

Determination of Near-Coincident Cells for Hexagonal Crystals. Related DSC Lattices

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Abstract

Crystallographic data concerning geometric properties of hexagonal lattices of C_α , Zn, Be_α , Ti_α , Zr_α , Mg and Cd are obtained from two different computation techniques. These properties are related to the relative orientations of identical hexagonal lattices 1 and 2 which superimpose two multiple cells $M1$ and $M2$ within a given small deformation. These orientations are listed for ratios $\Sigma = |\text{volume of cells } M1 \text{ (or } M2)/\text{volume of the unit cell}|$ varying from 1 to 25. Their number are limited by choosing all the principal strains transforming $M1$ into $M2$ less than or equal to 1%.

Introduction

Three techniques have been used to determine the relative orientations of identical hexagonal crystals which give rise to a near coincidence of two cells of the two crystal lattices 1 and 2, cells denoted hereinafter $M1$ and $M2$ respectively. [This has been referred to by previous workers as a 'coincidence' or 'near-coincidence site lattice' or '*orientation de macle*',* where the number Σ_1 (or Σ_2) is defined by the ratio volume of $M1$ (or $M2$)/volume of the unit cell.] Two techniques depend either upon searching for vectors of common length arising from rational values of $(c/a)^2$ (Fortes, 1973; Warrington, 1975) or in searching for coincidences arising from rotation about specific axes, chosen *a priori*, of (low) crystallographic index (Bruggeman, Bishop & Hartt, 1972). The first method derives from that used by Warrington & Bufalini

(1971) for cubic crystals; the second from the use of a 'generation function' typified by Ranganathan (1966) and Goux (1961). The third technique (Bonnet & Cousineau, 1977), tested on Zn/Zn and Ni_3Al (cubic)/ Ni_3Nb (orthorhombic), depends on a numerical method of calculation capable of treating the case of general lattices and envisaged in part by Santoro & Mighell (1973). It takes into account the experimental [rather than idealised or rational values of $(c/a)^2$] values of the lattice parameters. The technique determines relative orientations that, with additional imposed constraints (which may be chosen arbitrarily small) on $M1$, will give full or true coincidence with $M2$.

Determination of relative orientations

In searching for a 'constrained coincidence' the worker must compromise and set limits on the deviation from exact coincidence that is to be allowed. In the numerical method (Bonnet & Cousineau, 1977) this is represented by a maximum value of $S = |\varepsilon_1| + |\varepsilon_2| + |\varepsilon_3|$ where $\varepsilon_1, \varepsilon_2, \varepsilon_3$ are the principal strains of the pure deformation D transforming lattice 1 into lattice 2. D^{-1} transforms lattice 2 into a fictitious lattice denoted lattice 2', which can be exactly superposed onto lattice 1 (Bonnet & Durand, 1975). The unit cell of this CSL (coincidence site lattice) is defined either by $M1$ or by the deformed cell $M2$, denoted $M2'$. In order to save computer time and attempt to make the search efficient, limits are set on $\Delta\theta$, the value by which the angle of rotation about some determined axes is incremented, and on ΔU , the rounding term to obtain integer elements of the matrix $|u|_{F1}$ transforming $M1$ into $M2'$. The determinant of this matrix, expressed in the coordinate system $F1$ attached to the hexagonal unit cell of lattice 1, is equal to Σ_1/Σ_2 (see the above reference). For identical crystals and small deviation from exact coincidence, $\Sigma_{12} = \Sigma_2 = \Sigma$.

* We note for the benefit of our readers whose mother tongue is English that the term '*orientation de macle*' as defined by Friedel (1964) is more general a concept than the nearest English equivalent of 'twin' used in its restrictive sense.

