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Die 62 allgemeinen Auslöschungseinheiten.

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In unserem Buche über *Fouriersynthese von Kristallen* (Nowacki, 1952, S. 163/4) wurde das Problem der '*allgemeinen Auslöschungseinheiten*' erwähnt. Bekanntlich ist es bei gegebener Lauesymmetrie und gegebenen Auslöschungen nicht möglich, alle 219 = 230 − 11 wesentlich verschiedenen Raumgruppen auseinanderzuhalten; man wird vielmehr auf die 120 Auslöschungseinheiten ('diffraction groups') geführt. Nimmt man nun an, dass die Lauesymmetrie unbekannt sei, so fragt es sich, welche Gesamtheiten von Raumgruppen man unterscheiden und ermitteln kann, wenn man ausschliesslich Auslöschungen verwendet. Wir führen zu diesem Zweck den Begriff der '*allgemeinen Auslöschungseinheit*' ein, indem wir darunter die Gesamtheit aller Raumgruppen verstehen, welche — unabhängig von der Lauesymmetrie — dieselben Auslöschungen aufweisen. Es wurde eine Bestimmungstabelle ausgearbeitet, welche erlaubt, bei gegebenen Auslöschungen alle dazu gehörigen Raumgruppen zu finden und zwar für sämtliche mögliche Orientierungen der Koordinatenachsen und für jede Aufstellungswahl. Das Resultat ist, dass es 62 allgemeine Auslöschungseinheiten im Gegensatz zu den 120 gewöhnlichen gibt.

Die Existenz der allgemeinen Auslöschungseinheiten ist z.T. eine Folge der Tatsache, dass die Strukturamplitude

$$F(h, k, l) = \sum_j \exp 2\pi i(hx_j+ky_j+lz_j)$$

(alle Punkte werden als gleichwertig vorausgesetzt) die Symmetrie eines Kristalles in einer nur eingeschränkten Weise enthält. Alle symmorphen Raumgruppen z.B. bilden eine einzige allgemeine Auslöschungseinheit, weil bei ihnen überhaupt keine Auslöschungen auftreten.

Im allgemeinen ist es unmöglich, Symmetrien durch Auslöschungen allein zu bestimmen; für die 31 + 2 Raumgruppen C_{2h}^5, D_2^3, C_{2v}^{19}, $D_{2h}^{4,6,8,10,14,15,22}$, C_{4h}^6, $D_4^{(4,8),6}$, C_{4v}^{12}, D_{2d}^4, $D_{4h}^{3,4,8,11,12,15,16,19,20}$, $O^{4,(7,6),8}$, T_d^6 und $O_h^{2,8,10}$ hingegen ist dies möglich.

Die allgemeinen Auslöschungseinheiten können bei Pseudosymmetrien und bei unsicher bekannter Lauesymmetrie praktisch wichtig werden, von der prinzipiellen Frage, wie weit man mit Auslöschungen allein kommt, abgesehen.

Die ausführliche Arbeit zusammen mit der Bestimmungstabelle wird in den *Schweizerischen Mineralogischen und Petrographischen Mitteilungen* erscheinen.

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The crystallographic relationship between the phases γ and ε in the system iron–manganese.

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Between compositions 10% and 30% manganese a close-packed hexagonal phase (ε) may be formed in iron–manganese alloys (Schmidt, 1929–30). Its formation in powder specimens has been explained in terms of athermal nucleation (Parr, 1952); and similar arguments apply to the formation of ε in solid specimens. To retain ε in powders the sample has to be water-quenched from the face-centred (γ) phase field; and in view of the slow diffusion rate in iron–manganese alloys (Jones & Pumphrey, 1949) it is reasonable to suppose that the transformation involves a 'martensite' reaction (Troiano & McGuire, 1943). Although solid specimens will retain ε on slow cooling (Parr, 1952) as well as on quenching, the phase is identical in structure and behaviour in solids and powders, and presumably forms by the same mechanism.

