It seems likely then that the plane of the nitro group in 9-nitroanthracene in solution or in the vapour phase might be free to oscillate between angles of 64° and 116° with the anthracene plane, but that in the crystal the most stable configuration is at 85°. The small amount of resonance interaction between the nitro group and the aromatic π-electrons, at 64° tilt, is not sufficient to hold the nitro group in this position in opposition to crystal forces, which apparently give minimum energy and best packing when the angle is 85°.

The measured bond lengths indicate that the symmetry of the anthracene nucleus is *mmm*, and the mean bond lengths are compared in Table 3 with those in anthracene (Sinclair, Robertson & Mathieson, 1950; Cruickshank, 1956). On the basis of the estimated standard deviations, the lengths of the bonds *A–B* differ significantly, but since there are no other significant differences between corresponding carbon–carbon bond lengths in the two molecules, and the values of the standard deviations are probably rather low, it is doubtful whether there is any real difference between the *A–B* bonds. The carbon–nitrogen bond distance corresponds to a single bond, and the N–O bond lengths are identical with those in aliphatic nitro compounds.

Intermolecular distances

The shortest intermolecular distance is 3·05 Å between atom B' of the standard molecule and atom O_2 of the molecule with coordinates $(-\frac{1}{2}+x, \frac{1}{2}-y, z)$. While this distance appears to be a little shorter than those usually found in structures of this type, it is almost exactly equal to the sum of the van der Waals radii (1·7 Å for the half-thickness of the aromatic rings plus 1·4 Å for the van der Waals radius of oxygen). The aromatic planes of those molecules related by the glide plane are almost exactly parallel, the distance between them being 3·50 Å, and the shortest carbon–carbon distances between these molecules are 3·71 Å and 3·79 Å. The shorter intermolecular contacts are illustrated in Fig. 5.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1959). **12**, 242

X-ray scattering factors of Al^{2+}, Al^{3+}, Mn^{2+}, Fe, Zr^{4+}, Au^{+} and U^{6+}.

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(*Received* 29 *September* 1958)

Some years ago we published a set of X-ray scattering factors (Berghuis *et al.*, 1955), computed from electron density data which had become available since the publication of the *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). The present paper gives some more data, being the transforms of electron densities either published since 1935 or kindly submitted by the authors. The list is by no means complete: a growing interest in more accurate X-ray scattering factors has led several authors to compute transforms of recent self-consistent field (SCF) data (Piper, 1957; Freeman, 1959; Freeman & Wood, 1959; Ibers, 1957, 1958*a*, *b*; Hurst, Miller & Matsen, 1958). Also, *f*-factors of a large number of both atoms and ions have recently been computed from the Thomas–Fermi–Dirac field (TFD) by Thomas & Umeda (1957), while Tomiie & Stam (1958) calculated a number of scattering factors from Slater functions. We computed form factors for Al^{2+} and Al^{3+} from wave functions given by Katterbach (1953) who states that he gives a more accurate solution of the Hartree–Fock equation than Krichagina & Petrashen (1938) whose results were used by Freeman (1958); Katterbach also took into account polarization of the $2p$ shell in Al^{2+}. Our new data for Al^{3+} agree completely with those of Freeman (1959) derived from another source (Froese, 1957); those for Al^{2+} are occasionally slightly lower than Freeman's. See Table 1, in which our results (lefthand column for each atom or ion) are compared with those of other investigators. For Mn^{2+} we used the same input data as Freeman; between $\sin\theta/\lambda = 0{\cdot}10$ and $0{\cdot}40$ our values are consistently about one percent lower than Freeman's,

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* Report No. R 312/439.

