Acknowledgment

Thanks are due to Drs. G. Groetzinger and Philip Schwed for valuable discussions.

Discussion of this paper, if any, will appear in JOURNAL OF METALS, November 1955, and in AIME Metals Branch Transactions, Vol. 203, 1955.

References

¹E. Orowan: *Proceedings Royal Society* (1939) **171**, p. 79.

²B. Welber and R. Webeler: *JOURNAL OF METALS* (1953) **5**, p. 1558.

³B. Welber: *Journal of Applied Physics* (1952) **23**, p. 876.

⁴R. Landauer: *Journal of Applied Physics* (1952) **23**, p. 779.

⁵B. Wiener, G. Groetzinger, and P. Schwed: Private communication; *Physical Review* (1954) **93**, p. 922.

⁶P. J. E. Forsyth: *Journal Institute of Metals* (1954) **82**, p. 449.

⁷E. Passaglia and W. F. Love: *Physical Review* (1954) **95**, p. 666.

Technical Note

Crystal Structure of Neodymium Metal

by F. H. Ellinger

THE crystal structure of neodymium has been reported by Quill¹ and by Klemm and Bommer^{2,3} to be hexagonal-close-packed, Strukturbericht-type A3, with $a_o = 3.650\text{\AA}$, $c_o = 5.890\text{\AA}$, $c/a = 1.614$. Klemm and Bommer,³ however, pointed out that the observed intensities of the lines of the neodymium powder pattern agreed only in part with the intensities calculated for the type A3 structure, and that the neodymium powder pattern showed extra lines which could not be traced to impurities. They found that these extra lines could be accounted for by doubling the c -axis, but apparently they did not consider their evidence to be sufficiently conclusive to justify reporting the doubled c -axis. In the present work, the structure of neodymium was found to be double hexagonal-close-packed.

The neodymium metal used in the present investigation was obtained through the courtesy of F. H. Spedding of the Ames Laboratory. Its major impurity was stated to be 0.03 pct Ca. The author's spectrographic analysis indicated high purity and carbon was determined to be less than 30 ppm. X-ray powder specimens were prepared from filings stress relieved in vacuum at 200°C for 50 hr. Powder photographs were taken in an 114.6 mm diam camera (Straumanis film mounting) at room temperature and in a 19 cm diam Unicam high temperature camera at elevated temperatures. Copper x -radiation was used for all the photographs.

The powder pattern of neodymium was found to index to a hexagonal unit cell with dimensions, as determined from the high angle $K\alpha$ doublets, of: $a_o = 3.655 \pm 0.001\text{\AA}$; $c_o = 11.796 \pm 0.004\text{\AA}$; and $c/a = 3.227$ at room temperature. The measured density of neodymium shows that this cell contains 4 atoms, the calculated density is accordingly $D_x = 7.02$ g per cu cm. The diffraction data for the first 15 lines of the powder pattern are listed in Table I. In a double hexagonal-close-packed unit cell, the 4 atoms would be in the positions $(0,0,0)$, $(0,0,\frac{1}{2})$, $(\frac{1}{3}, \frac{2}{3}, \frac{1}{4})$, and $(\frac{2}{3}, \frac{1}{3}, \frac{3}{4})$ of space group $P6_3/mmc$. On the basis of these positions, the relative intensities of the reflections were calculated using the expression:

$$I \propto |F|^2 p \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$$

where F is the structure factor and p is the multiplicity factor.

F. H. ELLINGER, Member AIME, is associated with Los Alamos Scientific Laboratory, University of California, Los Alamos, N. M. TN 208E. Manuscript, Dec. 7, 1953.

Table I. X-Ray Diffraction Data for Neodymium Metal, Radiation: Cu $K\alpha$

HK L	Observed		Calculated Intensity
	d, Å	Intensity*	
10.0	3.136	w	48
10.1	3.032	m	262
00.4	2.921	m	214
10.2	2.767	s	614
10.3	2.452	mw	148
10.4	2.141	vw	37
10.5	1.883	w	65
11.0	1.820	mw	86
10.6	1.664	m	130
20.0	nil	nil	6
20.1	1.563	vw	36
11.4	1.549	ms	185
20.2	1.525	mw	97
10.7	1.483	w	29
00.8 } 20.3 }	1.469	w +	{ 25 29

* s is strong; m, medium; w, weak; and v, very.

Since absorption was not taken into consideration, comparison of observed and calculated intensities should be made only for neighboring reflections.

Each atom has 12 neighbors, 6 in the basal plane at a distance of 3.655Å and 3 above and 3 below at the closer distance of 3.626Å. These distances correspond to an average radius of the neodymium atom of 1.820Å.

The description of this structure in terms of A, B, and C close-packed layers of atoms is ABACABAC · · · · ·. The structure repeats every fourth layer and the stacking sequence of the second, third, and fourth layers corresponds to cubic-close-packing of atoms.

A series of powder photographs taken at successively increasing temperatures up to 680±10°C revealed that the double hexagonal-close-packed structure is stable up to this temperature.

Acknowledgments

The author wishes to thank W. H. Zachariasen and A. S. Coffinberry for their helpful comments on this work and also Marion Gibbs for measuring the diffraction films. This work was sponsored by the United States Atomic Energy Commission.

¹L. L. Quill: *Ztsch. anorg. allgem. Chemie* (1932) **208**, p. 273.

²W. Klemm and H. Bommer: *Ztsch. anorg. allgem. Chemie* (1937) **231**, p. 138.

³W. Klemm and H. Bommer: *Ztsch. anorg. allgem. Chemie* (1939) **241**, p. 264.