To gain an insight into the relevant merits of the alternative methods, the results for C and for the hexagonal metals Zn,* Be_α, Ti_α, Zr_α, Mg, Cd were derived by the above technique and that of the rational (c/a)² route of Warrington (1975). The latter technique assumes that all constrained coincidences lie close to perfect coincidence of ideal crystals with nearby rational values of (c/a)²; it is necessary, of course, to search for all relevant values of (c/a)² that approximate to within an arbitrary deviation from the experimental value. This value is measured with great accuracy for all the hexagonal crystals here chosen. The two techniques give consistent results and find all relevant coincidence provided that Δu is made large enough and that the integer ratios (c/a)² contain all values up to sufficiently large integers. The tables presented show that, for example for zinc, it was necessary to increase Δu from 0.3 to 0.4. On the other hand, many additional solutions for the necessary and quoted values of (c/a)² are found to be excluded from the table by the imposed condition of S_{max}.

Presentation of the results

Tables 1 and 2 have been prepared using the crystal parameters reported by Donnay & Ondik (1973) except for Ti (Mitchell, 1979) and C_α (Cullity, 1967), and the following values of calculation variables:

Be_α, Ti_α, Zr_α c/a = 1.589 ± 0.004;
Mg c/a = 1.624, Cd c/a = 1.885, C_α c/a = 2.723;
S_{max} = 25, ΔL = 0.5 Å, S_{max} = 0.021, Δu = 0.4,
Δθ = 0.003.

For the rational (c/a)² technique all values of m/n where m and n are integers up to m = 117 and n = 20 were investigated; many ratios (typically from high m and n) where c/a lies within a deviation of the experimental value of c/a do not give rise to solutions for Σ ≤ 25.

The values of the rotation axis and angle correspond to the disorientation value [i.e. the lowest rotation angle that may describe a given relative orientation provided that the axis lies within the unit stereographic triangle; since the two crystals are otherwise identical this includes, therefore, a reduction *via* the inverse rotation as well as all possible symmetry rotations, see, for instance, Mackenzie (1958) and Bonnet (1980)].

For a complete understanding of the geometric quantities mentioned in the tables, the reader must refer to the work of Bonnet & Cousineau (1977). [uvw] and θ_d are the pairs of disorientation axis/angle for which a cell M2 is near coincident to a cell M1. The value ε describes the intensity of the deformation, since in each

* In Bonnet & Cousineau (1977), the two last solutions Σ = 21 are equivalent. One of them has to be removed for the benefit of a Σ = 23 (c²/a² = 27/8) described in this paper.

Table 1. *Near-coincident cells for the hexagonal metals Be_α, Cd, Mg, Ti_α, Zn, Zr_α and other related crystallographic quantities*

The rotation axes and angles are expressed as disorientation values. Entries are ordered in increasing Σ value and increasing rotation angle *except* where, for a given rotation axis and more than one ideal c/a value, more than one CSL is produced at closely similar rotation angles. In such cases successive entries quote Σ values and rotation angles and the axis symbol is not repeated. The axis is not repeated where it is unchanged in succeeding entries in the column, thus four entries for Cd 7/2, Σ = 9 to Cd 18/5, Σ = 23 all share the same rotation axis [210]. The values of ε quoted are for the metal appearing in the same line of column one.

