 - \gamma$ | $\varphi = \pi - \gamma$ |

numerically intensive and is required by the Fortran compiler. Also, if other memory-resident applications are used, 16 Mbytes of memory are necessary. 16 Mbytes of space is required on disk C to install the package and run the programs. VGA or Super VGA color graphics are highly recommended and a laser printer for output is suggested.

## 3. Program structure

The main *BEARTEX* window (Fig. 2), described below, gives access to 30 different programs in separate windows (such as in Fig. 3) in the present version. After execution of a program, output files are generated which are used in other programs or can be exported.

The basic components are Fortran programs that operate in DOS under Windows, using a supplied DOS extender. The Fortran programs are compiled with Microsoft Power Station Fortran version 1. The interactive windows interface was created with VisualBasic 3.0. The general structure is to produce preliminary input on a 'configuration file' which is then modified by the user in the window dialog and produces a new configuration file containing the modified data for the main program. The applications can also be run in a DOS environment but require as input the configuration files. In general, one does not need to know either this system structure, Fortran or even DOS. The 30 programs have been given four-digit names for identification (*WIMV*, *TENS etc.*).

As with all software, errors may occur. Usually they are related to the data file input. A default example is supplied which has been tested and can be used to verify that the system has been properly installed. Online help provides specific information on each program and contains a section on troubleshooting.

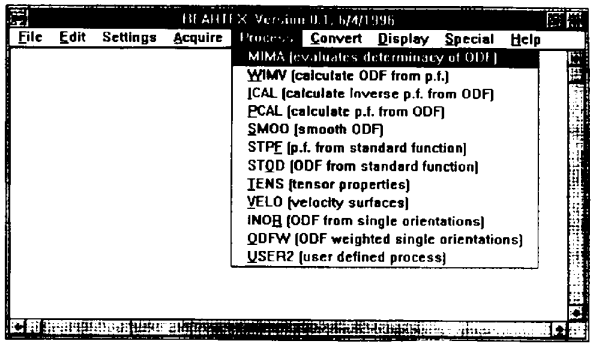


Fig. 2. Display of the main *BEARTEX* window, showing programs in the PROCESS option.

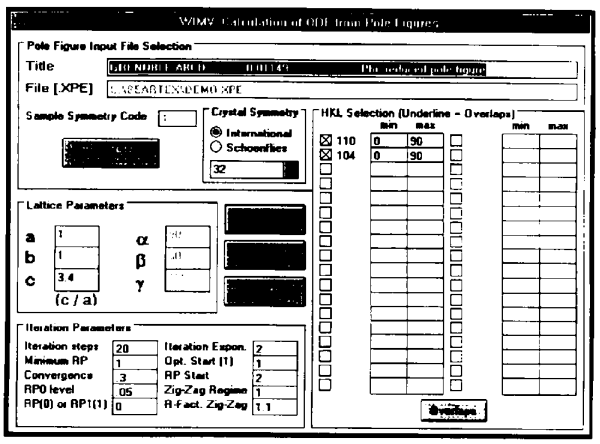


Fig. 3. Window to change parameters for *WIMV* which calculates the orientation distribution from pole figures.

## 4. *BEARTEX* options and programs

The main *BEARTEX* window consists of nine menus. Fig. 2 shows the PROCESS option. (i) FILE is the standard Windows menu for opening, saving and printing text files. (ii) EDIT allows the user to copy, cut and paste text. (iii) SETTINGS is for changing the screen fonts, colors and sound. (iv) ACQUIRE is a set of programs related to the acquisition of X-ray diffraction data. Subroutines may be required to interface with specific goniometer hardware. Also included are programs for data corrections, for both bulk samples and thin films. *GONO* drives a three- or four-axis pole figure goniometer (DOS BASIC program); *HEXF* prepares a file with angle positions for equal-area pole figure coverage; *CORR* corrects pole figure data for background and defocusing; *FICO* calculates a theoretical defocusing curve, also applicable for thin films; *HROT* prepares a file for rotated angle positions for hexagonal grid data; *ABXX* corrects and processes data for detailed pole figure scans (*e.g.* epitaxic films); *THET* calculates $d(hkl)$ from $2\theta$ and $2\theta$ from $d(hkl)$ for various wavelengths.

(v) PROCESS contains programs to calculate the OD from pole figures and perform various operations with the OD. *MIMA* evaluates whether the OD is fully defined with a set of measured pole figure areas; *WIMV* calculates OD from pole figures for any crystal and triclinic sample symmetry; *PCAL* calculates any pole figure from the OD; *ICAL* calculates any inverse pole figures from the OD; *SMOO* smooths and sharpens the OD ('filtering'); *STPF* calculates model pole figures from sets of standard Gauss components; *STOD* calculates model OD from sets of standard Gauss components; *INOR* calculates an OD-like representation of large sets of single-orientation data; *TENS* determines polycrystal tensor properties from single-crystal properties and OD; *VELO* calculates longitudinal and transverse wavespeed surfaces from stiffness tensors; *ODFW* assigns texture weights to individual orientations; *CLMN* calculates harmonic coefficients from the OD; *COMP* performs an intensity integration within a sphere of texture-component positions.

