PHYSICAL REVIEW B VOLUME 31, NUMBER 7 1 APRIL 1985

High-pressure structural phase transition in Mg

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(Received 9 August 1984)

Mg was studied by energy-dispersive x-ray diffraction at room temperature and is found to transform to the bcc structure around 50 GPa, in agreement with recent theoretical predictions by McMahan and Moriarty.

Recent total-energy calculations for various solid modifications of the third-period metals Na, Mg, Al, and Si (Ref. 1) by McMahan and Moriarty[2,3] have predicted new high-pressure phase transitions for these metals, which are all controlled by *d*-state effects. The light alkaline-earth metal Mg is expected to transform from hcp to bcc around 50 GPa and to fcc at still higher pressures. These results stimulated us to extend our previous high-pressure investigations[4] on Mg into the 50-GPa regime.

The present high pressure x-ray diffraction studies on Mg were performed at Hamburger Synchrotronstrahlungslabor (HASYLAB) at Deutsches Elektronen-Synchrotron using synchrotron radiation.[5] Small samples were mounted in a gasketed diamond anvil cell of the Syassen-Holzapfel type[6] together with a ruby splinter for pressure determination by the ruby fluorescence technique. The linear pressure scale with $d\lambda/dp = 3.65$ Å/GPa was adopted.[7] Isopropanol was used as the pressure transmitting medium. Uncertainties of the nominal pressure may be as high as 5 GPa in the upper pressure range due to nonhydrostatic conditions.

Figure 1(a) shows a diffraction pattern of hcp Mg at 28.5 GPa with the indexing of the dominant peaks 100, 101, and 110. On increasing pressure an additional diffraction line starts to develop above 49 GPa between the 100 and 101 reflex. This new line is definitely not the 002 reflex of hcp. On further compression this new line grows up in intensity and two additional new peaks appear, while the intensity of the hcp lines strongly decreases. In the diffraction pattern at 58 GPa, the highest pressure of various different preparations, the hcp diffraction lines have been almost suppressed [Fig. 1(b)]. On decreasing pressure to 49 GPa the intensity of these reminiscent hcp lines decreases at first further by cold working, indicating that Mg has almost completely transformed into the new phase [Fig. 1(c)]. The new lines can be indexed to a bcc structure with $a = 2.9530 \pm 0.002$ Å at 58 GPa. This structural assignment is very well supported also by the comparison of observed and calculated relative intensities (Table I), where no change in texture during the phase transition has been assumed. We found a large hysteresis in this phase transition on unloading. The intensity ratios between the hcp 101 and the bcc 110 reflection at 56 GPa and unloaded 44 GPa are almost equal. We, therefore, estimate the hcp-bcc transition pressure to 50 ± 6 GPa. The volume change at the transition is rather small with $\Delta V/V \simeq 1\%$.

Table II gives a comparison of the experimental values for transition pressures and volumes (at room temperature) with the theoretical predictions[2,3] (for 0 K) from McMahan and Moriarty. The overall agreement between experiment and theory appears remarkable.

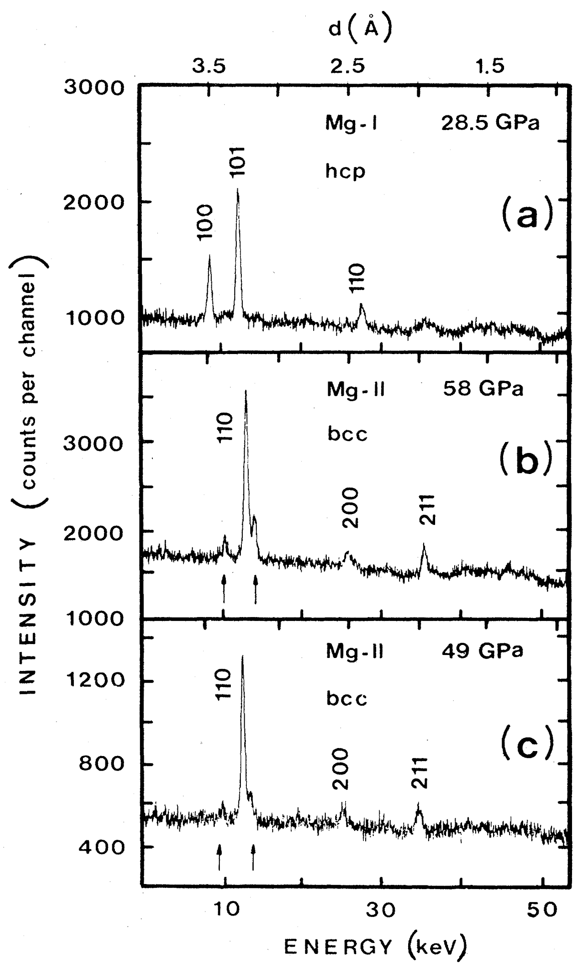

FIG. 1. X-ray diffraction patterns of Mg I (hcp) and Mg II (bcc) at various pressures. In (b) and (c) the 100 and 101 diffraction lines of the reminiscent hcp phase are marked by arrows. The exposure time was ≃ 2000 sec.

McMahan and Moriarty[2,3] have also performed total-energy calculations without taking into account any *d* states, and it is interesting to note that in this case Mg would

TABLE I. Observed and calculated d spacings and intensity ratios for bcc Mg at 58 GPa.

hkl	d_{obs} Å	d_{calc} Å	I_{obs} (%)	I_{calc} (%)
110	2.0871	2.0881	100	100
200	1.4770	1.4765	10	17
112	1.2057	1.2056	15	25

TABLE II. Experimental (300 K) and theoretical (0 K) reduced volumes and transition pressures for the hcp-bcc transition in Mg. GPT: generalized pseudopotential technique; LMTO: linear muffin-tin orbitals method.

V/V_0			P/GPa		
Expt.	GPT	LMTO	Expt.	GPT	LMTO
0.59 ± 0.02	0.58	0.56	50 ± 6	50	57

remain hcp even at 10 times normal density. The observed transition from hcp to bcc in Mg around 50 GPa gives, therefore, further experimental evidence for the important role the almost empty d states play in effecting the stability of the high-pressure structures in the third-period metals like Na, Mg, Al, and Si. The only previous experimental indication for these d band effects has been noticed recently[8] in a comparison of the high-pressure structures of Si and Ge.[9]

This work was supported in part by the Bundesministerium für Forschung und Technologie and performed at Hamburger Synchrotronstrahlungslabor at Deutsches Elektronen-Synchrotron.

[1]According to Ref. 3 Si should transform to hcp at 41 GPa and become a natural member of the third-period simple metals; see Ref. 9.
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