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THE DISTRIBUTION OF DISORIENTATION ANGLES IF ALL RELATIVE ORIENTATIONS OF NEIGHBOURING GRAINS ARE EQUALLY PROBABLE

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In investigating the grain structure of metals it is of interest to determine the degree to which the relative orientations of neighbouring grains deviate from random. For grains with the same crystal lattice one can determine experimentally the disorientation angle between neighbouring grains, i.e. the minimum angle needed to rotate one lattice so that it becomes parallel to the other. The frequency of these angles is then compared to the density of disorientation angles computed under the assumption of no correlation between the orientations of neighbouring grains. This density has been determined for the cubic system by Handscomb [1] and by Mackenzie [2]. Two related papers are Mackenzie [3] and Warrington-Boon [4]. In this paper we consider the non-cubic crystal systems and determine mean, standard deviation, median, density and distribution of the disorientation angle.

TABLE 1
M the Highest Order of a Symmetry Axis and N the Number of Rotations in the Holohedry.

crystal system	tri-clinic	mono-clinic	ortho-rhombic	rhombo-hedral	tetra-gonal	hexa-gonal
M	1	2	2	3	4	6
N	1	2	4	6	8	12

Following Handscomb [1], we find for the density of disorientation angles p(d), where d is measured in degrees

$$p(d) = (N/90)\cdot \sin^2(d/2)\cdot f(d), \qquad (1)$$

where f(d) is the fraction of the surface of the sphere with radius sin(d/2) that lies within the following concentric solid: a prism with regular N-gons as bases, squares as lateral faces, and with all edges of length $2\cdot\cos(d/2)\cdot\tan(90^\circ/M)$ in the hexagonal, tetragonal, rhombohedral and orthorhombic system. In the monoclinic system the solid becomes a (concentric) layer of thickness $2\cdot\cos(d/2)$, and in the triclinic system it becomes all space. It follows that for

$$0^\circ \le d \le 180^\circ/M \quad , \; p(d) = (N/180)(1-\cos d) \qquad (2)$$

$$180^\circ/M \le d \le 180^\circ\cdot M/N \quad , \; p(d) = (N/180)\cdot\tan(90^\circ/M)\cdot\sin d \qquad (3)$$

Eq. (2) is sufficient to deal with the triclinic system, Eqs. (2) and (3) to deal with the monoclinic system, so that we can restrict ourselves in the following to the four remaining systems, where N=2M.

$$90^\circ \le d \le 2 \text{ arc tan } \left(\sqrt{1+\tan^2(90^\circ/M)}\right),$$
$$p(d) = (M/90)\left[(M+\tan(90^\circ/M))\cdot\sin d - M(1-\cos d)\right] \qquad (4)$$

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$$2\,\mathrm{arc\,tan}\left(\sqrt{1+\tan^2(90^\circ/M)}\right) \le d \le 2\,\mathrm{arc\,tan}\left(\sqrt{1+2\tan^2(90^\circ/M)}\right),$$

$$\begin{aligned} p(d) = {} & (M/90)\Big[(M+\tan(90^\circ/M))\cdot\sin d - M(1-\cos d) + (M/180)\Big\{(1-\cos d) \\ & \cdot\Big(\mathrm{arc\,cos}\frac{1-\tan^2(d/2)\cos(180^\circ/M)}{\tan^2(d/2)-1} + 2\,\mathrm{arc\,cos}\frac{\tan(90^\circ/M)}{\sqrt{\tan^2(d/2)-\tan^2(90^\circ/M)}\sqrt{\tan^2(d/2)-1}}\Big) \\ & -2\sin d\cdot\Big(2\,\mathrm{arc\,cos}\frac{\tan(90^\circ/M)}{\sqrt{\tan^2(d/2)-1}} + \tan(90^\circ/M)\cdot\mathrm{arc\,cos}\frac{1}{\sqrt{\tan^2(d/2)-\tan^2(90^\circ/M)}}\Big)\Big\}\Big] \end{aligned} \quad (5)$$