The close-packed arrangement of atoms in face-centred cubic and close-packed hexagonal structures suggests that face-centred cubic → close-packed hexagonal shear transformations are such that $(111)_\gamma$ is parallel to $(0001)_\varepsilon$. Nishiyama (1936) proposed a mechanism in which this relationship exists, and $(110)_\gamma$ is parallel to $(11\bar{2}0)_\varepsilon$. Shear takes place in a$[211]_\gamma$ direction.

The oscillation photograph reproduced in Fig. 1 of a water-quenched sample of an 18·5% manganese alloy in needle form, was taken in a 5 cm. camera. Because pairs of spots indicate parallel planes of atoms (Barrett, Geisler & Mehl, 1941, 1943) it is immediately evident from the photograph that $(13\bar{1})_\gamma$ is parallel to $(11\bar{2}2)_\varepsilon$. The plane $(13\bar{1})_\gamma$ lies in a zone which includes $(111)_\gamma$ and $(01\bar{1})_\gamma$; and $(11\bar{2}2)_\varepsilon$ lies in a zone which includes $(0001)_\varepsilon$ and $(11\bar{2}0)_\varepsilon$. The angles between planes in the zones are:

γ Planes		ε Planes	
(111)		(0001)	
	58° 29′		58° 14′
$(13\bar{1})$		$(11\bar{2}2)$	
	31° 31′		31° 46′
$(01\bar{1})$		$(11\bar{2}0)$	

Therefore the relationship between the γ and ε structures should lead to pairs of spots 222_γ and 0004_ε. This correspondence does exist, although it does not appear so clearly on Fig. 1 as the relationship between 311_γ and $11\bar{2}2_\varepsilon$. Because of almost identical interplanar spacings the diffraction spots 220_γ and $11\bar{2}0_\varepsilon$ appear to be on a single arc; but as $(13\bar{1})_\gamma$ is parallel to $(11\bar{2}2)_\varepsilon$, and $(111)_\gamma$ is parallel to $(0001)_\varepsilon$, it follows that $(01\bar{1})_\gamma$ is parallel to $(11\bar{2}0)_\varepsilon$.

The relationship demanded by the Nishiyama mechanism is therefore satisfied. A superimposed volume

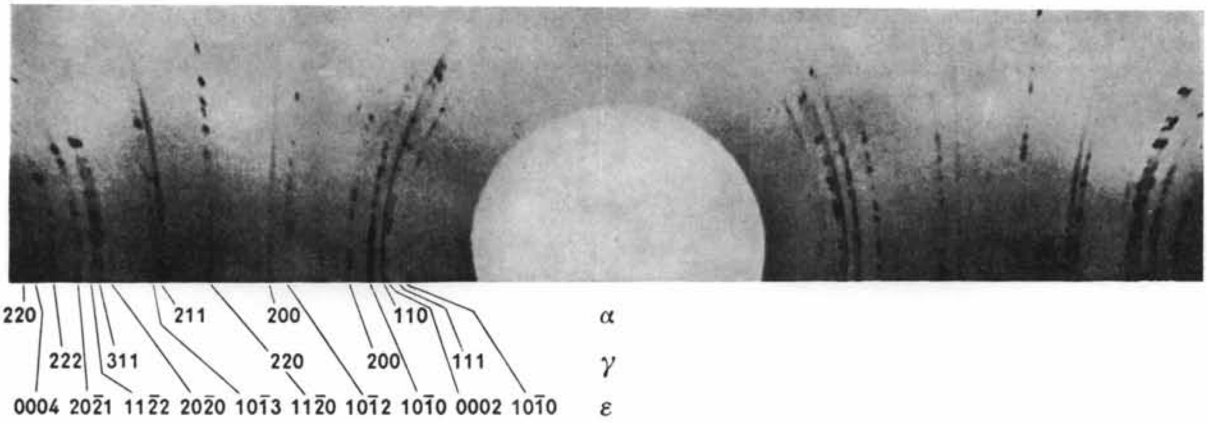

Fig. 1. Oscillation photograph of quenched needle.