Table 1. *Atomic scattering factors*

	Al^{2+}		Al^{3+}		Mn^{2+}		Fe		Zr^{4+}		Au^{+}			U^{6+}
sin θ/λ	*SX* (1)	Freeman (2)	*SX* (1)	Freeman (3)	*SX* (4)	Freeman (4)	*S* (5)	Freeman (6) & Wood	*S* (7)	*TFD* (8)	*S* (9)	Henry (10)	*TFD* (8)	*S* (11)
0·00	11·00	11·00	10·00	10·00	23·00	23·00	26·00	26·00	36·00	36·00	78·00	78·00	78·00	86·00
0·05	10·84	—	9·93	—	22·64	—	25·19	—	35·60	35·67	76·98	—	76·97	85·15
0·10	10·40	10·39	9·74	9·74	21·68	21·91	23·36	23·96	34·47	34·72	74·22	74·26	74·14	82·77
0·15	9·81	—	9·43	—	20·40	—	21·37	—	32·79	33·24	70·42	—	70·19	79·29
0·20	9·17	9·17	9·01	9·01	18·96	19·19	19·52	20·36	30·80	31·39	66·24	66·32	65·88	75·23
0·25	8·55	—	8·52	—	17·43	—	17·81	—	28·71	29·34	62·11	—	61·74	71·07
0·30	7·95	7·97	7·98	7·97	15·84	15·96	16·21	17·05	26·70	27·25	58·24	58·35	57·96	67·10
0·35	7·37	—	7·40	—	14·32	—	14·73	—	24·87	25·23	54·70	—	54·52	63·46
0·40	6·79	6·83	6·82	6·81	12·96	13·06	13·39	14·15	23·25	23·39	51·49	51·62	51·35	60·16
0·50	5·70	5·73	5·69	5·68	10·77	10·80	11·16	11·77	20·56	20·31	45·96	46·07	45·70	54·33
0·60	4·71	4·75	4·69	4·68	9·16	9·19	9·52	9·95	18·37	17·92	41·33	41·42	40·97	49·20
0·70	3·88	3·91	3·86	3·84	8·09	8·09	8·36	8·64	16·42	15·97	37·30	37·46	36·97	44·65
0·80	3·22	3·25	3·20	3·19	7·33	7·33	7·55	7·72	14·63	14·29	33·71	33·66	33·53	40·67
0·90	2·71	2·73	2·70	2·69	6·77	6·77	6·97	7·06	12·98	12·89	30·49	30·52	30·60	37·25
1·00	2·33	2·35	2·32	2·31	6·32	6·32	6·51	6·57	11·51	11·70	27·57	27·62	28·04	34·27
1·10	2·05	2·07	2·04	2·04	5·91	5·92	6·10	6·15	10·24	10·68	25·01	25·27	25·83	31·63
1·20	1·84	—	1·84	—	5·54	—	5·73	—	9·07	9·80	22·81	23·28	23·87	29·23
1·30	1·69	1·70	1·69	—	5·15	—	5·37	—	8·32	9·03	20·94	—	22·16	27·03

S: self-consistent field; *X*: with exchange.

Reference to the input data:

(1) Katterbach (1953).
(2) Krichagina & Petrashen (1938).
(3) Froese (1957).
(4) Hartree (1955).
(5) Manning & Goldberg (1938).
(6) Wood & Pratt (1957).
(7) Altmann (1955) and Altmann, additional unpublished data.
(8) Thomas & Umeda (1957).
(9) Douglas, Hartree & Runciman (1955).
(10) Henry (1954*b*).
(11) Ridley (1957).

Table 2.

Atomic scattering factors for Al^{2+} and Al^{3+}

$\sin\theta/\lambda$	1*s*	2*s*	2*p*	Total Al^{3+}	3*s*	Total Al^{2+}
0·00	2·00	2·00	6·00	10·00	1·00	11·00
0·05	2·00	1·98	5·95	9·93	0·90	10·84
0·10	2·00	1·93	5·81	9·74	0·66	10·40
0·15	1·99	1·85	5·58	9·43	0·38	9·81
0·20	1·99	1·75	5·28	9·01	0·16	9·17
0·25	1·98	1·62	4·92	8·52	0·03	8·55
0·30	1·97	1·48	4·52	7·98	−0·03	7·95
0·35	1·97	1·33	4·11	7·40	−0·04	7·37
0·40	1·95	1·18	3·68	6·82	−0·03	6·79
0·50	1·93	0·88	2·88	5·69	0·01	5·70
0·60	1·90	0·62	2·17	4·69	0·02	4·71
0·70	1·87	0·41	1·59	3·86	0·02	3·88
0·80	1·83	0·24	1·13	3·20	0·02	3·22
0·90	1·79	0·13	0·79	2·70	0·01	2·71
1·00	1·74	0·05	0·53	2·32	0·01	2·33
1·10	1·69	0·00	0·35	2·04	0·00	2·05
1·20	1·64	−0·02	0·22	1·84	0·00	1·84
1·30	1·59	−0·03	0·13	1·69	0·00	1·69