TABLE 2

The Limits for the Validity of Eqs. (2-5) for p(d). ($X=\tan^2(90^\circ/M)$)

crystal system	$180^\circ/M$	$180^\circ M/N$	$2\,\mathrm{arc\,tan}(\sqrt{1+X})$	$2\,\mathrm{arc\,tan}(\sqrt{1+2X})$
triclinic	180°	180°	---	---
monoclinic	90°	180°	---	---
orthorhombic	90°	90°	109.47°	120°
rhombohedral	60°	90°	98.21°	104.48°
tetragonal	45°	90°	94.53°	98.42°
hexagonal	30°	90°	91.99°	93.84°

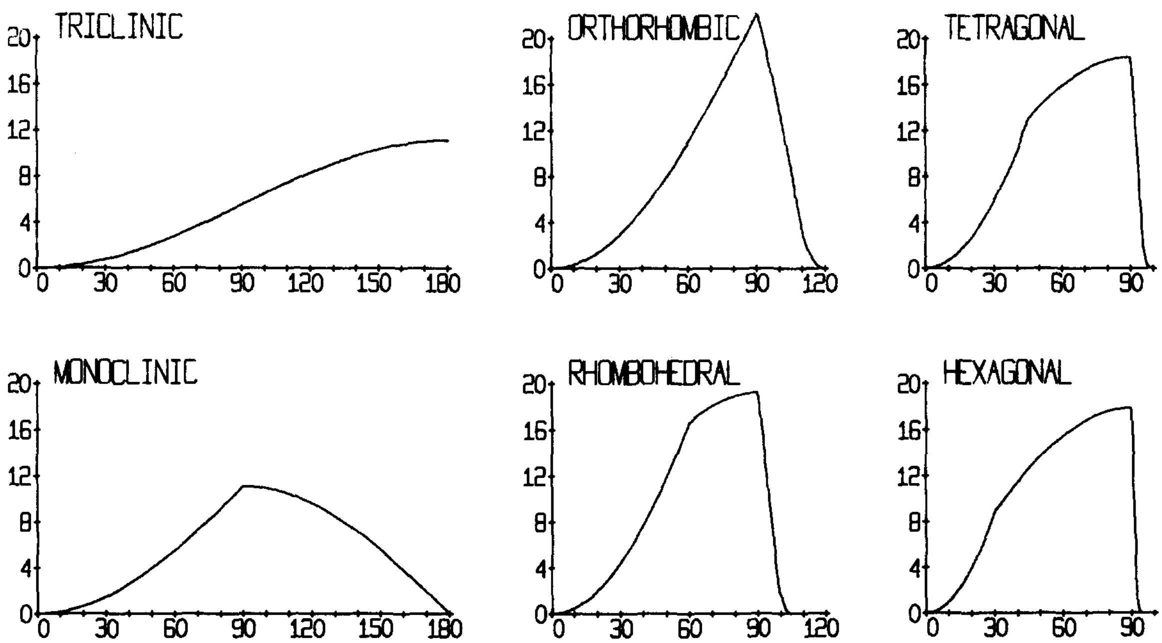

FIG. 1

The density function p(d) for the disorientation angle. The ordinate gives the density in per mille as a function of the angle in degrees. (A similar graph for the cubic system is given in [2].)

