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Abstract

A new high-pressure phase and the equation of state of YbH_2. J. Staun Olsen (Physics Laboratory II, University of Copenhagen, Copenhagen), B. Buras (Physics Laboratory II, University of Copenhagen, Copenhagen and Risø National Laboratory, Roskilde)*), L. Gerward (Laboratory of Applied Physics III, Technical University of Denmark, Lyngby), B. Johansson (Institute of Physics, University of Aarhus, Aarhus), B. Lebech (Risø National Laboratory, Roskilde), H. L. Skriver (Risø National Laboratory, Roskilde) and S. Steenstrup (Physics Laboratory II, University of Copenhagen, Copenhagen).

Physica Scripta (Sweden)

High-pressure x-ray diffraction studies have been performed on YbH_2 up to 28 GPa. A first order phase transition from an orthorhombic structure to a collapsed hexagonal structure with $c/a = 1.34$ has been observed at about 15 GPa. The transition is accompanied by a 5.2% decrease in volume. Fitting the V(P) data to Murnaghan's equation of state yields the bulk modulus $B_0 = 40.2$ GPa and its pressure derivative $B_0' = 4.75$ for the orthorhombic phase. For the hexagonal phase we find the bulk modulus to be $B = B_0 = 138$ GPa independent of pressure, i.e. $B_0' = 0$.

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1. Introduction

In several rare-earth compounds and intermetallics the valence state of the rare-earth ion may be changed between the $4f^{n+1}(5d6s)^2$ and $4f^n(5d6s)^3$ configurations by chemical manipulations or by application of high pressure [1]. By now quite a number of such unstable valence systems have been studied, although naturally the main emphasis has been on chemically manipulated systems rather than on compressed systems. Furthermore, no attention has been directed towards those cases where the valence change may be accompanied by a change in crystal structure.

At zero pressure the rare-earth dihydride, YbH_2, shares the orthorhombic CaH_2 type structure with EuH_2, and in both compounds the ground state configuration is $4f^{n+1}(5d6s)^2$. In contrast, the ground state configuration of the other rare-earth dihydrides is $4f^n(5d6s)^3$, and they all crystallize in the fcc fluorite structure. Hence, if the valence state of Yb is changed to $4f^n(5d6s)^3$ under pressure one would expect YbH_2 to transform into an fcc structure.

The present report describes the results of x-ray diffraction experiments using synchrotron radiation and a diamond anvil high-pressure cell. Some preliminary results of this work have been presented previously [2]. The work clearly demonstrates a structural phase transformation at about 15 GPa. As the results will show, the high-pressure phase does not have the expected fcc structure but a collapsed hexagonal structure with c/a = 1.34. Refined values for the unit cell parameters are given as functions of pressure. The bulk modulus and its pressure derivative have been obtained by fitting the experimental V(P) data to Murnaghan's equation of state.

2. Experimental

A diamond anvil cell was utilized for the high-pressure studies and the YbH_2 powder was enclosed in an inconel gasket. A 4:1 methanol-ethanol mixture was added to the powder to allow for hydrostatic pressure conditions. The pressure was determined from the pressure induced shift of the fluorescence lines from a small ruby added to the powder.

The x-ray experiments were performed using synchrotron radiation from the electron storage ring DORIS at DESY-HASYLAB in Hamburg. The electron energy was 4 GeV. The pressure cell was placed on the energy-dispersive diffractometer [3] or the triple-axis spectrometer [4] working in the energy-dispersive mode. Diffraction from the gasket was avoided by reducing the incident beam cross section to 0.1x0.1 mm². The scattering angle, $2\Theta_0$, was about 14.5°.