Crystals (c/a) ²	Σ	uvw θ _d (°)	ε (×10 ³)	U _{F1} (×Σ)	M1 U1 _{F1}	DSC-1 _{F1} (×Σ)
All	7	001	0	8 $\bar{3}$ 0	0 3 1	3 1 0
				3 5 0	0 2 3	2 3 0
Any		21.79		0 0 7	1 0 0	0 0 7
Be 5/2	7	210	2	7 0 0	$\bar{2}$ 0 $\bar{1}$	0 0 $\bar{7}$
Ti			4	2 3 $\bar{10}$	$\bar{1}$ $\bar{1}$ 2	$\bar{1}$ 5 $\bar{1}$
Zr		64.62	7	$\bar{2}$ 4 3	0 1 1	1 2 1
	18/7	25	6	25 0 0	$\bar{2}$ 0 $\bar{1}$	0 0 $\bar{25}$
			7	11 36	$\bar{1}$ $\bar{1}$ $\bar{9}$	$\bar{1}$ 18 $\bar{21}$
		63.90	7	14 11	0 $\bar{1}$ $\bar{4}$	1 7 $\bar{4}$
Cd 7/2	9	210	6	9 0 0	$\bar{2}$ 0 $\bar{1}$	0 0 $\bar{9}$
			2	5 $\bar{14}$	$\bar{1}$ $\bar{1}$ 3	$\bar{1}$ 7 $\bar{1}$
		56.25	2	4 5	0 1 1	1 2 1
Zn 7/2	9		6	9 0 0	2 0 1	0 0 9
			2	5 $\bar{14}$	$\bar{1}$ $\bar{1}$ $\bar{3}$	$\bar{1}$ 7 1
		56.25	2	4 5	0 1 $\bar{1}$	1 $\bar{2}$ $\bar{1}$
Zn 17/5	22		6	22 0 0	2 0 0	0 0 22
			5	12 34	1 1 9	$\bar{1}$ 17 20
		56.94	5	10 12	0 $\bar{1}$ 2	1 5 2
Cd 18/5	23		5	23 0 0	2 0 $\bar{1}$	0 0 $\bar{23}$
			5	13 36	1 1 8	$\bar{1}$ 18 3
		55.58	5	10 13	0 $\bar{1}$ 3	$\bar{1}$ 5 3
Mg 21/8	9	100	-2	9 $\bar{2}$ $\bar{7}$	1 1 4	$\bar{1}$ 5 4
			0	5 $\bar{14}$	0 1 7	2 1 8
		56.25	0	4 5	0 1 2	2 1 $\bar{1}$
Mg 27/10	23		10	23 5 $\bar{18}$	$\bar{1}$ 1 9	1 $\bar{11}$ 9
			0	13 36	0 1 18	2 1 18
		55.58	0	10 13	0 $\bar{1}$ 5	2 1 5
Zn 27/8	9	100	10	9 $\bar{3}$ $\bar{9}$	$\bar{1}$ 1 1	3 3 6
			0	3 18	0 3 3	6 3 3
		70.53	0	4 3	0 1 2	$\bar{1}$ 1 $\bar{1}$
Mg 8/3	10	210	-6	10 0 0	2 0 0	0 0 10
			4	2 $\bar{16}$	1 $\bar{2}$ 1	2 4 6
		78.46	3	6 2	0 $\bar{1}$ 2	1 3 2
Cd 18/5	11	100	6	11 5 $\bar{12}$	$\bar{1}$ $\bar{1}$ 2	1 3 8
			0	1 24	0 2 5	2 5 5
		84.78	0	5 1	0 1 3	$\bar{1}$ 3 3
Be 5/2	11		2	11 5 $\bar{10}$	1 $\bar{1}$ 3	1 8 3
Ti			4	0 1 $\bar{20}$	0 2 5	2 5 5
Zr		84.78	7	0 6 1	0 $\bar{1}$ 3	1 3 3
Cd 7/2	13		8	13 6 $\bar{14}$	$\bar{1}$ $\bar{1}$ 3	$\bar{1}$ 10 3
			0	1 28	0 2 7	2 7 7
		85.59	0	6 1	0 1 3	1 3 3
Ti 18/7	13		10	13 6 $\bar{12}$	1 $\bar{1}$ 3	1 9 4
Zr			7	0 1 24	0 2 5	2 5 5
		85.59	0	7 1	0 $\bar{1}$ 4	1 4 4
Cd 39/11	24		1	24 $\bar{11}$ $\bar{26}$	1 1 7	$\bar{1}$ 19 5
			0	2 52	0 2 14	2 14 14
		85.22	0	11 2	0 $\bar{1}$ 5	1 5 5

Table 1 (cont.)