TABLE 3
The Density p(d) of the Disorientation Angle d

Disori-entation angle d°	Density p(d) in per mille for the non-cubic crystal systems					
	tri-clinic	mono-clinic	ortho-rhombic	rhombo-hedral	tetra-gonal	hexa-gonal
0	0	0	0	0	0	0
5	0.02	0.04	0.08	0.13	0.17	0.25
10	0.08	0.17	0.34	0.51	0.68	1.01
15	0.19	0.38	0.76	1.14	1.51	2.27
20	0.34	0.67	1.34	2.01	2.68	4.02
25	0.52	1.04	2.08	3.12	4.16	6.25
30	0.74	1.49	2.98	4.47	5.95	8.93
35	1.00	2.01	4.02	6.03	8.04	10.25
40	1.30	2.60	5.20	7.80	10.40	11.48
45	1.63	3.25	6.51	9.76	13.02	12.63
50	1.98	3.97	7.94	11.91	14.10	13.68
55	2.37	4.74	9.48	14.21	15.08	14.63
60	2.78	5.56	11.11	16.67	15.94	15.47
65	3.21	6.42	12.83	17.44	16.68	16.19
70	3.66	7.31	14.62	18.08	17.30	16.79
75	4.12	8.24	16.47	18.59	17.78	17.25
80	4.59	9.18	18.36	18.95	18.13	17.59
85	5.07	10.14	20.29	19.17	18.34	17.80
90	5.56	11.11	22.22	19.25	18.41	17.86
91				17.48	15.28	10.82
92				15.68	12.09	3.66
93				13.85	8.84	0.55
94				12.00	5.53	
95	6.04	11.07	18.09	10.08	2.61	
96				8.14	1.14	
97				6.17	0.35	
98				4.17	0.03	
99				2.58		
100	6.52	10.94	13.49	1.58		
101				0.89		
102				0.43		
103				0.15		
104				0.01		
105	6.99	10.73	8.45			
110	7.46	10.44	3.10			
115	7.90	10.07	0.63			
120	8.33	9.62	0			
130	9.13	8.51				
140	9.81	7.14				
150	10.37	5.56				
160	10.78	3.80				
170	11.03	1.93				
180	11.11	0				

TABLE 4

The Distribution $P(d) = \int_0^d p(x)dx$ of the Disorientation Angle

Disori- entation angle d°	Distribution P(d) for the non-cubic crystal systems: tri- clinic	mono- clinic	ortho- rhombic	rhombo- hedral	tetra- gonal	hexa- gonal
5	0.00004	0.00007	0.00014	0.00021	0.00028	0.00042
10	0.00028	0.00056	0.00113	0.00169	0.00225	0.00338
15	0.00095	0.00190	0.00379	0.00569	0.00759	0.01138
20	0.00224	0.00449	0.00897	0.01346	0.01794	0.02691
25	0.00437	0.00873	0.01746	0.02619	0.03492	0.05238
30	0.00751	0.01502	0.03005	0.04507	0.06009	0.09014
35	0.01187	0.02374	0.04748	0.07122	0.09496	0.13812
40	0.01762	0.03523	0.07047	0.10570	0.14093	0.19247
45	0.02492	0.04984	0.09968	0.14953	0.19937	0.25279
50	0.03394	0.06788	0.13575	0.20363	0.26721	0.31862
55	0.04481	0.08962	0.17925	0.26887	0.34021	0.38946
60	0.05767	0.11534	0.23068	0.34601	0.41782	0.46476
65	0.07262	0.14525	0.29050	0.43134	0.49944	0.54396
70	0.08978	0.17955	0.35910	0.52021	0.58446	0.62646
75	0.10920	0.21841	0.43681	0.61195	0.67222	0.71161
80	0.13097	0.26194	0.52388	0.70587	0.76205	0.79878
85	0.15512	0.31025	0.62049	0.80124	0.85328	0.88731
90	0.18169	0.36338	0.72676	0.89734	0.94521	0.97651
95	0.21068	0.41887	0.82776	0.97101	0.99734	
100	0.24208	0.47393	0.90692	0.99779		
105	0.27587	0.52815	0.96194			
110	0.31200	0.58112	0.99074			
115	0.35040	0.63243	0.99898			
120	0.39100	0.68169	1			
130	0.47838	0.77259				
140	0.57317	0.85106				
150	0.67418	0.91471				
160	0.78002	0.96161				
170	0.88917	0.99033				
180	1	1				

TABLE 5

The Median, the Mean and the Standard Deviation of the Disorientation Angle

Crystal system	tri- clinic	mono- clinic	ortho- rhombic	rhombo- hedral	tetra- gonal	hexa- gonal
median	132.35°	102.39°	78.68°	68.88°	65.03°	62.25°
mean	126.48°	102.30°	75.16°	66.63°	63.01°	60.07°
standard deviation	37.01°	33.76°	20.85°	19.28°	19.50°	20.21°

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