(vi) CONVERT contains programs to change file formats, Euler angle conventions of OD and section types. The preferred file format for pole figures is the 'new' Berkeley format which is a minor modification of the format used in *popLA*. *CHBI* converts the standard binary OD file into ASCII Berkeley format. *CHPF* converts pole figures. The user

must provide a subroutine for individual changes. *CHOD* converts OD. The user must provide a subroutine for individual changes. *CSEC* calculates (from a binary file) various OD sections in different angle conventions. *HKLX* converts (for cubic crystals only) Euler angles to (*hkl*) [*uvw*] and vice versa.

(vii) DISPLAY contains programs for the graphic display of texture data on the monitor (in different color patterns with the possibility of preparing a PCX file with a screensaver) and for contour plots on a Hewlett Packard LaserJet printer or PostScript printers. *CONT* gives a contour plot in polar coordinates of OD sections or pole figures; *POXX* gives a color display of OD and pole figures on a monitor; *XYCO* gives contour plots of OD sections in rectangular format; *PTXX* gives a plot of individual orientations (or components).

(viii) SPECIAL has several options to access other systems. *RINITIALIZE* deletes all configuration files and restarts the system with default files; *DOS* shells to DOS without leaving *BEARTEX*; *LOCAL* opens a menu window to access local programs running under DOS; *POPLA* activates the *popLA* menu under DOS if *popLA* is already installed.

(ix) HELP is a menu containing help on various topics.

## 5. Data formats

The calculations in *BEARTEX* rely mainly on discrete methods. Orientation space is divided into discrete $5 \times 5 \times 5^\circ$ cells and pole figures into $5 \times 5^\circ$ cells. The most important data file is the experimental pole figure file that needs to be imported and, if necessary, converted from other conventions. Other data files used in various programs are explained in the online help and documentation provided with the system.

### 5.1. *Pole figures*

The *popLA* package has made an admirable attempt to standardize data formats with the so-called 'old Berkeley' format based on a format previously used at the University of Metz, France. Most of the *BEARTEX* programs will accept this format. However, the standard for *BEARTEX* is a slightly modified version, which became necessary because of application to low-crystal-symmetry materials (with larger than one-digit and negative *hkl*'s) and a more general choice of pole figure ranges. The pole figure file contains information about lattice parameters and crystal symmetry so that it does not need to be re-entered during processing.

Pole density or diffraction intensity data are supplied as integers in $5 \times 5^\circ$ intervals on azimuth and pole distance. For a pole figure with triclinic sample symmetry, the data consist of 19 (pole distance) rings, each with 72 (azimuthal) values. To obtain integers, *e.g.* from values normalized to multiples of a random distribution, data are multiplied with a constant factor (generally 100). Fig. 4 is an example of a 110 pole figure file used to calculate the OD.

### 5.2. *Standard OD format*

The OD is stored as a binary file using the Roe/Matthies Euler angle convention and $\gamma$ sections. There should be no problems with these binary files since they are produced in the package. They can be converted (in *CHBI*) to Berkeley format for representation and inspection.

### 5.3. *Detailed $\alpha$–$\beta$ scan of a pole figure region*

For detailed $\alpha$–$\beta$ scans of regions on the pole figure, a simple array is used in free format. Each line contains a string of values for $\beta$ for one value of $\alpha$ with arbitrary increments of $\alpha$ and $\beta$.

### 5.4. *OD component file*

The user may either use or create a file with individual orientations or OD components, defined by three Euler angles. These could come from individual orientation measurements (*e.g.* electron backscattered diffraction patterns, EBSP) or from a simulation program.

File extensions contain information about data format and data type (*e.g.* X?? are ASCII pole figure or OD data for viewing and plotting, Y?? are ODs in binary format).

## 6. Brief description of the programs

### 6.1. *ACQUIRE*

*GONO* is a data-collection program which drives functions of a four-axis pole figure goniometer (motors and counter) from a PC. It is written in QuickBASIC and it is used at Berkeley and Los Alamos to drive a Scintag microprocessor and a CENTROID stepper motor controller. (A source code is supplied and it should be easy to modify the driver subroutines for other systems.) There are options for (*a*) pole figure coverage (hexagonal or $5 \times 5^\circ$), (*b*) experimental determination of defocusing curves, (*c*) single-angle scans ($\theta$–$2\theta$, $\omega$, $\chi$, $\phi$) and (*d*) detailed $\chi$–$\phi$ scans over a selected area, mainly used for epitaxic thin films. Output consists of uncorrected pole figure data.

*HEXF* calculates an equal-area hexagonal grid angle file (spherical goniometer coordinates) for a given resolution for efficient pole figure measurements (Matthies & Wenk, 1992). These data files are used in *GONO* to drive the pole figure goniometer. The user chooses the angular resolution of pole figure and the maximum pole distance. For most textures 7.5° or 10° are adequate.