Atomic scattering factors for Mn^{2+}

$\sin\theta/\lambda$	1*s*	2*s*	3*s*	2*p*	3*p*	3*d*	Total
0·00	2·00	2·00	2·00	6·00	6·00	5·00	23·00
0·05	2·00	2·00	1·97	5·99	5·81	4·87	22·64
0·10	2·00	1·99	1·88	5·97	5·36	4·49	21·68
0·15	2·00	1·97	1·73	5·93	4·82	3·95	20·40
0·20	2·00	1·95	1·54	5·87	4·28	3·33	18·96
0·25	2·00	1·92	1·33	5·80	3·69	2·70	17·43
0·30	1·99	1·88	1·11	5·71	3·03	2·12	15·84
0·35	1·99	1·84	0·89	5·61	2·37	1·62	14·32
0·40	1·99	1·79	0·69	5·49	1·79	1·21	12·96
0·50	1·98	1·69	0·35	5·23	0·91	0·62	10·77
0·60	1·97	1·56	0·12	4·93	0·31	0·27	9·16
0·70	1·96	1·43	−0·01	4·60	0·02	0·08	8·09
0·80	1·95	1·29	−0·06	4·26	−0·10	−0·01	7·33
0·90	1·94	1·15	−0·06	3·90	−0·11	−0·05	6·77
1·00	1·93	1·01	−0·03	3·54	−0·06	−0·07	6·32
1·10	1·91	0·88	0·00	3·19	0·01	−0·07	5·91
1·20	1·90	0·75	0·02	2·85	0·08	−0·06	5·54
1·30	1·88	0·63	0·05	2·53	0·12	−0·05	5·15

Atomic scattering factors for Zr^{4+}

$\sin\theta/\lambda$	1*s*	2*s*	3*s*	4*s*
0·00	2·00	2·00	2·00	2·00
0·05	2·00	2·00	1·99	1·93
0·10	2·00	2·00	1·96	1·75
0·15	2·00	1·99	1·91	1·48
0·20	2·00	1·98	1·85	1·16
0·25	2·00	1·97	1·77	0·83
0·30	2·00	1·96	1·68	0·54
0·35	2·00	1·94	1·57	0·30
0·40	2·00	1·92	1·46	0·12
0·50	1·99	1·88	1·22	−0·05
0·60	1·99	1·83	0·97	−0·07
0·70	1·99	1·77	0·74	−0·02
0·80	1·98	1·71	0·53	0·03
0·90	1·98	1·64	0·35	0·07
1·00	1·97	1·57	0·20	0·08
1·10	1·97	1·49	0·10	0·07
1·20	1·96	1·41	0·02	0·05
1·30	1·95	1·32	−0·02	0·03

Table 2 (*cont.*)

$\sin\theta/\lambda$	2*p*	3*p*	4*p*	3*d*	Total
0·00	6·00	6·00	6·00	10·00	36·00
0·05	6·00	5·97	5·76	9·95	35·60
0·10	5·99	5·88	5·08	9·81	34·47
0·15	5·97	5·74	4·11	9·58	32·79
0·20	5·96	5·55	3·03	9·27	30·80
0·25	5·93	5·31	2·01	8·89	28·71
0·30	5·90	5·03	1·15	8·45	26·70
0·35	5·86	4·72	0·52	7·96	24·87
0·40	5·82	4·38	0·11	7·44	23·25
0·50	5·73	3·66	−0·20	6·33	20·56
0·60	5·61	2·94	−0·13	5·23	18·37
0·70	5·48	2·25	0·03	4·18	16·42
0·80	5·33	1·64	0·16	3·25	14·63
0·90	5·17	1·12	0·21	2·45	12·98
1·00	4·99	0·70	0·20	1·79	11·51
1·10	4·81	0·39	0·17	1·26	10·24
1·20	4·62	0·17	0·12	0·73	9·07
1·30	4·42	0·02	0·08	0·52	8·32

