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① X-ray ② Compressibility ③ Ruthenium ④ Iron    H. T. Hall

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

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**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 $2\theta$ 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

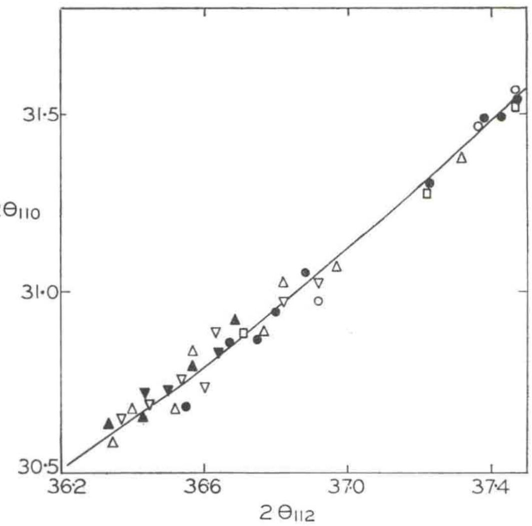


FIG. 1. Diffraction angle $2\theta_{110}$ vs. $2\theta_{112}$ for ruthenium.

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*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 |

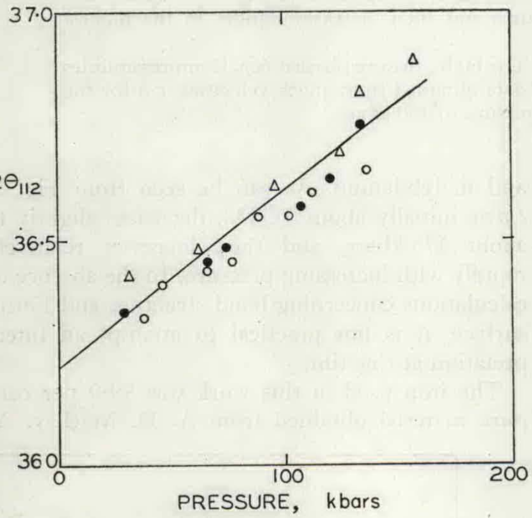


FIG. 2. Diffraction angle $2\theta_{112}$ vs. pressure for ruthenium.

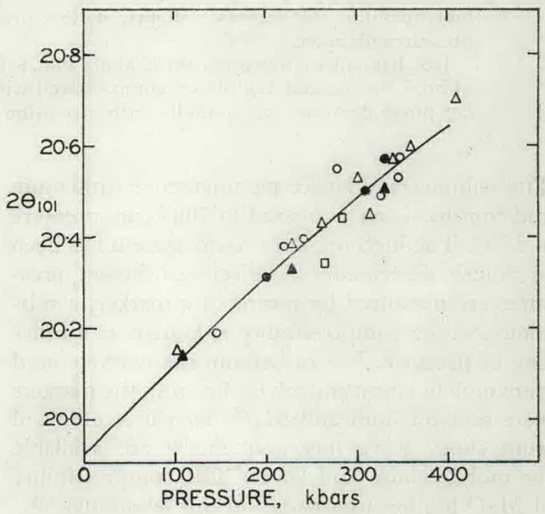


FIG. 3. Diffraction angle $2\theta_{101}$ vs. pressure for ruthenium.

*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 |

25°C and one atmosphere pressure, iron has the bcc structure. Shock velocity measurements[(4)] and static electrical resistance measurements[(5)] have shown a phase transition at 130 kbars. JAMIESON and LAWSON[(6)] found a single strong line in an X-ray spectrum of the high pressure phase which was interpreted to indicate that it is *hcp*. We found strong lines corresponding to the 101, 110, 110 lines and weaker lines located consistent with interpretation as 112, 002 and 103.

Figure 6 shows a typical plot of 101 line vs. pressure. In Table 2 are listed $V/V_0$ for both *bcc* and *hcp* phases, as well as values for *c*, *a* and *c*/*a* for the *hcp* phase. $V/V_0$ values are plotted in Fig. 7. The transition is quite sluggish and compressibility values were obtained for the *bcc* phase well

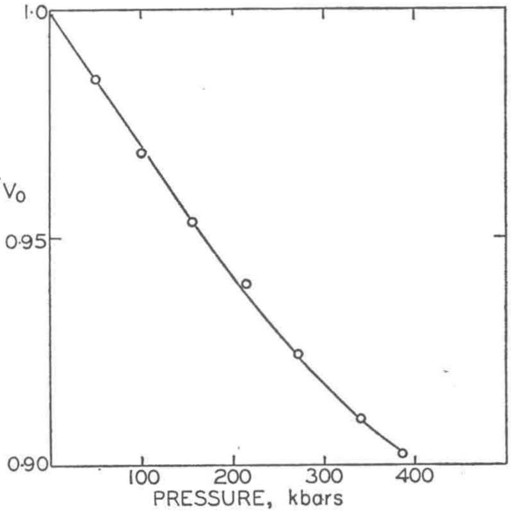


FIG. 4. Fractional change in volume vs. pressure for ruthenium.

