Using the f.c.c. nickel lines as an internal standard, the spotted rings could be indexed as the reflections of a h.c.p. structure with

$$a=2{\cdot}622\,,\quad c=4{\cdot}320\ \text{Å};\quad c/a=1{\cdot}648. \qquad (1)$$

In Table 1, the measured *d* values of the spotted reflections are listed together with *d* values calculated with the use of the relation

$$d=\frac{a}{\sqrt{\frac{4}{3}\,(h^2+hk+k^2)+(a/c)^2l^2}} \qquad (2)$$

with the above *a* and *c* parameters, and, for comparison, with *d* values for the hexagonal $Ni_3N$. Note that all observed spotted reflections could be indexed with extremely good agreement between observed and calculated lines, while the agreement between the measured *d* values and those of $Ni_3N$ is only fair; note especially the $Ni_3N$ value 1·155 Å and the missing 1·098 Å value. In addition to the lack of *d*-value agreement, the *a* and *c* values are also different. Jack (1950) gives for $Ni_3N$

$$a=2{\cdot}667\,,\quad c=4{\cdot}3122\ \text{Å};\quad i.e.\ c/a=1{\cdot}617\,,$$

which are quite noticeably different from the values found above. NiO, on the other hand, which might have formed during evaporation in the relatively poor vacuum, crystallizes at room temperature in the rhombehedral structure (Pearson, 1958, p. 1021), which, after transformation to the equivalent hexagonal description, yields $a=2{\cdot}955$, $c=4{\cdot}207$ Å, and thus a much smaller $c/a$ ratio than the structure found in the investigated nickel films. Therefore, the evidence is very strong that the observed structure is in fact a hexagonal phase of nickel.

The grain growth was observed only when a high-intensity electron beam was used; furthermore, the effect was observed near tears in the films, which then were curling during viewing. Therefore, it is believed that the transformation of f.c.c. nickel to the hexagonal form is due to a combination of heating and straining. A more detailed presentation of the proposed mechanism will be given elsewhere.

*Note added in proof*: In a recent article, Wright & Goddard (1965) reported that nickel may be electro-deposited to form a single-crystal hexagonal structure, provided that correct bath conditions and suitable substrates are used. The lattice parameters were determined as $a=2{\cdot}50\pm0{\cdot}01$ Å; $c/a=1{\cdot}59\pm0{\cdot}01$. It was observed that – in agreement with our own observations – the growth conditions are extremely critical for the formation of the h.c.p. structure, which was found to be unstable at room temperature.

Table 1. *Measured and calculated d values*

| Expected hexagonal lines | Measured *d* values of the spotted rings | Calculated *d* calues using equations (1) and (2) | *d* values for $Ni_3N$ from ASTM card No. 10–280 |
|---|---|---|---|
| (*hk·l*) | (Å) | (Å) | (Å) |
| (10·0) | 2·27 | 2·271 | 2·311 |
| (00·2) | 2·159 | 2·160 | 2·144 |
| (10·1) | Superimposed on Ni ring (111) | 2·010 | 2·035 |
| (10·2) | 1·565 | 1·564 | 1·576 |
| (11·0) | 1·311 | 1·311 | 1·333 |
| (10·3) | 1·216 | 1·218 | 1·219 |
| | | | 1·155 |
| (20·0) | 1·135 | 1·135 | 1·133 |
| (11·2) | 1·119 | 1·120 | 1·115 |
| (20·1) | 1·098 | 1·098 | |
| (00·4) | 1·081 | 1·080 | 1·076 |
| (20·2) | Superimposed on Ni ring (222) | 1·005 | 1·018 |

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# A knowledge availability survey of the crystal structural data for pyrimidine derivatives.