*CORR* corrects experimentally determined pole figures for background, defocusing, volume and absorption. The data may be in the form of pole figures in $5 \times 5^\circ$ Berkeley or hexagonal format. A correction curve as a function of $\alpha$ ($90^\circ - \chi$) with 19 values in 5° increments must be supplied (either empirical or calculated by *FICO*). One can select to smooth, normalize (to multiples of a random distribution), filter to eliminate large spikes and average axially symmetric pole figures over a desired angular range. Output consists of corrected pole figures.

```
CALCITE Gre433  Neutron Diffraction ILL Grenoble
Any information                                    Background:
Any information
Any information
Any information
  1  1   0    0.   90.    5.    0. 360.    5. 1 1 1 2 3    0          .0
 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122
 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122
 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122 122
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 108 109 109 110 111 112 113 113 115 115 116 117 118 120 121 122 124 125
 125 126 126 126 126 126 125 125 124 124 123 123 123 122 121 121 120 120
 120 120 120 119 120 120 121 122 123 123 124 124 125 125 125 125 125 124
 123 122 121 120 118 117 116 114 113 112 110 109 108 107 107 106 106 107
  96  97  98 100 101 102 103 105 106 107 109 111 113 115 116 119 120 123
 124 124 124 123 121 120 119 119 118 116 115 114 113 113 113 113 112 111
 etc.
```

Fig. 4. An example of the first lines of a pole figure data file used to calculate the OD. Values are in $5 \times 5^\circ$ intervals on azimuth and pole distance.

Table 2. *Crystal symmetries considered in the Beartex package*

| System | Cubic | | Tetragonal | | Orthorhombic | Monoclinic | Triclinic | Hexagonal | | Trigonal | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Point group | *O* | *T* | *D*4 | *C*4 | *D*2 | *C*2 | *C*1 | *D*6 | *C*6 | *D*3 | *C*3 |
| | 432 | 23 | 422 | 4 | 222 | 2 | 1 | 622 | 6 | 32 | 3 |
| Code | 7 | 6 | 5 | 4 | 3 | 2 | 1 | 11 | 10 | 9 | 8 |

*FICO* produces theoretical correction curves for defocusing, absorption and volume consisting of 19 $\alpha$ values in 5° intervals. They are based on goniometer geometry and absorption properties of the analyzed material. Theoretical correction curves are particularly important for thin films but can also be used for bulk samples.

*HROT* calculates a rotated 5 × 5° grid to be used in *CORR* with hexagonal grid data. The program applies four consecutive rotations about orthogonal axes *x*, *y*, *z* and *x* explained in the program.

*ABXX* corrects experimentally determined $\alpha$–$\beta$ ($\chi$–$\phi$) scans for background, defocusing and absorption. It also integrates over two peaks which can be chosen on a graphical display. It is used for strong textures like those found in epitaxic films. An appropriate correction curve must be supplied (*e.g.* produced by *FICO*).

*THET* converts *d*(*hkl*) to 2$\theta$ and *vice versa*. Choose a wavelength from the list or enter your own. Then select *d*(*hkl*) or 2$\theta$, respectively.

### 6.2. *PROCESS*

*MIMA* evaluates the coverage of orientation space. Inputs are the extents of experimental pole figures *hkl*, lattice geometry and crystal symmetry; outputs are the numbers of 'pole figure projection paths' intersecting in a 5 × 5 × 5° orientation space cell. In order to define an orientation, the minimum number of intersections must be three. For OD determination a larger number of intersections, preferably ten or more, are recommended. It is assumed that data have been measured in full azimuthal rings. In this case, a representation of the OD definition depending on two Euler angles ($\beta$ and $\gamma$) is sufficient. The results possess symmetry properties similar to an inverse pole figure (Helming, 1991). Fig. 5(*a*) shows the results of *MIMA* for an OD analysis of a cubic material from three incomplete pole figures.

*WIMV* is the most demanding program in the package. It determines the orientation distribution from one to 100 complete or incomplete pole figures using the discrete *WIMV* algorithm (Matthies & Vinel, 1982) and provides an automatic conditional ghost correction. This algorithm uses all available experimental information and finds, among all possible solutions for the OD, the one which has the smallest discrepancy between experimental and recalculated pole figures and the sharpest texture. The discrepancy is evaluated with the averaged relative deviation RP value (Matthies, Wenk & Vinel, 1988) over the measured pole figures

$$\mathrm{RP} = \frac{1}{N}\sum_i \frac{|P_i^{\mathrm{obs}} - P_i^{\mathrm{calc}}|}{P_i^{\mathrm{obs}}},$$

where $P_i^{\mathrm{obs}}$ and $P_i^{\mathrm{calc}}$ are the observed and recalculated pole densities, respectively, and the summation is over all the $N$ measured points $i$ in all pole figures considered.

The texture strength is quantified with the texture index $F_2$ (Bunge, 1982)

$$F_2 = \frac{1}{8\pi^2}\sum_i [f(g_i)]^2 \Delta g_i,$$

where $f(g_i)$ is the OD value at point $g_i = (\alpha, \beta, \gamma)_i$ and $\Delta g_i$ the 5° cell volume of the orientation space.

In addition to average RP values, the program gives information on RP for individual pole figures which can be used to identify poor data. Two RP values are distinguished: RP0 is the summation over all points with $P_i^{\mathrm{obs}}$ above a defined minimum (usually 0.05 multiples of a random distribution or m.r.d.); RP1 considers only values larger than 1 m.r.d. and is indicative of deviations in the pole figure maxima.