Atomic scattering factors for Au^{+}

$\sin\theta/\lambda$	1*s*	2*s*	3*s*	4*s*	5*s*	2*p*	3*p*
0·00	2·00	2·00	2·00	2·00	2·00	6·00	6·00
0·05	2·00	2·00	2·00	1·99	1·96	6·00	6·00
0·10	2·00	2·00	1·99	1·97	1·83	6·00	5·98
0·15	2·00	2·00	1·98	1·92	1·63	5·99	5·96
0·20	2·00	2·00	1·97	1·87	1·38	5·99	5·92
0·25	2·00	1·99	1·96	1·79	1·11	5·98	5·88
0·30	2·00	1·99	1·94	1·71	0·84	5·98	5·83
0·35	2·00	1·99	1·92	1·61	0·58	5·97	5·77
0·40	2·00	1·98	1·89	1·51	0·37	5·96	5·69
0·50	2·00	1·97	1·83	1·28	0·06	5·94	5·53
0·60	2·00	1·96	1·76	1·04	−0·07	5·91	5·33
0·70	2·00	1·95	1·68	0·81	−0·09	5·88	5·11
0·80	2·00	1·93	1·59	0·59	−0·04	5·84	4·86
0·90	1·99	1·91	1·49	0·40	0·01	5·80	4·60
1·00	1·99	1·89	1·39	0·24	0·06	5·76	4·32
1·10	1·99	1·87	1·29	0·11	0·08	5·71	4·02
1·20	1·99	1·84	1·18	0·03	0·08	5·65	3·72
1·30	1·99	1·82	1·07	−0·03	0·07	5·59	3·42

$\sin\theta/\lambda$	4*p*	5*p*	3*d*	4*d*	5*d*	4*f*	Total
0·00	6·00	6·00	10·00	10·00	10·00	14·00	78·00
0·05	5·97	5·84	9·99	9·95	9·36	13·92	76·98
0·10	5·89	5·37	9·98	9·81	7·71	13·69	74·22
0·15	5·77	4·67	9·94	9·59	5·65	13·32	70·42
0·20	5·59	3·82	9·90	9·27	3·71	12·82	66·24
0·25	5·37	2·93	9·84	8·89	2·16	12·20	62·11
0·30	5·11	2·08	9·78	8·44	1·05	11·50	58·24
0·35	4·82	1·34	9·70	7·93	0·35	10·73	54·70
0·40	4·50	0·73	9·61	7·38	−0·05	9·92	51·49
0·50	3·80	−0·01	9·39	6·20	−0·28	8·23	45·96
0·60	3·08	−0·25	9·14	5·00	−0·17	6·59	41·33
0·70	2·38	−0·20	8·85	3·84	0·01	5·09	37·30
0·80	1·73	−0·04	8·52	2·80	0·14	3·79	33·71
0·90	1·17	0·11	8·17	1·91	0·20	2·73	30·49
1·00	0·70	0·20	7·80	1·19	0·20	1·83	27·57
1·10	0·35	0·22	7·40	0·64	0·17	1·16	25·01
1·20	0·10	0·20	6·99	0·26	0·13	0·64	22·81
1·30	−0·07	0·15	6·57	0·01	0·08	0·27	20·94

Atomic scattering factors for U^{6+}

$\sin\theta/\lambda$	1*s*	2*s*	3*s*	4*s*	5*s*	6*s*
0·00	2·00	2·00	2·00	2·00	2·00	2·00
0·05	2·00	2·00	2·00	1·99	1·98	1·90
0·10	2·00	2·00	2·00	1·98	1·91	1·61
0·15	2·00	2·00	1·99	1·95	1·79	1·21
0·20	2·00	2·00	1·98	1·91	1·64	0·78
0·25	2·00	1·99	1·97	1·86	1·47	0·40
0·30	2·00	1·99	1·96	1·80	1·27	0·13
0·35	2·00	1·99	1·94	1·74	1·07	−0·03

Table 2 (*cont.*)

0·40	2·00	1·99	1·92	1·66	0·87	−0·10
0·50	2·00	1·98	1·88	1·50	0·50	−0·05
0·60	2·00	1·97	1·83	1·31	0·21	0·05
0·70	2·00	1·96	1·77	1·12	0·02	0·09
0·80	2·00	1·95	1·70	0·92	−0·07	0·07
0·90	2·00	1·94	1·63	0·73	−0·09	0·03
1·00	1·99	1·92	1·55	0·56	−0·06	0·00
1·10	1·99	1·90	1·47	0·40	−0·01	−0·01
1·20	1·99	1·89	1·39	0·27	0·03	−0·02
1·30	1·99	1·87	1·30	0·16	0·07	−0·01