Fig. 2. Photomicrograph of quenched needle (× 4 000).

contraction of 2% is largely in a direction normal to the shearing movement:

Parameter of γ: $a = 3\cdot585$ Å;
whence $\frac{1}{2}a_\gamma\sqrt{2} = 2\cdot535$ Å, $\frac{2}{3}a_\gamma\sqrt{3} = 4\cdot140$ Å.
Parameters of ε: $a = 2\cdot528$ Å, $c = 4\cdot080$ Å.

The mechanism is of the type which produces a 'Widmanstätten' pattern of strain bands; and the contraction associated with the transformation limits the growth of ε around each nucleus. A photomicrograph (Fig. 2) confirms both the strain pattern and the absence of massive precipitate, although individual phases cannot be distinguished.

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Some implications of a theorem due to Shannon.

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Shannon (1949), in the field of communication theory, has given the following theorem: If a function $d(x)$ is known to vanish outside the points $x = \pm a/2$, then its Fourier transform $F(X)$ is completely specified by the values which it assumes at the points $X = 0, \pm 1/a, \pm 2/a, \ldots$. In fact, the continuous $F(X)$ may be filled in merely by laying down the function $\sin \pi aX/\pi aX$ at each of the above points, with weight equal to the value of $F(X)$ at that point, and adding.

Now the electron-density function $d(x)$ describing a single unit cell of a crystal vanishes outside the points $x = \pm a/2$, where a is the length of the cell. The reciprocal-lattice points are at $X = 0, \pm 1/a, \pm 2/a, \ldots$, and hence the experimentally observable values of $F(X)$ would suffice, by the theorem, to determine $F(X)$ everywhere, if the phases were known. (In principle, the necessary points extend indefinitely in reciprocal space, but by using, say, Gaussian atoms both $d(x)$ and $F(X)$ can be effectively confined to the unit cell and the observable region, respectively.)

For centrosymmetrical structures, to be able to fill in the $|F|^2$ function would suffice to yield the structure, for sign changes could occur only at the points where $|F|^2$ vanishes. The structure corresponding to the $|F|^2$ function is the Patterson of a single unit cell. This has twice the width of the unit cell, and hence to fill in the $|F|^2$ function would require knowledge of $|F|^2$ at the half-integral, as well as the integral h's. This is equivalent to a statement made by Gay (1951).

I think the conclusions which may be stated at this point are:

1. Direct structure determination, for centrosymmetric structures, could be accomplished as well by finding the sizes of the $|F|^2$ at half-integral h as by the usual procedure of finding the signs of the F's at integral h.
2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where $|F|^2$ was observed at non-integral h, it would suffice to have only the values at half-integral h.

The extension to three dimensions is obvious.

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Unit-cell dimensions and space groups of synthetic peptides. I. Glycyl-L-tyrosine, glycyl-L-tyrosine hydrochloride, glycyl-DL-serine and glycyl-DL-leucine.

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The data presented here form part of an extended survey of crystalline peptides recently begun by the Wool Industries Research Association. The objects of the investigation are first to obtain some knowledge of the factors influencing the crystallization of these materials; secondly, from their unit-cell dimensions to obtain information regarding the types of molecular arrangements present, and thirdly to select materials suitable for a more detailed X-ray examination.

Source of peptides.

Glycyl-L-tyrosine was obtained from Roche Products, Welwyn Garden City, England, and the monohydrochloride was prepared from it by treatment with excess of 2N.HCl, followed by evaporation at room temperature. (Found 12·1% Cl; calculated 12·9%.)

Glycyl-DL-leucine and glycyl-DL-serine were synthesized by the chloracetyl chloride method first described by