The degree of 'texture disorder' is evaluated by the calculation of the entropy $S$ (Matthies, 1991)

$$S = -\frac{1}{8\pi^2}\sum_i f(g_i)\ \ln f(g_i)\Delta g_i.$$

Pole figure data need formally to extend over full azimuthal circles ('triclinic format'). In the case of higher sample symmetry (with measurements only over a 180° or 90° sector), the pole figure file has to be expanded into this now-redundant form. The extent in polar angle can be chosen from a minimum to a maximum. *WIMV* is applicable to any crystal symmetry (divided into 11 rotation groups, equivalent to the rotation parts of the 11 Laue groups) (Table 2).

The number and extent of pole figures must cover the whole three-dimensional orientation space (*cf. MIMA*). If diffraction peaks *hkl* are overlapped, they can be treated by assigning intensity ratios.

There are many options to choose from in order to get a better refinement of the OD (Fig. 3). It is possible to eliminate a pole figure from a list in addition to limiting its extent for the analysis. The iteration procedure is controlled with various parameters which depend mainly on the sharpness of the texture and the quality of the experimental data.

Output from *WIMV* is the OD on a binary file. *WIMV* also provides a file of normalized experimental and recalculated pole figures which is used to assess the quality of the experimental data and to reveal problems of inconsistency in the OD refinement (Figs. 5*b* and 5*c*).

*PCAL* calculates any pole figure *hkl* from a binary OD file produced by *WIMV*, *STOD*, *INOR* or *SMOO*. The lattice plane is defined by Miller indices.

*ICAL* calculates any inverse pole figures from a binary OD file. The sample direction is defined by vector components with 'pseudocubic' *hkl* indices; 100, 010 and 001 describe the *x*, *y*, and *z* axes of the sample coordinate system, respectively.

*SMOO* provides a smoothed and/or sharpened OD from a binary OD file. This is particularly useful for coarse-grained samples and data with poor counting statistics. The program smooths a rugged orientation distribution in three dimensions and subsequently sharpens it, if desired (Matthies & Vinel, 1994). The combination of both steps effectively corresponds to a filtering procedure. For smoothing, a bell curve width and

two parameters related to counting statistics can be chosen. The exponential sharpening process maintains peak maxima, in spite of smoothing, reproducing the texture index $F_2$ of the original input OD with stochastic elements.

*STPF* calculates, for given symmetries, pole figures from sets of individual components described by standard Gauss functions. Components are defined by Euler angles, weights and widths of bell curves. Arbitrary pole figure *hkl*'s can be selected. Different *hkl*'s can be overlapped to a composite pole figure by providing weight ratios. The ratios, including the isotropic component ('Phon'), must add up to 1.0.

*STOD* calculates model orientation distributions from standard Gauss functions. As in *STPF*, input consists of lattice parameters and symmetry plus Euler angles, weights and widths for the desired OD components (see above). There is a choice of OD output files between 'true' $f$ (corresponding to the sum of the even and odd parts in the harmonic formulation), 'reduced' $\tilde{f}$ (even) and the difference between the two $\tilde{f}$ (odd).

*INOR* calculates an OD-like distribution from individual orientations in histogram form of $5 \times 5^\circ$ boxes. Correspondingly, the algorithm is fast but less precise than the standard precision routine *STOD*. It is meant for large data-sets such as automatically acquired EBSP data. Individual orientations are defined by three Euler angles, just as in *STPF* and *STOD*, and can be weighted. The program can also be used to construct misorientation distributions if individual misorientation data are used as input.

*TENS* determines second- and fourth-rank symmetric tensor properties of textured polycrystal aggregates by averaging of single-crystal properties based on the OD, using the conventional approximations (Voigt, Reuss and Hill) and the geometric mean algorithm (Matthies & Humbert, 1995) with self-consistent elements. For input, the single-crystal tensor needs to be provided. For a fourth-rank elastic tensor, $6\times6$ stiffnesses in Voigt notation are the standard input (preferably in GPa units). For random texture, no OD input file is required.

The output is a file that contains tensors for the polycrystal in $6 \times 6$ notation and the order given in Table 3.

*VELO* calculates velocity surfaces for longitudinal and the two transverse waves ($p$, $s1$ and $s2$ in geophysical terminology) from the stiffness tensor such as the one prepared by *TENS* (in GPa) and the density (g cm$^{-3}$). The output is wave velocity surfaces, both as absolute values (km s$^{-1}$ $\times$ 100) and normalizing the largest value to 1000.

*ODFW* assigns weights to individual orientations, defined by Euler angles, based on OD values. This may be used for texture simulations to assign the texture of the starting material to a limited set of starting grains. Two input files must be provided, one with individual orientations and a second one with the OD. Individual orientations may be in Roe/Matthies, Kocks, Bunge or Canova convention and output is in the same convention as input.