Crystals (c/a) ²	Σ	uvw θ_d (°)	ε ($\times 10^3$)	U_{F1} ($\times \Sigma$)	$M1$ $U1_{F1}$	$DSC-1_{F1}$ ($\times \Sigma$)
Cd 18/5	21	210	6	21 0 0	2 0 1	0 0 21
		64-62		6 9 $\overline{36}$	1 3 $\bar{1}$	3 $\bar{6}$ 12
7/2	25		7	25 0 0	2 0 1	0 0 25
		63-90		7 11 $\overline{42}$	1 3 4	3 7 16
Cd 7/2 Zn	21	510	7	22 5 $\overline{14}$	1 3 2	1 9 $\overline{12}$
		70-53		7 3 6 $\overline{42}$	3 2 $\bar{1}$	3 $\bar{6}$ 6
Mg 21/8	21	14 7 2	2	23 6 7	3 2 1	1 10 3
		73-40		13 3 $\overline{28}$	2 $\bar{1}$ 3	4 2 9
Zn 27/8	21	210	7	21 0 0	2 $\bar{1}$ $\bar{1}$	0 0 $\overline{21}$
		44-41		4 12 7	0 $\bar{1}$ 2	2 1 6
Be 51/20 Ti Zr	22	100	6	22 5 $\overline{17}$	1 0 8	1 11 8
		56-94		5 0 12 $\overline{34}$	0 $\bar{1}$ $\overline{17}$	2 0 $\overline{16}$
Be 18/7 Mg Ti Zr	23	100	7	23 2 $\overline{12}$	1 3 0	3 2 11
		34-30		7 0 19 $\overline{24}$	1 6 $\bar{1}$	6 4 $\bar{1}$
Be 5/2 Ti Zr	23	100	2	23 8 $\overline{20}$	1 3 2	2 5 9
		72-28		4 0 7 $\overline{40}$	0 5 4	4 10 5
Be 5/2 Ti Zr	23	210	2	23 0 0	2 0 1	0 0 23
		55-58		3 5 13 $\overline{30}$	1 3 3	3 5 14
Be 5/2 Ti Zr	23	20 10 3	2	25 7 10	2 1 2	1 12 9
		86-26		4 17 2 $\overline{30}$	0 4 1	3 10 4
Cd 18/5	23	100	6	23 8 $\overline{24}$	1 1 4	3 4 $\overline{13}$
		72-28		0 7 48	0 3 8	6 8 3
Cd 7/2	23	210	7	23 0 0	2 $\bar{1}$ 0	0 0 $\overline{23}$
		77-44		9 5 $\overline{42}$	1 1 7	3 7 $\overline{13}$
Cd 7/2 Zn	23	100	4	23 2 $\overline{14}$	1 $\bar{1}$ 3	1 7 8
		34-30		4 0 19 $\overline{28}$	0 2 7	2 14 7
Mg 21/8	23	100	2	23 9 $\overline{21}$	1 2 4	3 5 13
		77-44		0 5 42	0 3 7	6 10 3
Mg 21/8	23	210	1	23 0 0	2 1 1	0 0 23
		34-30		2 19 $\overline{21}$	1 1 11	1 $\overline{11}$ 11
Zn 27/8	23	18 9 2	10	25 6 9	3 $\bar{1}$ 0	1 11 3
		79-98		15 1 36	2 3 3	4 2 11
Mg 21/8	25	100	2	25 7 $\overline{21}$	1 $\bar{1}$ 4	3 5 $\overline{14}$
		63-90		0 11 42	0 3 7	6 10 3
Mg 8/3	25	210	2	25 0 0	2 $\bar{1}$ $\bar{1}$	0 0 $\overline{25}$
		23-07		1 23 16	1 4 5	1 8 9
Zn 7/2	25	210	7	25 0 0	2 0 $\bar{1}$	0 0 $\overline{25}$
		63-90		7 11 $\overline{42}$	1 3 4	3 7 16

Table 1 (cont.)

