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RECOVERING ODFS WITH MAXIMUM ENTROPY AND THEIR GEOSCIENTIFIC INTERPRETATION

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SPECIFICS OF QUANTIATIVE TEXTURE ANALYSIS IN GEOSCIENCES

While in material sciences the major emphasis is on how to control a process both in the laboratory as well as in production to cause a required preferred crystal orientation and corresponding macroscopic physical properties, the problem in geosciences is in many instances just the opposite and much more difficult: which processes caused an observed pattern of preferred crystal orientation. The answer to this question cannot be achieved by quantitative texture analysis only but requires a complete study of the microstructure and the entire geologic situation on different scales. Quantitative texture analysis in geosciences can but add an additional parameter to narrow down the multiple ambiguities of the geological problem. Therefore, this parameter itself should be conservatively estimated, i.e. as safe as possible given the data.

Another application may be in geophysics concerning the relationship between preferred crystal orientation and velocity anisotropy which has been quantitatively established for instance for metals, mantle amphibolites and peridotites etc. This implies for the interpretation of seismic data that travel times are not related by some simple function to distance (depth) but depend on the local geologic structure, and it is by no means clear which properties are responsible to generate a seismic reflector surface; anisotropy may well be one of them. Unless elastic properties are known for rocks composing the crustal/mantle segment of interest, interpretation of reflection seismic data is therefore ambiguous. Quantitative texture analysis may provide a missing parameter to sufficiently characterize rocks for the purpose of safe, i.e. less ambiguous interpretation of seismic data.

ENTROPY OPTIMIZATION IN TEXTURE ANALYSIS

Thus, the orientation distribution is a basic mathematical approach of describing and quantifying anisotropy, and recovering an odf from experimental pdfs is the crucial prerequisite of quantitative texture analysis. Motivated by its specific purposes in geosciences we should apply mathematical models and additional modeling assumptions which provide a solution that allows safe interpretation.

The entropy maximizing solution is proposed here because it yields the (truly nonnegative) odf as uniform (with respect to entropy) as possible consistent with the experimental data thus avoiding artificial components, also "ghosts" caused by the specific properties of the diffraction experiment [1,2,3]. Its use is theoretically justified by Jaynes' concentration theorem; when applied to the QTA problem, it states that all feasible odfs are strongly concentrated near the particular feasible odf with maximum entropy. The approach of finite series expansion and entropy optimization has been coded in a FORTRAN package called MENTEX (Maximum ENTropy TEXture).

APPLICATIONS OF THE MENTEX METHOD

Tables 1 and 2 summarize the results of MENTEX when applied to the three incomplete pdfs of reflections (100), (110), (111) arbitrarily truncated at 75 degrees of the data sets 'MIX2' and 'Santa Fe' introduced by Matthies. The main difference of the two model odfs is that $S(f_{MIX2}) > S(f_{MIX2})$ but $S(f_{SAFE}) < S(f_{SAFE})$. In both cases, the mathematical model odf and the odf recovered from the corresponding pdfs agree well.

Table 1: Summary of numerical results of the mathematical model MIX2

Problem MIX2 Data MIX2IPDF	min	max	comment	
odf f	0.54	5.75		
even f	0.06	4.89	S(f) > S(f)	
odf f	0.5768	5.5355	after 30 iterations	
			RP0	RP1
pdf (100) inc$^{1)}$	0.5940	1.8650	0.3435	0.3299
(100) rec	0.5898	1.8744		
pdf (110) inc$^{1)}$	0.6750	2.2910	0.2941	0.2341
(110) rec	0.6720	2.2861		
pdf (111) inc$^{1)}$	0.6510	1.8600	0.2653	0.1961
(111) rec	0.6532	1.8670		
pdf (311)$^{2)}$inc$^{1)}$	0.8200	1.3390	0.4208	0.2949
(311) calc	0.8236	1.3286		

REMARKS: 1) arbitrarily truncated at 75 degrees
2) not used as input for MENTEX

Table 2: Summary of numerical results of the mathematical model Santa Fe

Problem Santa Fe Data SAFEIPDF	min	max	comment	
odf f	0.73	5.03		
even f	0.09	3.98	S(f) < S(f)	
odf f	0.7218	5,2346	after 30 iterations	
			RP0	RP1
pdf (100) inc$^{1)}$	0.7300	1.7590	0.1831	0.2260
(100) rec	0.7273	1.7588		
pdf (110) inc$^{1)}$	0.7310	1.6890	0.2014	0.1699
(110) rec	0.7295	1.6909		
pdf (111) inc$^{1)}$	0.7310	1.5400	0.1372	0.1200
(111) rec	0.7300	1.5415		
pdf (311)$^{2)}$inc$^{1)}$	0.7600	1.2530	0.3408	0.2909
(311) calc	0.7563	1.2622		

REMARKS: 1) arbitrarily truncated at 75 degrees
2) not used as input for MENTEX

Encouraged by these results, MENTEX has also been used to analyze preferred orientation of minerals in naturally and experimentally deformed ores. As a typical example the analysis of an experimentally deformed pyrite ore is presented. The specimen is constituted of pyrite grains with a mean diameter of 0.06mm. A sample has been strained 24% by axial compression at a strainrate of 2*10exp(-4) , at 600°C under a confining pressure of 300MPa [4]. After deformation the grain size has been determined to be 0.04mm [5]. This grain size reduction indicates cataclastic flow as one component of deformation modes. In order to check if there were also operating intracrystalline glide modes the preferred orientation of pyrite has been determined by neutron diffraction [6]. From these measurements the eight complete pole figures of reflections (111), (200), (210), (220), (222), (211), 311), and (321) were available. From these the (111)-, (200)- and (220) pole figures were used to calculate a MENTEX odf. Fig. 1 shows the (200)

