

① X-ray
② Compressibility

③ Ruthenium
④ Iron

H. J. Hall

J. Phys. Chem. Solids Pergamon Press 1964. Vol. 25, pp. 865-868. Printed in Great Britain.

THE EFFECT OF PRESSURE ON THE VOLUME AND LATTICE PARAMETERS OF RUTHENIUM AND IRON*

R. L. CLENDENEN and H. G. DRICKAMER

Department of Chemistry and Chemical Engineering and Materials Research Laboratory
University of Illinois, Urbana, Illinois

(Received 24 February 1964)

Abstract—The volume changes and lattice parameters of ruthenium and iron have been measured to 400 kbars pressure. The compressibility of ruthenium is comparable to that of rhodium and molybdenum. c/a decreases slightly at low pressures and then increases rapidly to the highest pressures obtained.

Iron has a phase transition at 130 kbars and 25°C. The high pressure phase is *hcp*. Compressibilities of both the *bcc* and *hcp* phases compare well with data obtained from shock velocities. c/a for the *hcp* phase decreases very rapidly with increasing pressure to 400 kbars.

THE volumes and lattice parameters of ruthenium and iron has been measured to 400 kbars pressure at 25°C. The high pressure X-ray system has been previously described.⁽¹⁾ As discussed therein, pressures are measured by means of a marker, a substance whose compressibility is known as a function of pressure. For ruthenium the markers used were molybdenum and silver. For iron the markers were molybdenum and MgO. Densities obtained from shock wave measurements⁽²⁾ are available for molybdenum and silver. The compressibility of MgO has been measured in this laboratory.⁽³⁾

The ruthenium used in this study was 99.9 per cent pure material obtained from A. D. Mackay. Ruthenium has the *hcp* structure. The 100, 101, 110 and 112 lines were used for calculating lattice parameters. The data were smoothed by plotting the 2θ for the 112 line. Figure 1 is a typical plot. Line locations vs. pressure are shown in Figs. 2 and 3. Smoothed values of V/V_0 , c , a , and c/a are shown in Table 1. Figure 4 shows a plot of V/V_0 and Fig. 5 a plot of c/a vs. pressure. No densities are available for ruthenium from shock wave data, but the compressibility obtained from our data is very similar to the shock wave results for rhodium

and molybdenum. As can be seen from Fig. 5, c/a is initially about 1.5838, decreases slightly to about 175 kbars, and then increases relatively rapidly with increasing pressure. In the absence of calculations concerning band structure and Fermi surface, it is not practical to attempt an interpretation at this time.

The iron used in this work was 99.9 per cent pure material obtained from A. D. Mackay. At

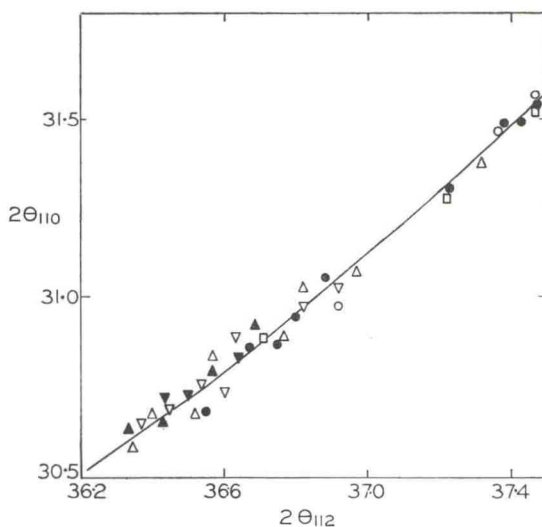


FIG. 1. Diffraction angle $2\theta_{110}$ vs. $2\theta_{112}$ for ruthenium.

* This work was supported in part by the United States Atomic Energy Commission and in part by the Petroleum Research Fund.

Table 1. Effect of pressure on volume and lattice parameters of ruthenium

P (kbars)	V/V_0	c	a	c/a
0	1.000	4.275	2.700	1.584
50	0.985	4.255	2.688	1.584
100	0.970	4.236	2.677	1.582
150	0.956	4.215	2.664	1.582
200	0.943	4.195	2.652	1.582
250	0.931	4.177	2.640	1.582
300	0.919	4.163	2.628	1.584
350	0.909	4.152	2.618	1.586
400	0.901	4.144	2.608	1.589

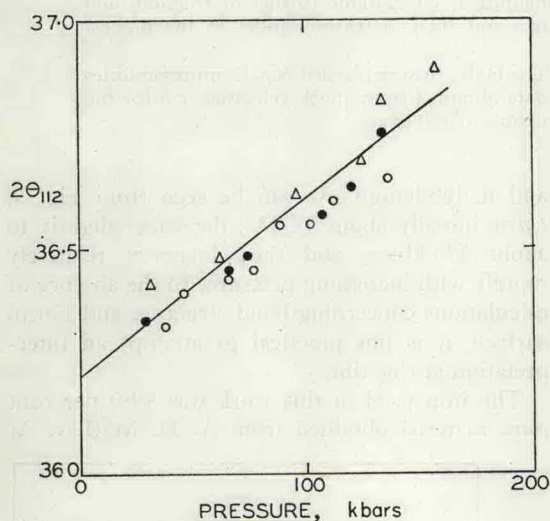
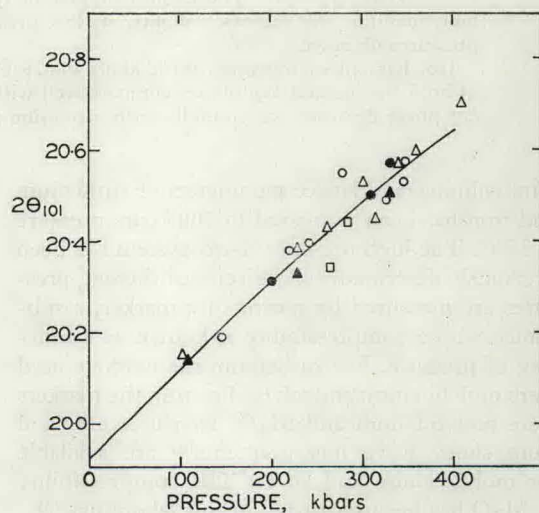
FIG. 2. Diffraction angle $2\theta_{112}$ vs. pressure for ruthenium.FIG. 3. Diffraction angle $2\theta_{101}$ vs. pressure for ruthenium.

Table 2. Effect of pressure on volume and lattice parameters of iron

P (kbars)	V/V_0 (bcc)	V/V_0 (hcp)	c	a	c/a
0	1.00				
50	0.974				
100	0.952				
150	0.932	0.910	4.050	2.465	1.643
200	0.914	0.883	3.975	2.452	1.621
250	0.896	0.864	3.920	2.443	1.605
300	0.879	0.852	3.882	2.435	1.594
350		0.840	3.852	2.428	1.586
400		0.829	3.828	2.421	1.580