*CLMN*. In *BEARTEX* the OD is obtained with discrete (direct) methods. However, for comparison a representation

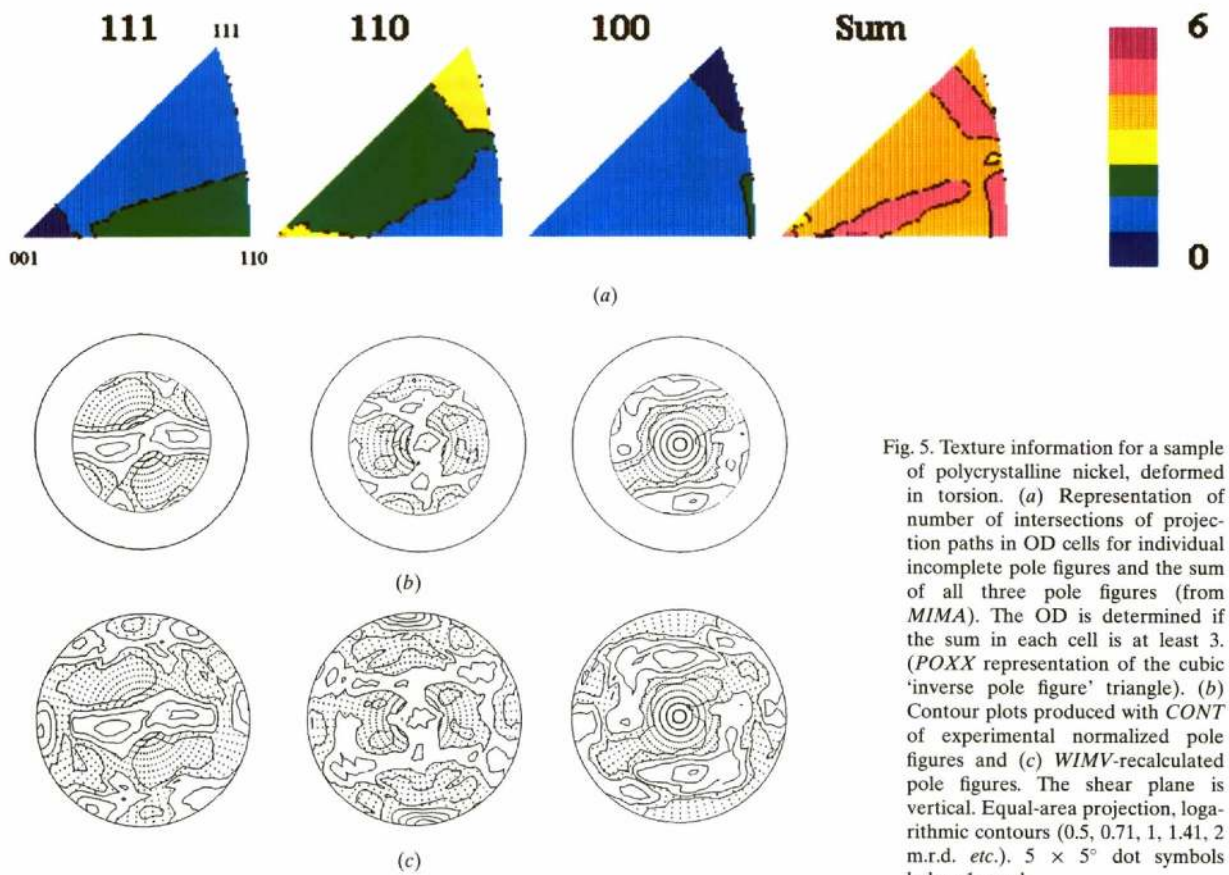



Fig. 5. Texture information for a sample of polycrystalline nickel, deformed in torsion. (*a*) Representation of number of intersections of projection paths in OD cells for individual incomplete pole figures and the sum of all three pole figures (from *MIMA*). The OD is determined if the sum in each cell is at least 3. (*POXX* representation of the cubic 'inverse pole figure' triangle). (*b*) Contour plots produced with *CONT* of experimental normalized pole figures and (*c*) *WIMV*-recalculated pole figures. The shear plane is vertical. Equal-area projection, logarithmic contours (0.5, 0.71, 1, 1.41, 2 m.r.d. *etc.*). $5 \times 5^\circ$ dot symbols below 1 m.r.d.

Table 3. *Stiffness ($C_{ij}$) and compliance ($S_{ij}$) tensors calculated by TENS*

Single crystal (input)
Voigt average
Reuss average
Hill average
Geometric mean

of the OD with spherical harmonics may be useful. *CLMN* calculates by numerical integration of the OD both even and odd harmonic coefficients in Tesseral formulation for all crystal and sample symmetries. The maximum order of the expansion is 47.

*COMP* estimates by integration the intensity of a spherical component (including all symmetrically equivalent spheres). The user must supply an OD and triplets of angles defining the center and the surface of the spherical component.

### 6.3. *CONVERT*

*CHBI* converts the binary OD file produced in *WIMV*, *SMOO* or *STOD* into an ASCII file in Berkeley format for representation with *POXX* or *CONT*. OD values are multiplied by 100.

*CHOD* converts OD data from old into new, or new into old Berkeley format. The source code is supplied and the user can modify it (subroutine *CHANGE*) to transform data (*e.g.* renormalize, change order, rotate *etc.*). It uses a three-dimensional data array.

*CHPF* converts pole figure data in a similar way to *CHOD*. It uses a two-dimensional data array.