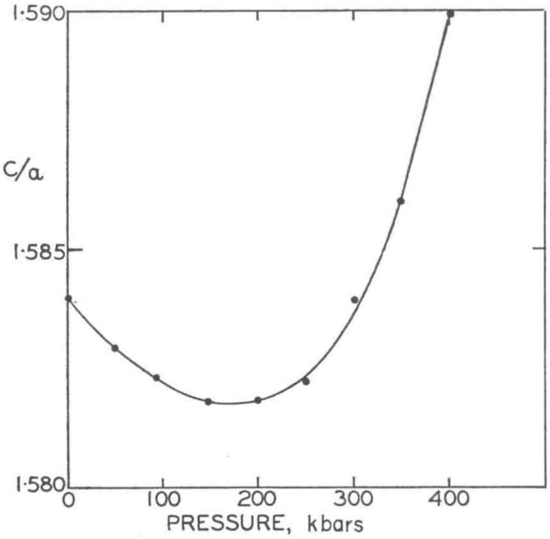


FIG. 5. Lattice parameter ratio *c*/*a* vs. pressure for ruthenium.

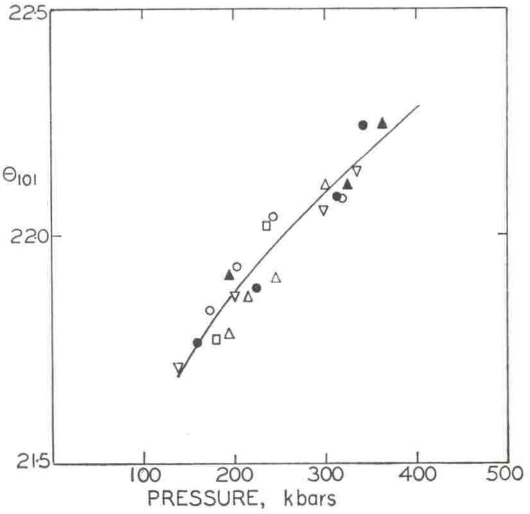


FIG. 6. Diffraction angle $2\theta_{101}$ vs. pressure for *hcp* iron.

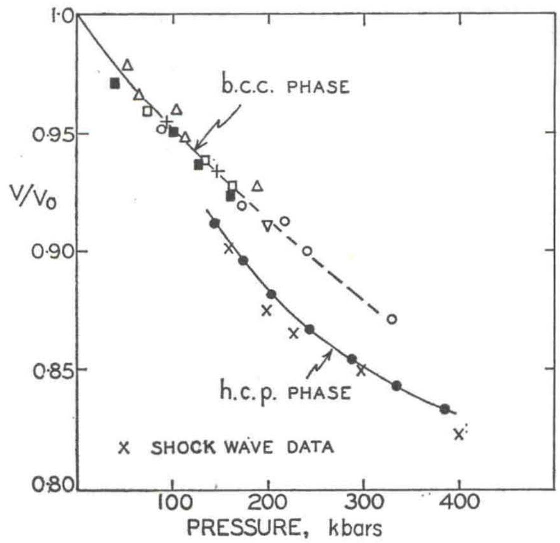


FIG. 7. Fractional change in volume vs. pressure for iron.

beyond its region of stability, in one case to over 300 kbars. It can be seen that the densities obtained from shock wave measurements coincide exactly with out results for the *bcc* phase, and check very reasonably for the *hcp* phase.

As can be seen from Table 2 and Fig. 8, $c/a$ is about 1·645 at 150 kbars and decreases rather rapidly with increasing pressure, reaching a value of 1·580 at 400 kbars. This high compressibility of the $1/c$ axis corresponds to a relatively rapid expansion of the Brillouin zone in the $1/c$ direction and a relatively slow expansion in the $1/a$ direction. In the absence of any other information one could interpret this to mean a rather strong interaction of the Fermi surface with the 100 faces of the Brillouin zone, corresponding to the close approach of the Fermi surface and the zone boundary.[7]

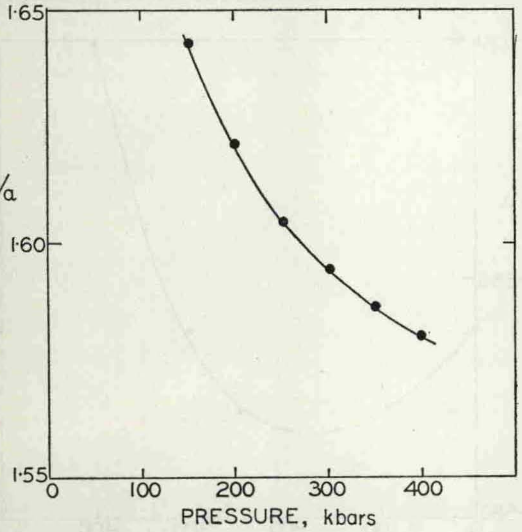


FIG. 8. Lattice parameter ratio $c/a$ vs. pressure for *hcp* iron.

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