$\sin\theta/\lambda$	$2p$	$3p$	$4p$	$5p$	$6p$
0·00	6·00	6·00	6·00	6·00	6·00
0·05	6·00	6·00	5·98	5·92	5·62
0·10	6·00	5·99	5·93	5·69	4·61
0·15	6·00	5·97	5·85	5·32	3·25
0·20	5·99	5·95	5·73	4·84	1·89
0·25	5·99	5·92	5·58	4·27	0·79
0·30	5·98	5·88	5·41	3·66	0·08
0·35	5·98	5·84	5·20	3·02	−0·24
0·40	5·97	5·79	4·98	2·40	−0·29
0·50	5·96	5·67	4·47	1·29	−0·02
0·60	5·94	5·53	3·92	0·47	0·21
0·70	5·91	5·37	3·33	−0·02	0·24
0·80	5·89	5·18	2·75	−0·22	0·14
0·90	5·86	4·99	2·19	−0·23	0·04
1·00	5·82	4·77	1·67	−0·12	−0·03
1·10	5·79	4·54	1·22	0·02	−0·04
1·20	5·75	4·31	0·83	0·15	−0·03
1·30	5·70	4·06	0·50	0·24	0·00

$\sin\theta/\lambda$	$3d$	$4d$	$5d$	$4f$	Total
0·00	10·00	10·00	10·00	14·00	86·00
0·05	10·00	9·97	9·84	13·96	85·15
0·10	9·98	9·89	9·35	13·85	82·77
0·15	9·96	9·75	8·60	13·66	79·29
0·20	9·93	9·55	7·63	13·41	75·23
0·25	9·89	9·31	6·53	13·09	71·07
0·30	9·85	9·02	5·36	12·71	67·10
0·35	9·79	8·69	4·21	12·27	63·46
0·40	9·73	8·32	3·14	11·79	60·16
0·50	9·58	7·49	1·38	10·70	54·33
0·60	9·40	6·58	0·27	9·52	49·20
0·70	9·20	5·63	−0·25	8·29	44·65
0·80	8·96	4·68	−0·35	7·06	40·67
0·90	8·71	3·78	−0·21	5·89	37·25
1·00	8·43	2·94	0·01	4·80	34·27
1·10	8·13	2·20	0·22	3·81	31·63
1·20	7·82	1·56	0·36	2·93	29·23
1·30	7·49	1·03	0·43	2·18	27·03

whereas they agree perfectly at higher $\sin\theta/\lambda$ values. This might possibly be due to different interpolation of the wave functions.

The form factor of Fe was computed some time ago from the somewhat old SCF data of Manning & Goldberg (1938). While these values are presumably better than the old TF values, they are appreciably lower in the medium $\sin\theta/\lambda$ range than Freeman & Wood's (1959) recent and more reliable data (SCF with exchange). We publish our results nevertheless, in order to point out the effect of exchange in this region of the periodic system.

Scattering factors for Zr^{4+}, Au^{+} and U^{6+} are computed from SCF electron densities *without* exchange. Although we are aware that exchange effects may also be quite important in this region, it was thought worth while to compare the results with Thomas & Umeda's (TFD, i.e., with exchange). This comparison turns out very similar to Ibers's recent result on Hg (Ibers, 1958), in that the SCF and TFD values agree within a few units in the first decimal place, except at the highest $\sin\theta/\lambda$ values, where SCF values are about one unit lower; this amounts to a deviation of about -5% for Au^{+}, of -8% for Zr^{4+}. The agreement with Henry's (1954*a*) SCF computation for Au^{+} is good.

Since after our first paper we have had several requests for the transforms of the individual orbitals, we also give, in Table 2, these partial data, normalized for the number of electrons in each orbital. In the case of Fe, only the transform of the total electron density was computed, so that individual electron form factors are not available for this atom; these have, however, already been given by Freeman (1959).

The computations were carried out on the electronic digital computer ARMAC of the Mathematical Centre (except those for Fe which were still done on IBM-machines). We used a subroutine (due to Mr E. W. Dijkstra) for integration according to Simpson's Formula with automatic choice of the optimum interval-length with respect to a given tolerance. The tolerances were chosen so as to give results correct to about four figures. The integration-variables were those for which the wave-function P was tabulated: r in atomic units for Au^{+} and Mn^{++}, $\varrho = \ln 10^3 r$ for Fe, U^{6+} and Al^{2+} and Al^{3+} and $\xi = 3\log_{10} r$ for Zr^{4+}. Thus there were three somewhat different types of integrands. In the latter two cases the contribution in the neighbourhood of $r = 0$ was evaluated from the series-expansion of P.

The integrals were split up into sections in which the input data were tabulated equidistantly. The values in non-tabular points were calculated by interpolation with first and second differences.