Figure 1 and 2 show examples of energy-dispersive diffraction spectra from the low-pressure phase and the high-pressure phase, respectively. For each diffraction peak the interplanar spacing d can be obtained from the Bragg equation, written in terms of the photon energy E associated with the peak:

$$E\ d\ \sin\Theta_0 = hc/2 = 6.199\ \text{keV}\cdot\text{Å} \qquad (1)$$

where Θ_0 is the fixed Bragg angle, h Planck's constant and c the velocity of light. The peak positions E have been determined by fitting the observed peaks to a Gaussian shape. In this way also overlapping peaks have been resolved, a problem that is particularly important for the orthorhombic diffraction spectra with many lines.

3. Unit cell parameters

The location of the Bragg peaks in the energy-dispersive diffraction spectrum may be used to identify the Bravais lattice, the unit cell size and in some cases the space group. Information about the detailed arrangement of atoms within the unit cell is contained in the intensity of the

Bragg peaks. However, because of the small sample size and a possible pressure induced texture variation in the sample it is very difficult to obtain reliable intensity data from the high-pressure diffraction spectra.

3.1 The orthorhombic phase at $P < 15$ GPa

The structure of YbH_2 at atmospheric pressure is orthorhombic with the space group Pnma (D_{2h}^{16}). The unit cell contains 4 YbH_2 units. With the origin at $\bar{1}$ the Yb atoms occupy the positions 4(c) with $x = 0.24$ and $z = 0.11$. (For a description of the space group see e.g. the International Tables for X-ray Crystallography Vol. I [5]).

The results of this work show that the orthorhombic phase is stable up to about 15 GPa. The observed positions of the Bragg peaks have been fitted by a least-squares method to the calculated positions corresponding to an orthorhombic structure using the lattice constants a, b and c as fitting parameters. The Bragg angle has to be determined independently, because $\sin\Theta_0$ is a common constant for all diffraction lines. Thus the least squares fit will give a precise determination of the ratios a:b:c, whereas the absolute values of the unit cell parameters may be uncertain by a common multiplicative factor because of the experimental uncertainty of $\sin\Theta_0$.

The refined unit cell parameters are given in Table 1 and shown in Fig. 3. The goodness of the fit is characterized by a factor G defined as

$$G(\%) = 100 \cdot \sum_{i=1}^{N} |E_i(\mathrm{obs}) - E_i(\mathrm{calc})| / \sum E_i(\mathrm{obs}) \qquad (2)$$

where E_i(obs) and E_i(calc) are the energies of the i:th diffraction peak measured experimentally and calculated from the fit, respectively. It is seen that the G-factor is about 0.3%.

It has been shown [6,7] that peak positions and hence lattice constants can be determined with a precision of about 0.05% in energy-dispersive diffractometry provided the experimental conditions are optimized. For example, the observed and calculated peak energies of a silicon powder diffraction spectrum reported by Fukamachi, Hosoya and Terasaki [7] give G = 0.06% in the 18-40 keV range. However, as discussed by Buras [8], the diamond-anvil high-pressure cell of the present work imposes some limitations on the x-ray diffraction studies. The main restrictions are due to the absorption in the diamonds, the limited scattering angle and the small sample size. In view of these limiting factors the fits obtained in the present work must be considered as highly satisfactory.

The unit cell parameters of orthorhombic YbH_2 at atmospheric pressure are compared with published values in Table 2. It is seen that the agreement is within 0.3% in all cases.

3.2 The hexagonal phase at 15 GPa < P < 28 GPa

As mentioned in the Introduction the diffraction spectra of the high-pressure phase of YbH_2 can be indexed according to a hexagonal close-packed arrangement of the Yb-atoms. The scattering power of the hydrogen atoms is too small to have any observable effect on the x-ray diffraction spectra. The unit cell parameters a and c have been determined from least squares fittings to the observed spectra in a similar way as described in the preceding section. The refined unit cell parameters are given in Table 3. Also in this case the goodness of the fits must be considered as highly satisfactory.

