popLA - AN INTEGRATED SOFTWARE SYSTEM FOR TEXTURE ANALYSIS

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The quantitative analysis of texture data is a computationally intensive task requiring mathematically sophisticated techniques. The small market has made commercial distribution of texture analysis software expensive and, on the whole, unsatisfactory. Additionally, most of the software that has been made available has been specific to one or another brand of x-ray hardware and associated computer. In some cases, proprietary data structures have made information interchange almost impossible.

The intent of this paper is to make available, at nominal cost, popLA (preferred orientation package - Los Alamos), a texture analysis software system that has been assembled by the authors for their own use. The system is designed to be implemented on the most widely available computer hardware, the IBM™ PC and compatibles operating under MS-DOS. It provides graphical output on a PC monitor, hardcopy on a laser printer or plotter, and data files in ASCII format to provide for easy information interchange and to be used in properties prediction. It requires a PC compatible personal computer running under DOS version 3.1 or later, and equipped with a hard disk, mathematics coprocessor, 480kB of available RAM and, for screen graphics, an EGA or VGA monitor. Hardcopy can be to a laser printer compatible with either the HP Laserjet series II graphics commands or the Adobe Postscript language, or to any plotter or plotter emulator compatible with the HPGL plotter graphics language. Some of the features of the package are described below. For a more detailed description, see ref. ⁶

DATA REQUIREMENTS AND DATA STRUCTURE

The software requires input in the form of experimental pole figure files containing data that have been corrected for background, defocussing etc. The pole figures may be complete, or partial (reflection) pole figures to a tilt of at least 70°. The following operations are available for the pole figure data: symmetry analysis and rotation or tilting to compensate for sample misalignment, smoothing, symmetrization, and (in the case of incomplete pole figures) completion in a crystallographically consistent way by harmonic analysis.

The data file structure is consistent between pole figures and ODF files, containing a header which identifies the sample, pole figure or section, and the

domain over which the data are available, scaling factor etc. This file structure allows one display program to handle both pole figures and ODFs, and also facilitates easy data transfers between different laboratories. The data themselves are four-digit integers scaled (as far as their values allow) so that random = 100. Table 1 shows the header and first few lines of a {111} pole figure measured to 80° tilt angle.

TABLE 1. Beginning of typical {111} pole figure file. The second line contains parameters describing the data domain, "random" level etc.

CU ROLLED 80%				Measured to 80 degrees tilt											
(111)	5.0	80.0	5.0360.0	1	1	2-1	3	100	13						
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
2	3	2	3	2	2	3	2	2	3	2	2	2	2	3	2
3	4	4	4	3	3	4	3	2	2	3	3	2	3	3	2
3	4	3	3	3	3	2	2	3	3	2	3	3	3	5	4
4	3	3	4	3	5	3	3	3	3	2	4	3	4	2	4
3	4	3	2	3	4	3	1	4	4	3	3	4	5	6	6
7	6	5	6	6	5	5	4	4	4	4	3	3	4	3	3
2	3	3	3	3	2	3	4	4	4	4	5	6	6	5	7
8	8	7	8	8	7	8	7	7	5	5	4	5	4	4	2
5	4	5	4	4	5	4	5	5	6	8	9	10	13	16	20
33	35	33	28	21	18	13	11	9	8	6	5	5	4	4	3
3	3	3	4	4	4	4	5	6	8	9	11	13	18	22	29
40	38	35	33	27	21	19	17	13	10	9	8	8	6	4	5
5	6	6	6	6	6	7	9	11	14	19	28	37	53	75	103
204	220	212	185	142	102	68	43	29	19	15	9	8	7	7	5
4	5	5	5	6	6	7	8	12	15	24	33	51	78	116	160
262	254	223	179	134	96	70	46	38	27	21	15	12	10	8	7

ODF ANALYSIS

ODF analysis is available using both the spherical harmonic method^{1,2} (even terms only) for cubic, tetragonal, hexagonal and orthorhombic crystals, and by a WIMV based method³ for cubic, tetragonal, trigonal, hexagonal, and orthorhombic crystals. ODF output is as an ASCII file containing ODF sections in the conventions of Bunge¹, Roe² or Kocks⁴ according to the user's choice. The ODF files may be used to produce graphical output (see below) or "weighted grains" files that may be used for subsequent use in modelling texture evolution and anisotropy of properties⁵.

GRAPHICAL OUTPUT

Graphical output of pole figure and ODF data is available in a variety of formats. Polar plots of pole figures and ODF sections (both normal and oblique⁴) may be made in stereographic or equal-area projection⁹. Both grey-shades and color graphics are available with an appropriate computer monitor, and grey shades are available in hardcopy on a laser printer (Figures 1-3). Plotter output is available as contour plots in equal area or stereographic projection for both pole figures and

ODF sections, or in the more conventional form of Cartesian plots for ODF sections.

Figure 1. Measured equal-area incomplete pole figures (above) from a misaligned sample, and the same data (below) after rotation, symmetrization and completion.

PROPERTIES PREDICTIONS

Anisotropy of properties is of recurring interest in texture research, and some capability for properties prediction is included in popLA. The "weighted grains" files provide an economical route to self-consistent methods of property calculations and are used by the "LApp" plastic properties code, a PC version of which is included with popLA. Additionally, programs are supplied for the rapid assessment of R-values or yield surface sections in cubic metal sheets can be made from the spherical harmonic coefficients using the Taylor⁷ model of polycrystalline plasticity as described by Viana et. al⁸.

INTEGRATION

The authors have attempted as far as possible to maintain a consistent "user interface" for the software. Prompts are provided at all points where user input is needed, and where appropriate, default inputs are suggested. The consistent file

Figure 2. Orientation distribution of copper deformed in plane strain compression to a von Mises strain of 1.1, presented as constant ν sections in equal-area projection. Also shown is the same distribution after conversion to weighted discrete grains.

Figure 3. Neutron pole figures from a deformed calcite (trigonal) sample, and the corresponding constant ν (oblique) sections of the orientation distribution. The sample was assumed to have monoclinic statistical symmetry. The data were analysed by the WIMV method.

structure allows easy transfer of data from one program to another within the package. Additionally, a menu is available from which the various programs may be invoked without the need to remember the many individual program names.

ACKNOWLEDGEMENTS

The authors wish to thank L. Stixrude, M.A. Przystupa, T.G. Schofield, A.C. Biondo, R.E. Bolmaro, T. Ozturk, J. Hirsch, C.N. Tome and G.R. Canova, whose programming contributions are incorporated in the package. The major portion of this work was supported by the Division of Basic Energy Sciences, U.S. Department of Energy and by the Institute of Geophysics and Planetary Physics of the University of California and Los Alamos National Laboratory.

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To obtain the popLA package, write to :

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