As in our previous computations we chose

$$\sin\theta/\lambda = 0{\cdot}00\ (0{\cdot}05)\ 0{\cdot}40\ (0{\cdot}10)\ 1{\cdot}30\,.$$

This work was carried out under the auspices and with financial support of the International Union of Crystallography, in preparation of Vol. III of *The International Tables for X-ray Crystallography.*

We express our gratitude to the Netherlands Organization for Pure Research (Z. W. O.) for generous support, to Prof. A. van Wijngaarden and to Dr J. A. Ibers for stimulating discussions. We further wish to thank Messrs. Freeman, Altmann and Piper and Mrs Ridley, who very kindly put their unpublished results at our disposal.

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Relation of symmetry to structure in twinning.

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(*Received* 6 *October* 1958)

In a recent paper with the above title Holser (1958) deals with twin structures belonging to the class which may be characterized as consisting of two crystals with a two-dimensionally periodic layer—the boundary layer—in common. He makes an attempt to derive the possible twinning operations compatible with this characterization. As he shows, such twinning may occur if the boundary layer has an element in its plane symmetry group which is not an element of the space group of the crystal. In this case the structure of the crystal possesses true partial symmetry operations* and should thus be classified as an OD-structure (Dornberger-Schiff, 1956).

The two examples shown schematically in Figs. 1 and 2 prove, however, that the existence of true partial symmetry elements of the plane symmetry group of the boundary layer is not the only source of twinning, as has been formulated by the author (p. 252).

In example 1 (Fig. 1) the only symmetry operation of the boundary layer (a rotation diad) is an operation of the crystal; in example 2 (Fig. 2) the boundary layer has no symmetry (except the translations). Thus in both cases the boundary layer does not possess any symmetry element which the crystal does not possess as well. In both cases there is, however, at least one true partial symmetry operation (partial glide planes in both cases) within the crystal which transforms the boundary layer into an adjacent layer; and these partial symmetry operations serve as twinning operations.

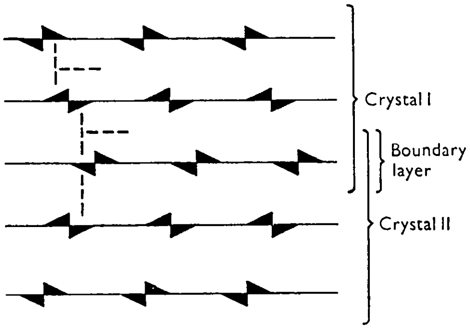

Fig. 1. Schematic drawing of a twinned structure. Symmetry of the boundary layer $P12(1)$. Symmetry of the OD-family characterized by the symbol

$$\begin{array}{c} P\;1\;2\;(1) \\ \{\,c_2\;1\;(a_x)\}\,. \end{array}$$

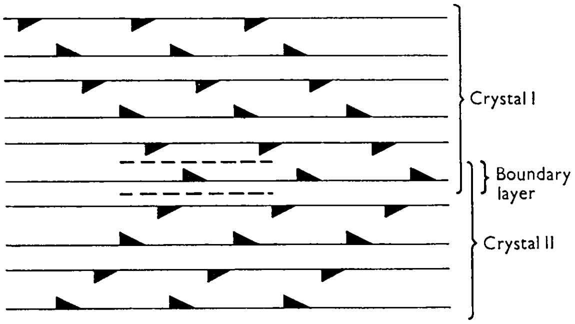

Fig. 2. Schematic drawing of a twinned structure. Symmetry of the boundary layer $P11(1)$. Symmetry of the OD-family characterized by the symbol

$$\begin{array}{c} P\;1\;1\;(1) \\ \{\,1\;1\;(a_x)\} \\ \{\,1\;1\;(a_{x'})\} \end{array}$$

A general investigation of possible twinning operations is in progress at our Institute, as part of a research programme on OD-structures. Any twin structure, characterized as above, is a member of a family of OD-structures consisting of two-dimensionally periodic layers—either all of the same kind or of not more than three different kinds—one of which is the boundary layer. The twinning operation is in every case a true partial symmetry operation of the crystal, which transforms the boundary layer either into itself or into one of the adjacent layers of the same kind. The deduction of a complete list of the possible twin laws may thus be achieved on the basis of a theory of OD-structures (Dornberger-Schiff and Grell-Niemann).

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* A 'true partial symmetry operation' is a symmetry operation transforming a particular layer of the structure either into itself or into another layer without transforming the crystal into itself.

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