*CSEC* provides different OD output options. The input is a binary OD file in Roe/Matthies convention, $\alpha$, $\beta$, $\gamma$, in $\gamma$ sections (sample coordinate system related), triclinic sample symmetry region, $5 \times 5 \times 5^\circ$ intervals. Output sections can be based on the sample coordinate system (Figs. 6*b* and 6*c*, default), or the crystal coordinate system. Oblique $\sigma$ sections provide minimal distortion in the center of spherical OD representations and in the form of texture components (*e.g.* Fig. 6*c*) but a single section does not directly reflect all rotational symmetries (Matthies, Helming & Kunze, 1990*a*,*b*). The user can choose different conventions of Euler angles, rotate the OD and impose a final sample symmetry.

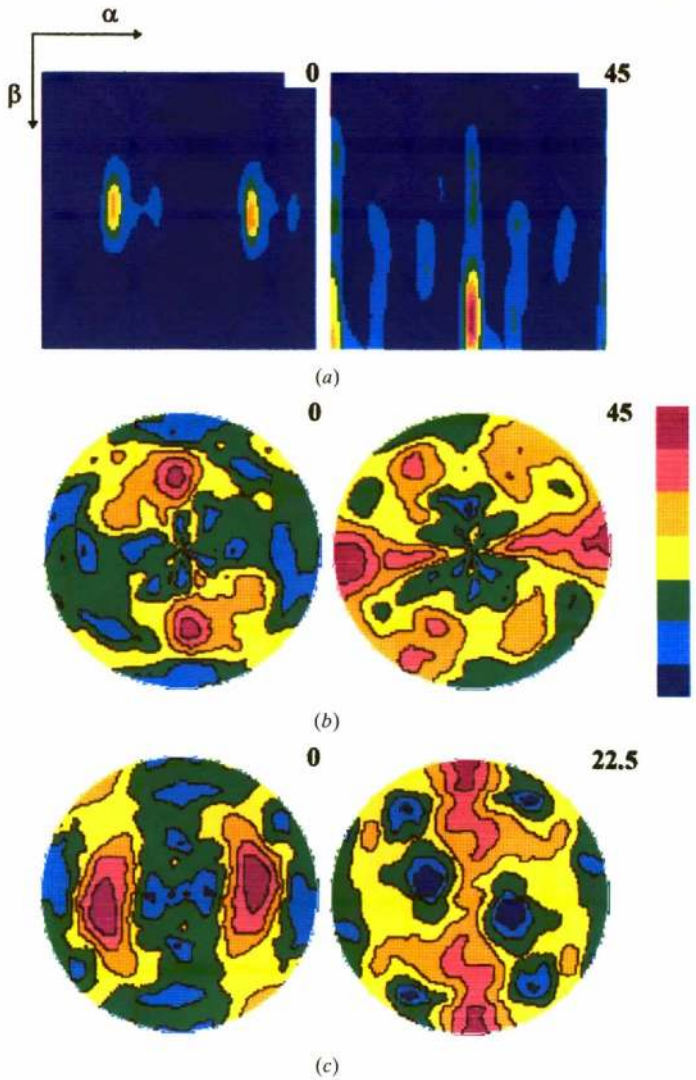



Fig. 6. Color plots of two OD sections for the sample illustrated in Fig. 5. (*a*) Rectangular representation of $\gamma$ sections (sample reference system). (*b*) Polar representation of $\gamma$ sections. (*c*) $\sigma$ sections (oblique sections with minimal distortion). For (*b*) and (*c*) equal-area projection, logarithmic scale with colors. Minimum is 0 m.r.d. and maximum is 10.7 m.r.d. (*POXX*).

*HKLX* is a utility to convert Euler angles to 'ideal orientation' nomenclature (*hkl*) [*uvw*], which some researchers use for cubic crystals.

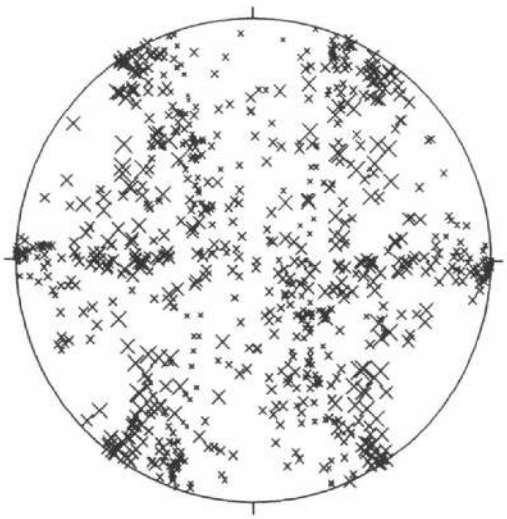


Fig. 7. Plot of individual orientations with the program *PTXX*. The orientations are the result of Taylor polycrystal plasticity simulations for an f.c.c. shear texture and can be compared with the pole figure recalculated from the experimental OD (Fig. 5*c*). The shear plane is vertical. 200 individual orientations given as Euler angles are represented in a (111) pole figure. The symbol size is proportional to the Taylor factor. Equal-area projection.