Crystals (c/a) ²	Σ	uvw θ_d (°)	ε ($\times 10^3$)	U_{F1} ($\times \Sigma$)	$M1$ $U1_{F1}$	$DSC-1_{F1}$ ($\times \Sigma$)
Zn 27/8	25	310	9	26 3 9	3 0 2	6 1 7
		63-89		5 10 $\overline{45}$	1 3 3	5 5 15
Zr 18/7	25	210	6	25 0 0	2 0 $\bar{1}$	0 0 $\overline{25}$
		63-90		7 11 $\overline{36}$	1 1 9	1 18 $\overline{21}$

calculated case $\varepsilon = -\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 = 0$. It is seen in Table 1 that a small deviation of the c/a ratio (e.g. for Be, Ti, Zr) may lead to a large change of the state of deformation. The cell $M1$ is calculated as a Niggli reduced cell (Krivy & Gruber, 1976). Miller indices of its j th base vector are given by the j th column of the matrix $[U1]_{F1}$. [Each base vector of $M2$ is defined analogously by the matrix $[U2]_{F2}$, where $F2$ is a coordinate system related to the hexagonal unit cell of lattice 2, coinciding with $F1$ for $\theta_d = 0$. The cells $M1$ and $M2$ can be directly derived from the matrix $[U]_{F1}$ by using an algorithm proposed by Bonnet (1976).] The same algorithm allows the determination of the DSC-1 and DSC-2 lattices which define the possible Burgers vectors of intrinsic grain-boundary dislocations, with reference to lattices 1 and 2 respectively (Bollmann, 1970; Bonnet & Durand, 1975). The rational components of the base vectors of the DSC-1 lattices are given in the last column of the tables by the matrices $[DSC-1]_{F1}$. The matrices $[U2]_{F2}$ and $[DSC-2]_{F2}$ can be obtained from

$$[U2]_{F2} = [U^{-1}]_{F1} \cdot [U1]_{F1}$$

$$[DSC-2]_{F2} = [U^{-1}]_{F1} \cdot [DSC-1]_{F1}$$

The tables show, in particular, that the disorientation axes are: for carbon [001], [100], [210], [310], [10,0,1], [10,5,1]; for the hexagonal metals [001], [100], [210], [510], [501], [14,7,2], [18,9,2], [20,10,3]. All the axes, for disorientations giving rise to CSL's for $\Sigma \leq 25$ lie in mirror planes of symmetry. Only for higher values of Σ are axes of lower symmetry required. When an axis not lying in a plane of symmetry occurs, the rotation and its inverse arise from different sets of solutions and no twin description exists. One such example (corresponding to the case of $\Sigma = 39$, [321] in cubic crystals) is $\Sigma = 49$ with $(c/a)^2 = 5/2$. Here the disorientation solutions are

$$\frac{1}{49} \begin{pmatrix} 41 & 9 & 30 \\ -5 & 24 & 80 \\ 14 & -28 & 21 \end{pmatrix} \text{ and } \frac{1}{49} \begin{pmatrix} 56 & -21 & 0 \\ 25 & 9 & -70 \\ -4 & 26 & 21 \end{pmatrix}$$

Table 2. Near-coincident cells for carbon α and other related crystallographic quantities

Exact coincidence $\Sigma = 7, 13, 19$ around the c axis are omitted.