Fig. 1a

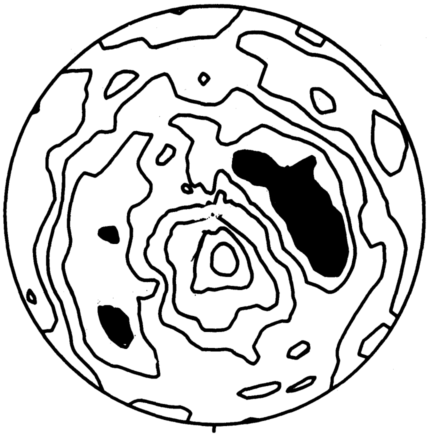

Fig. 1b

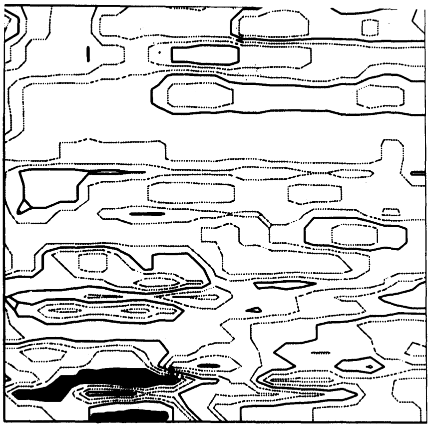

Fig. 2a

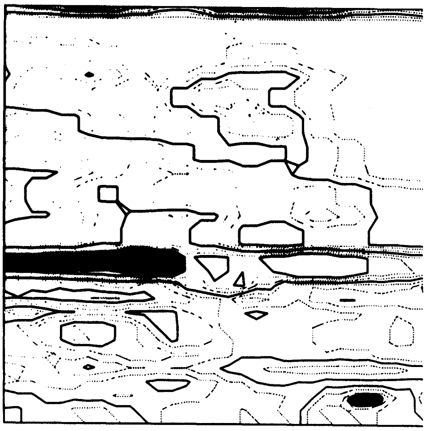

Fig. 2b

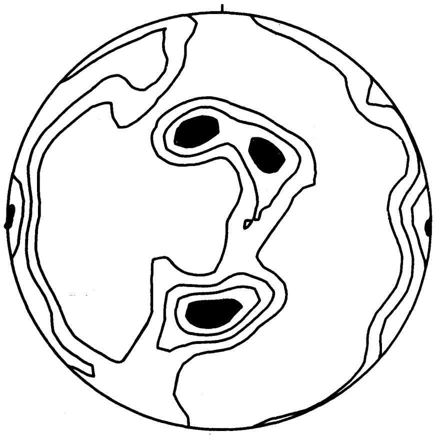

Fig. 3a

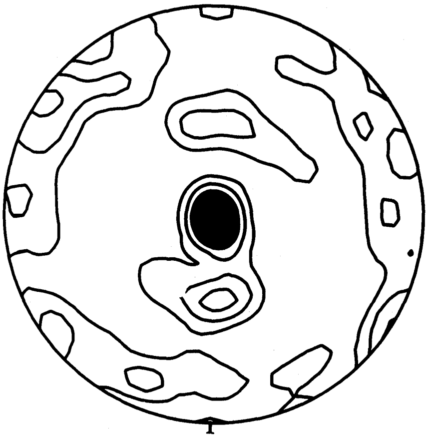

Fig. 3b

pole figures of an undeformed and an experimentally deformed pyrite sample which have both very weak preferred orientation and look rather similar; the same holds more or less for the other polefigures. Fig. 2 displays characteristic sections of the odf of both samples. Both odfs show elongated regions of larger and smaller densities parallel to the phi1-axis, changing their densities perpendicular to the phi1- and PHI-axes very rapidly. This is interpreted that there are numerous small volumes of large densities distributed within the Euler space of orientations. In order to gain some insight into their contribution to the corresponding pole figures, the Eulerian angles of their centers were determined from the odf and sorted into classes according to PHI: 0-15, 15-30, ... , 75-90. From these grouped data mathematical model pole figures were derived by means of the program POLSGL33 [7]. In general these modelled pole figures reveal similar orientation groups in both samples. The most remarkable difference was found in the orientaion class PHI=45-60: The deformed sample shows a (111) maximum in the center of the pole figures (fig. 3a) which is missing in the undeformed sample (fig. 3b). Therefore it is not unlikely that intracrystalline glide modes generated this preferred orientation with (111) perpendicular to the axis of compression. Other cubic ore minerals usually show a preferred orientation with (110) perpendicular to the axis of compression [8]. A detailed analysis of the preferred orientation in pyrite ores will be published elsewhere [5].

Summarizing our experience [9,10] with the maximum entropy method for pdf- to odf inversion we conclude that

- few and incomplete pdfs can be analyzed without additional effort and are sufficient to recover a reasonable estimate of the true odf,
- the relaxation parameter provides an apropriate means to account for small non-negligible experimental errors in the measured pdfs,
- a property of the odf itself is used as a stopping rule for the iterations,

- the recovered odf is nonnegative and explains the pdfs well,
- the recovered odf is a rather conservative estimate of the (unknown) true odf supporting a safe interpretation.

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