### 6.4. *DISPLAY*

*CONT* constructs contour plots of up to 16 OD sections or pole figures. The corresponding pole figures can be selected from a list. Standard output is a Hewlett Packard LaserJet printer but it is also possible to create an encapsulated PostScript file with plot commands on disk. Various options can be chosen, *e.g.* contour system and levels, $5 \times 5°$ dot patterns to outline fields with minima, stereographic or equal-area projection. A sum of all sections can be constructed as the last plot. In the case of $\gamma$ or $\sigma$ sections it represents a $z$-axis pole figure. Examples of pole figures are shown in Figs. 5(*b*) and 5(*c*).

*POXX* provides a VGA color display of (up to 16) pole figures or OD sections in polar coordinates (Figs. 6*b* and 6*c*). Pole figures can be selected from a list. A display in rectangular representation is also possible (Fig. 6*a*). Several options can be chosen (equal-area or stereographic projection, smoothing, linear or log intensity scale, color distribution with specified minimum and maximum, adding contours, selecting a special sector, including cubic). A cursor arrow allows one to determine angular positions in the pole figure. The screen can be photographed to prepare color slides for presentations or can be captured as a PCX or TIFF file for later editing and printing.

*XYCO* prepares a contour plot of up to 16 pole figures or OD sections in rectangular coordinates. Standard output is a Hewlett Packard LaserJet printer. Alternatively PostScript files can be produced.

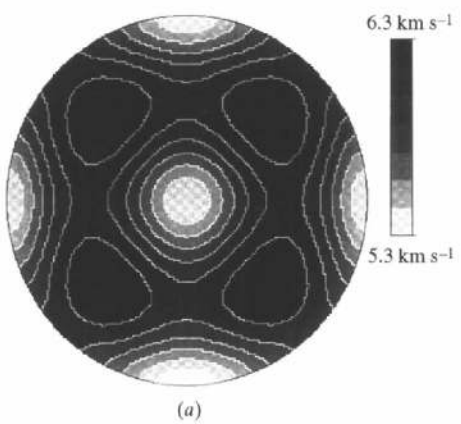
*PTXX* constructs pole figure representations of single orientations, *e.g.* from texture simulations. As in *CONT* the preferred output is on a Hewlett Packard LaserJet. The size of

Single crystal $C_{ij}$ (GPa)

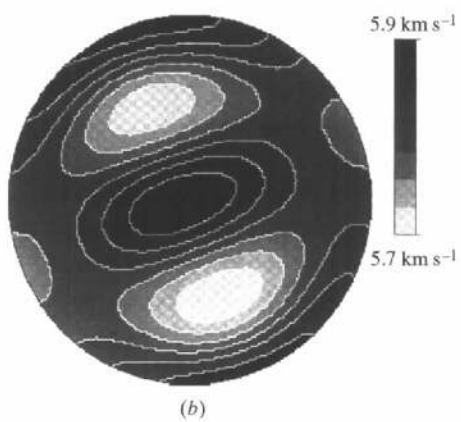
| | | | | | |
|---|---|---|---|---|---|
| 250.7 | 150.7 | 150.7 | | | |
| 150.7 | 250.7 | 150.7 | | | |
| 150.7 | 150.7 | 250.7 | | | |
| | | | 123 | | |
| | | | | 123 | |
| | | | | | 123 |

Geometric mean $C_{ij}$ (GPa)

| | | | | | |
|---|---|---|---|---|---|
| 298.3 | 127.7 | 126.2 | –0.4 | 0.3 | –2.0 |
| 127.7 | 305.7 | 118.7 | 0.7 | 0.2 | –1.0 |
| 126.2 | 118.7 | 307.2 | –0.2 | –0.5 | 3.1 |
| –0.4 | 0.7 | –0.2 | 78.5 | 2.8 | 0.2 |
| 0.3 | 0.2 | –0.5 | 2.8 | 85.3 | –0.4 |
| –2.0 | –1.0 | 3.1 | 0.2 | –0.4 | 86.7 |




(*a*)




(*b*)

Fig. 8. Elastic properties of (*a*) single crystal of nickel and (*b*) polycrystal deformed in torsion (same sample as described above). On top are stiffness tensors in Voigt notation. The polycrystal tensor was derived with the geometric mean (*TENS*). Below are *p*-wave velocity surfaces (*VELO*) represented as gray shades with *POXX*.

the output conforms with that of *CONT*. An *hkl* file which contains symmetrically equivalent *hkl*s and information on lattice and symmetry needs to be provided. Pole figures are plotted in either stereographic or equal-area projection. If the plot contains a single pole figure, the radius can be chosen. The sector which is plotted can be restricted. In the data-set, some orientations can be skipped. Data points with weights below a certain value can be omitted. If the component file contains individual weights (*e.g.* grain size, Taylor factor *etc.*) these weights can be used to control symbol sizes and symbol types (Fig. 7).

## 7. Typical procedure

The following is an example of a typical procedure for pole figure measurements and quantitative texture analysis with the *BEARTEX* package.

(i) Evaluate with *MIMA*, preferably before one starts measuring, how many experimental data points are necessary to determine an OD with sufficient quality (Fig. 5*a*) and evaluate whether enough data are available.