Crystals (c/a) ²	Σ	uvw θ_d (°)	ε ($\times 10^3$)	U_{F1} ($\times \Sigma$)	$M1$ $U1_{F1}$	DSC- 1_{F1} ($\times \Sigma$)
15/2	7	100	5	7 $\bar{2}$ $\bar{10}$	1 $\bar{1}$ $\bar{2}$	1 $\bar{1}$ 6
				0 3 $\bar{20}$	0 $\bar{2}$ $\bar{5}$	2 5 5
51/7	24	64.62	8	0 2 3	0 1 $\bar{1}$	$\bar{1}$ 1 1
				24 $\bar{7}$ $\bar{34}$	1 $\bar{1}$ $\bar{9}$	$\bar{1}$ $\bar{21}$ 3
15/2	11	100	3	0 10 $\bar{68}$	0 $\bar{2}$ $\bar{18}$	2 $\bar{18}$ $\bar{18}$
				0 7 10	0 1 3	1 3 3
15/2	11	35.10	3	11 $\bar{1}$ $\bar{10}$	1 1 5	$\bar{1}$ $\bar{6}$ $\bar{5}$
				0 9 $\bar{20}$	0 1 10	2 1 $\bar{10}$
15/2	11	210	6	0 2 9	0 $\bar{1}$ 1	2 1 $\bar{1}$
				11 0 0	2 1 0	0 0 $\bar{11}$
15/2	13	100	6	5 1 $\bar{30}$	1 3 3	3 5 8
				2 4 1	0 $\bar{1}$ 1	$\bar{1}$ 2 1
15/2	13	76.66	6	13 $\bar{5}$ $\bar{20}$	$\bar{1}$ $\bar{2}$ $\bar{3}$	2 9 $\bar{4}$
				0 3 40	0 4 $\bar{5}$	4 5 5
15/2	13	210	5	0 4 3	0 $\bar{1}$ 2	1 $\bar{2}$ 2
				13 0 0	2 1 0	0 0 $\bar{13}$
15/2	17	210	4	3 7 $\bar{30}$	1 2 5	5 3 8
				2 4 7	0 $\bar{1}$ 1	$\bar{1}$ 2 1
22/3	25	40.54	4	17 0 0	2 0 1	0 0 17
				2 13 $\bar{30}$	$\bar{1}$ $\bar{1}$ 8	1 15 16
23/3	17	210	5	2 4 13	0 1 1	$\bar{1}$ 2 1
				25 0 0	2 0 1	0 0 25
15/2	23	72.28	6	3 19 44	1 $\bar{1}$ $\bar{11}$	$\bar{1}$ 22 24
				3 6 19	0 1 $\bar{1}$	1 3 1
15/2	17	310	6	17 0 0	2 0 1	0 0 17
				6 5 44	1 2 6	2 11 2
15/2	19	10.5 1	5	3 6 5	0 1 $\bar{1}$	$\bar{1}$ 3 1
				23 0 0	2 0 1	0 0 23
15/2	17	79.84	6	8 7 $\bar{60}$	$\bar{1}$ $\bar{2}$ 8	2 $\bar{15}$ 4
				4 8 7	0 1 2	1 4 2
15/2	19	65.10	6	18 3 $\bar{10}$	3 2 2	1 8 10
				5 2 $\bar{50}$	1 3 4	5 6 $\bar{1}$
15/2	23	86.98	6	2 6 3	0 $\bar{1}$ 1	2 1 3
				21 6 10	3 1 $\bar{1}$	$\bar{1}$ 3 $\bar{17}$
117/16	25	87.71	7	11 5 40	2 1 4	4 7 $\bar{18}$
				2 6 9	0 1 1	1 3 2
36/5	23	42.34	10	19 9 $\bar{30}$	1 2 5	3 8 5
				0 1 $\bar{60}$	0 3 10	6 3 10
15/2	23	55.58	5	0 6 1	0 $\bar{1}$ 3	2 1 3
				25 $\bar{12}$ $\bar{39}$	$\bar{1}$ $\bar{2}$ 6	3 $\bar{14}$ 8
15/2	23	86.26	6	0 1 $\bar{78}$	0 3 13	6 3 $\bar{16}$
				0 8 1	0 1 4	2 1 3
15/2	23	10.0 1	6	23 3 $\bar{24}$	$\bar{1}$ 4 3	4 $\bar{15}$ 8
				0 17 48	0 8 7	8 7 7
15/2	23	86.26	6	0 5 17	0 1 2	1 2 2
				23 5 $\bar{30}$	$\bar{1}$ $\bar{3}$ $\bar{3}$	3 $\bar{14}$ 9
15/2	23	86.26	6	0 13 $\bar{60}$	0 6 5	6 5 5
				0 6 13	0 1 3	1 3 3
15/2	23	86.26	6	25 $\bar{17}$ $\bar{20}$	4 2 3	2 3 22
				7 2 $\bar{70}$	1 3 4	7 1 8
15/2	23	86.26	6	2 6 3	0 $\bar{1}$ 1	2 3 $\bar{1}$

