$$f = 8N^2z\left[\frac{1}{(4z^2+\mu^2)^2}+\frac{kc^2}{(4k^2z^2+\mu^2)^2}+\frac{c(1+k)}{[z^2(1+k)^2+\mu^2]^2}\right]. \qquad (3{\cdot}1)$$

The computed scattering factors are listed in Table 1. On comparison, it is found that the scattering factors obtained in this note are in perfect agreement for $Li^+$–$C^{4+}$ with the results of Womack *et al.*, obtained from a much more elaborate calculation. They differ for $H^-$ and He but the maximum deviation is 0·0007 electron for both the systems. The present work indicates that relatively good scattering factors can be obtained from relatively poor wave functions in support of Ibers's (1959) observation.

The authors are grateful to Prof. A. R. Verma for his interest in this work.

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# χ Phase in a niobium-rhenium alloy.

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(*Received* 21 *June* 1963)

## Introduction

The χ phase of Nb–Re is isomorphous with α Mn. It is cubic, with space group $I\bar{4}3m$, and the 58 atoms in the unit cell occupy four crystallographically distinct sites. Greenfield & Beck (1956) were unable to conclude from their X-ray diffraction data whether there is ordering among these sites, but Niemiec & Trzebiatowski (1956) found that the intensities of two low-angle powder arcs were consistent with an ordered distribution. A single-crystal investigation was undertaken to obtain further evidence.

## Experimental

The specimen had the composition Nb 25 at.%–Re 75 at.% and had been annealed in an argon arc furnace at 2200 °C for two hours.

The large linear absorption coefficient of 1660 $cm^{-1}$ for molybdenum radiation necessitates the use of a small crystal, and a fragment of cross section 0·01 × 0·04 mm was selected. The lattice parameter was determined by the method of Farquahar & Lipson (1946). The value obtained ($a = 9{\cdot}692 \pm 0{\cdot}002$ Å) was larger than the values given by Knapton (1958) ($a = 9{\cdot}683$ Å) and Niemiec & Trzebiatowski ($a = 9{\cdot}676$ Å) for an alloy of the same composition. To check that the fragment was representative, the lattice parameter was determined from powder data, a 9 cm diameter camera and Cu $K\alpha$ radiation being used, and the value obtained was $9{\cdot}693 \pm 0{\cdot}001$ Å. The calculated density is 17·2 $g.cm^{-3}$; the measured density was $17{\cdot}6 \pm 0{\cdot}3$ $g.cm^{-3}$.

A zero-layer Weissenberg photograph was taken with Mo $K\alpha$ radiation with the use of a multiple-film pack, and the spots were integrated slightly to facilitate the measurement of intensities. After an exposure time of 190 hours, only 63 (40%) of the independent reflexions within the limiting sphere were recorded, 28 of these being so faint that their measurement was considered unsatisfactory. The structure refinement was carried out with the remaining 35 reflexions, the intensities of which were measurable with an uncertainty of less than 15%. Corrections for absorption, which were essential, were computed by the method of Rogers & Moffett (1956), and these varied by a factor of three over the range within which data were collected.

## Structure determination

The four groups of sites in the α Mn structure are defined by five parameters, as shown in Table 1. Sites *a* and *c* have coordination number (C.N.) 16, and the $D_1$ and $D_2$ sites have C.N. 13 and 12 respectively.

Table 1. *Parameters defining sites in the* α Mn *structure*

| Multiplicity | | Parameters | | | |
|---|---|---|---|---|---|
| | | α Mn | | χ phase Nb–Re | |
| 2(*a*) | | — | — | — | — |
| 8(*c*) | | $x = 0{\cdot}317$ | | $x = 0{\cdot}314$ | |
| 24(*g*) | $D_1$ | $x = 0{\cdot}356$ | $z = 0{\cdot}042$ | $x = 0{\cdot}360$ | $z = 0{\cdot}040$ |
| | $D_2$ | $x = 0{\cdot}089$ | $z = 0{\cdot}278$ | $x = 0{\cdot}096$ | $z = 0{\cdot}277$ |

In accordance with the alloy composition, the unit cell contains 14·5 atoms of niobium and 43·5 of rhenium. Structure factors were first computed for the arrangements A and B of Table 2, the fractional coordinates given by Bradley & Thewlis (1927) for α Mn being used;

structure B, in which the sites with C.N. 16 are completely occupied by niobium, gave much the better agreement with observation. The scattering factors used were those of Thomas & Umeda (1957), and a complex correction for dispersion was made (Dauben & Templeton, 1955).

The coordinates of the ordered structure B were then refined by difference methods. An overall isotropic temperature factor of 0·25 Å² was applied, and, with the final parameters shown in Table 1, the $R$ value was 0·13.

To discover the effect of varying the degree of ordering between the $D_1$ and $D_2$ sites, calculations were carried out with the other arrangements given in Table 2. The results given there show that the residual steadily diminished as the niobium not accommodated in the $a$ and $c$ sites was increasingly concentrated in the $D_1$ site, until a minimum of 0·12 was reached when niobium was almost entirely absent from $D_2$. With this structure, the $R$ value computed over all the observed reflexions was 0·22.

Table 2. *Ordering of sites*

| Structure | Sites $a$ and $c$ | Ratio of Nb : Re<br>Site $D_1$ | <br>Site $D_2$ | $R$ value |
|---|---|---|---|---|
| A | | | | 0·24 |
| B | Nb | 2·25 : 21·75 | 2·25 : 21·75 | 0·13 |
| C | Nb | 1·5 : 22·5 | 3 : 21 | 0·14 |
| D | Nb | 3 : 21 | 1·5 : 22·5 | 0·13 |
| E | Nb | 3·75 : 20·25 | 0·75 : 23·25 | 0·12 |
| F | Nb | 4·5 : 19·5 | 0 : 24 | 0·12 |

Distribution of Nb and Re is random in structure A.

We are grateful to Dr Knapton of A.E.I., Aldermaston, for supplying the specimens, and to the Department of Scientific and Industrial Research for a grant for equipment.

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*Acta Cryst.* (1964). **17**, 63

## Crystallographic data for 1,2-dichloronaphthalene.

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(*Received* 17 *June* 1963)

Crystal data previously reported for 1,2-dichloronaphthalene (Trotter, 1960) actually corresponded to the 1,3-derivative (Trotter, 1961). The data for the 1,2-derivative have now been determined from precession films; crystals of 1,2-dichloronaphthalene are thick colourless plates, with (100) well developed, and smaller {011} forms.

*Crystal data* ($\lambda$, Mo $K\alpha = 0{\cdot}7107$ Å)

1,2-Dichloronaphthalene, $C_{10}H_6Cl_2$; $M$, 197·1; m.p., 37 °C.

Monoclinic,

$$a = 7{\cdot}26 \pm 0{\cdot}02,\ b = 8{\cdot}96 \pm 0{\cdot}02,\ c = 13{\cdot}72 \pm 0{\cdot}03\ \text{Å};\ \beta = 104{\cdot}2^\circ \pm 0{\cdot}1^\circ.$$

Volume of the unit cell: 865 Å³.

$D_m$ (flotation in aqueous KI): 1·51 g.cm$^{-3}$,

$D_x$ (with $Z = 4$): 1·51 g.cm$^{-3}$.

Absent reflexions: $h0l$ when $l$ is odd, $0k0$ when $k$ is odd. Space group is $P2_1/c(C^5_{2h})$.

No further work on this compound is planned.

The author is indebted to Dr Wolfgang Strehlow for suggesting measurement of these data and for the crystal sample, and to the National Research Council of Canada for financial support.

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