(ii) Prepare a suitable sample and measure a set of pole figure *hkl*'s. Measure the background at a position well removed from the diffraction peak (*GONO*). Use either $5 \times 5^\circ$ or a hexagonal grid for pole figure coverage. If using a hexagonal grid, *HEXF* creates a file with angles.

(iii) Raw data need to be corrected for defocusing, absorption, volume and background (*CORR* or *ABXX*). Correction curves can either be empirical, theoretical (*FICO*) or a combination of the two (*FICO*). For thin films, a combination of empirical correction functions for defocusing and theoretical (for absorption/volume) is recommended. *CORR* produces a file with corrected experimental pole figures and a preliminary normalization. These are the basis for the OD analysis (Fig. 5*b*).

(iv) If a hexagonal grid was used, the data can also be rotated (*HROT*).

(v) View experimental pole figures with *POXX* and assess the quality. Particularly uniform radial variations of intensity at the periphery of the measured region may be an indication of improper background or defocusing curve.

(vi) Calculate OD with *WIMV* from experimental data. If one has sufficient data, select those pole figure ranges that are most reliable, omit pole figures with weak diffraction intensities and avoid pole figures that are partially overlapped. Complete overlaps can be handled by the program. For very sharp textures one may have to change default iteration parameters. Check errors (RP) and compare normalized experimental pole figures with recalculated pole figures (Figs. 5*b* and 5*c*) to determine the quality of the OD. One may need to measure more pole figures or improve data correction.

(vii) The OD can be smoothed and sharpened, *e.g.* for coarse-grained samples (*SMOO*). Also, it can be converted to different angle conventions or different sections (*CSEC*). The standard format is $\gamma$ sections in the Euler angle conventions of Roe/Matthies $\alpha$, $\beta$, $\gamma$ (Figs. 6*a* and 6*b*). Oblique sections are preferred for minimizing distortions in the center of the figure and of the true component form (Fig. 6*c*). From the OD one can calculate any pole figures and inverse pole figures (*PCAL*, *ICAL*).

(viii) For interpretations of the texture it is often useful to compare the OD and recalculated pole figures with model textures based on standard Gauss functions (*STOD*, *STPF*) or with simulations (Fig. 7). The OD can also be used to give weights to individual orientations, *e.g.* as a starting texture for texture simulations (*ODFW*).

(ix) Once one has an OD one may calculate texture-weighted polycrystal physical tensor properties (*TENS*) with the single-crystal tensor data. In Fig. 8 the geometric mean of the elastic tensor of a sample of polycrystalline nickel, deformed in torsion, is compared with the single-crystal tensor of nickel. Wave velocity surfaces can be created with *VELO* and plotted with *POXX* (longitudinal velocities are shown in Fig. 8).

*BEARTEX* was developed for our own research needs over many years by Siegfried Matthies, Hans-Rudolf Wenk and John Donovan with significant contributions from Galina Vinel, Florian Heidelbach, George Johnson and Alene Pearson. We acknowledge contributions from the Texture School of the former ZfK Rossendorf, Dresden, Los Alamos National Laboratory, the University of Metz (France), and input and support from the Laboratoire de Cristallographie, Grenoble, particularly the help of Patrick Juen. Financial support from NSF (grant EAR 94-17580), the Center for Materials Science at Los Alamos, IGPP-LANL, MENESRIP France, and the France Berkeley Fund is gratefully acknowledged. We are appreciative of the thoughtful comments made by the reviewers.

### References

Bunge, H. J. (1982). *Texture Analysis in Materials Science*. London: Butterworths.

Helming, K. (1991). *Textures Microstruct.* **14–17**, 187–192.

Kallend, J. S., Kocks, U. F., Rollet, A. D. & Wenk, H.-R. (1991). *Mater. Sci. Eng.* A**132**, 1–11.

Kocks, U. F., Tomé, C. & Wenk, H.-R. (1998). *Texture and Anisotropy. Preferred Orientations in Polycrystals and Their Effect on Material Properties*. Cambridge University Press. In the press.

Matthies, S. (1991). *Textures Microstruct.* **14–18**, 1–12.

Matthies, S., Helming, K. & Kunze, K. (1990*a*). *Phys. Status Solidi B*, **157**, 71–83.

Matthies, S., Helming, K. & Kunze, K. (1990*b*). *Phys. Status Solidi B*, **157**, 489–507.

Matthies, S. & Humbert, M. (1995). *J. Appl. Cryst.* **28**, 254–266.

Matthies, S. & Vinel, G. W. (1982). *Phys. Status Solidi B*, **112**, K111–120.

Matthies, S. & Vinel, G. W. (1994). *Mater. Sci. Forum*, **157–162**, 1641–1646.

Matthies, S., Vinel, G. W. & Helming, K. (1987). *Standard Distributions in Texture Analysis*. Berlin: Akademie Verlag.

Matthies, S. & Wenk, H.-R. (1992). *Phys. Status Solidi A*, **133**, 253–257.

Matthies, S., Wenk, H.-R. & Vinel, G. W. (1988). *J. Appl. Cryst.* **21**, 285–304.

Wenk, H. R. (1985). *Preferred Orientation in Deformed Metals and Rocks. An Introduction to Modern Texture Analysis*. Orlando, FL, USA: Academic Press.