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Many of the biologically interesting molecules involved in life processes contain the pyrimidine ring. Consequently, up to February 1965, about one hundred twenty single-crystal structure determinations by X-rays or neutrons have been reported in more or less detail on compounds containing the pyrimidine ring, *i.e.* pyrimidines, barbiturates, purines, nucleosides, nucleotides, *etc.*

The crystal structural information obtained from these investigations (*i.e.* crystal data, valence and hydrogen bond lengths, angles, *etc.*) has been punched on cards in a format suitable for a uniform representation as well as for information retrieval by means of a card-sorting machine or a computer. These structural data, together with the explanatory report, are available to crystallographers at nominal mailing charges. Inquiries should be addressed to The Crystallography Laboratory, The University of Pittsburgh, Pittsburgh, Pa. The data are available in the following choice of format:

1. A print-out from punched cards
2. A punched-card deck
3. A magnetic tape from the punched cards.

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Mootz, E., Mootz, D. & Jeffrey, G. A. (1965), *A Knowledge Availability Survey of the Crystal Structural Data for Pyrimidine Derivatives.* Technical Report, University of Pittsburgh.

## Book Reviews

*Works intended for notice in this column should be sent direct to the Editor (A. J. C. Wilson, Department of Physics, The University, Birmingham 15, England). As far as practicable books will be reviewed in a country different from that of publication.*

**A systematic classification of types of intermetallic structures.** By P. I. Kripyakevich [This is not a book, but a translation of research/review papers from *Zh. Strukt. Khim.*, **4**, 117, 282.] 33 pp. 293 ref. New York: Consultants Bureau. Reprint in soft cover. Price $ 10.

Before discussing the paper by Kripyakevich, I wish to draw attention to a statement on the face page of the translation by Consultants Bureau Enterprises Inc. 'No part of this publication may be reproduced *in any form* [my italics] without written permission from the publisher.' Far too many scientific publications are issued nowadays with this protection. It is essential to science that scientists continue to exercise their prerogative of being able to quote reasonable pieces of scientific data and diagrams from other scientific publications without let or hindrance, and writing letters to publishers for permission whenever one wishes to exercise this prerogative is certainly beyond all reason. We must, therefore, make the businessman-publishers of scientific papers and works understand quite clearly that in exchange for our patronage (to the mutual benefit of both themselves and ourselves), we require that they subscribe to the *Fair Copying Declaration* of the Royal Society of London.

The author sets forth a classification of binary, ternary and quaternary compounds having metallic properties, that is based on coordination numbers, configurations of coordination polyhedra, and their method of combination, which can therefore be applied to all structural types. The classification is based on the type of coordination polyhedron of the atoms having the *lowest* coordination number, or smallest effective atomic radius when there are components with the same coordination number. This allows all known structure types to be separated into one of 17 classes with C.N. ranging between 2 and 14. Within a given class, further subdivision proceeds according to the relative arrangement of the coordination polyhedra in the structure, the C.N. of the remaining independent atoms, *etc.* If the smaller atoms have coordination polyhedra of two kinds, then the structure is classed according to that with the lower C.N. or the smaller effective radius if both have the same C.N. Thus for example $Sn_4Ni_3$ with C.N. 6 Ni in prisms and octahedra, is classified with the octahedra. The structure of a combination of atoms is characterized by a unit cell of specific symmetry, axial ratios and angles, occupied regular point-set(s) of a certain space group, and atomic coordinates. Thus when axial ratios and parameters vary beyond a certain range, so as to change the coordination significantly, a new 'structure' is obtained according to the classification, and so problems involving formally isotypic structures in which atoms have different coordination in degree and/or kind (*e.g.*, $F5_1$, $C11$, or $PH_4I$–BiIn–PbO–TeFe types) are removed.

In its present form, the intending user must personally develop the classification along lines suggested by the author, if he is to derive any benefit from it. This must take some considerable time and effort. The language is not always easy and there is a fair amount of symbolism to remember. The author does not say a word on the usefulness of the classification, and based as it is on the simplest coordination unit in the structure, it does not appear to be always useful in showing up relationships between different structural types and derivatives, nor does it appear to be of any help to the crystallographer who seeks systematically to examine, at an early stage in a structural analysis, whether a compound has an already known structure. Under these circumstances, I feel that it may not be useful to those who have only a secondary interest in structural relationships, and we may hope for a further paper by the author developing themes for the use of the classification which he has outlined.

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