Conclusions

The two techniques used provide consistent alternative routes to the determination of coincident cells (and constrained coincident cells) for noncubic crystals. They provide together a check that the input variables and constraints do not lead to spurious exclusion of any results. Both techniques have their limitations but it appears possible that the rational technique may become the more efficient when values of Σ higher than 25 are required for two identical crystals (if the symmetry is higher than monoclinic). The case of matching two different crystals as for a phase boundary has not yet been treated by the rational (c/a)² technique (or equivalent).

It is clear that there are indeed many solutions available even for quite small imposed constraints, even allowing for the fact that these are often grouped together with closely equal disorientations corresponding to different rational values of (c/a)². Which solution, if any, is to be preferred in a given case will be determined by energy considerations which may well depend upon the grain-boundary plane in question. In many such cases, however, it will require careful and precise experimental measurements to distinguish between the alternative possibilities which frequently concern the same rotation axis and closely related DSC lattices and hence grain-boundary dislocation Burgers vectors. Nevertheless, the conclusion remains that, for noncubic crystals, there are many possibilities of ordered structures in grain boundaries.

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Application of Cylindrical Distribution Functions to Wide-Angle X-ray Scattering from Oriented Polymers

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Abstract

A systematic approach is presented for obtaining cylindrical distribution functions (CDF's) of non-crystalline polymers which have been oriented by extension. The scattering patterns and CDF's are also sharpened by the method proposed by Deas and by Ruland. Data from atactic poly(methyl methacrylate) and polystyrene are analysed by these techniques. The methods could also be usefully applied to liquid crystals.

1. Introduction

There are two reasons for investigating the wide-angle X-ray scattering (WAXS) from oriented non-crystalline polymers. Firstly, it can aid in the interpretation of features in the scattering [or in the radial distribution function (RDF)] of unoriented polymers, by separating peaks into those from scattering within chains and those from scattering between chains (Lovell, Mitchell & Windle, 1980). Secondly, it may show changes in structure that take place when the polymer is deformed. In this paper we present a systematic approach to the calculation of cylindrical distribution functions (CDF's) which assists both these aims.

To investigate the structure of unoriented polymers, we have previously adopted the technique of comparing scattering calculated for models with that measured experimentally (*i.e.* the comparison is made in reciprocal space). Peaks in the experimental scattering can be separated into intrachain peaks, which intensify towards the extension direction (meridian) when the material is deformed, and interchain peaks, which

intensify perpendicular to the extension direction (towards the equator). This separation cannot easily be carried over into the RDF since features in the RDF come from more than one peak in the scattering. Hence a CDF (or at least its meridional and equatorial sections) must be prepared for the deformed materials before the RDF can be reliably separated into intrachain and interchain features.

To investigate the structure of oriented polymers, we have also made the comparisons in reciprocal space by using an azimuthal sharpening technique to improve the apparent degree of chain orientation (Lovell & Windle, 1976, 1977). This gives a pattern similar to a diffuse fibre pattern which may be more easily interpreted. Although unoriented polymers are frequently analysed with RDF's, few workers have prepared CDF's for oriented polymers since Norman (1954) first calculated the CDF of cellulose. This may be due to the difficulty of interpretation since, as we hope to show, CDF's are not much more difficult to prepare than RDF's.

We shall first compare the two methods which have been used for calculating CDF's and show how intermediate results in the procedure can assist in their interpretation. The approach is then illustrated with results from poly(methyl methacrylate) (PMMA) and polystyrene (PS) deformed close to their glass-transition temperatures.

2. Cylindrical distribution functions

The CDF is the cylindrical average of the normalized self-convolution of the electron density, and is defined by

$$W(\mathbf{r}) = 4\pi r[\rho(\mathbf{r}) - \rho_0]$$