Although the c/a-ratio[*)] of the distorted hexagonal packing in the orthorhombic phase is close to 1.63, the c/a-ratio for the hexagonal high-pressure phase is considerably less than the ideal hcp-value as seen in Fig. 4 and Table 3. At 14.3 GPa near the phase transition we find c/a = 1.34, indicating that the distorted hcp arrangement of the Yb atoms has transformed into a collapsed hcp arrangement. In accordance with this picture we observe

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[*)] Approximately equal to the a/b-ratio of the orthorhombic unit cell (see Section 5).

a discontinuity in volume that will be discussed in the following section. An attempt to explain the phase transformation process is presented in Section 5.

4. Equation of state

The volume per Yb atom has been calculated from the refined unit cell parameters found in the preceding sections. As seen in Figure 5 there is a discontinuity of the volume at the phase transition at about 15 GPa. Thus we conclude that it is a first order transition. At 14.3 GPa the volume per Yb atom is 28.9 Å^3 in the orthorhombic phase and 27.4 Å^3 in the hexagonal phase, indicating a 5.2% decrease in volume when the structure changes from orthorhombic to hexagonal.

The compressibility data of the orthorhombic phase were fitted to Murnaghan's equation of state [13]

$$P = (B_0/B_0') \left[(V_0/V)^{B_0'} - 1 \right] \qquad (3)$$

where B_0 is the isothermal bulk modulus and B_0' its pressure derivative at ambient pressure. The equation is based on the assumption that the bulk modulus is linear with pressure. A non-linear least squares method where

the parameters V_0, B_0 and B_0' were refined in an iterative procedure gave the following results

$$\begin{aligned} V_0 &= (35.63 \pm 0.07)\,\text{Å}^3 \\ B_0 &= (40.2 \pm 2.2)\,\text{GPa} \\ B_0' &= 4.75 \pm 0.45 \end{aligned} \qquad (4)$$

where the quoted errors are the asymptotic standard errors of the fit.

The Murnaghan equation gives a very good description of the experimental V(P) data for the orthorhombic phase as shown by the small standard deviation and by the calculated curve in Figure 5.

For the hexagonal phase ($P \geq 15$ GPa) we find a linear relation between ln V and P (Figure 5). This corresponds to the equation of state with $B_0' = 0$:

$$P = B_0 \ln(V_0/V) \qquad (5)$$

A least squares fit to equation (5) gives

$$\begin{aligned} V_0 &= (30.4 \pm 0.1)\,\text{Å}^3 \\ B_0 &= (138 \pm 3)\,\text{GPa} \\ B_0' &= 0 \end{aligned} \qquad (6)$$

where the qouted uncertainties are the standard deviations of the fit.

5. Interpretation of the phase transition

In our preliminary report [2], following the analogy with the structure of CaH_2 [14,15], we visualized the orthorhombic structure of YbH_2 as a distorted hexagonal structure and suggested that the observed phase transition at about 15 GPa can be interpreted as a transition from a distorted hexagonal lattice with $c/a \approx 1.6$ to a collapsed hexagonal lattice with $c/a = 1.34$. At that time, however, we based this suggestion of the knowledge of the positions of the Yb atoms only, because the positions of the hydrogen atoms were not known. In the meantime Fischer et al. [16] and Lebech et al. [12] have studied the structure of orthorhombic YbD_2 and YbH_2 at atmospheric pressure by means of neutron diffraction and suggested that the high pressure structure of YbH_2 is D^4_{6h} ($P6_3/mmc$) with the Yb atoms in (2c) and the hydrogen atoms in (2a) and (2d) positions. In order to enable a better insight into the phase transition process we give below a somewhat extended description of the line of thought that led to the above mentioned proposal and make some additional remarks.

The result of the neutron diffraction study [12] is depicted in Figure 6. Figure 6a shows the projection of the atoms in the orthorhombic phase at

14.3 GPa on the $(\vec{b}_o,\vec{c}_o)$ plane, and Figure 6b on the $(\vec{b}_o,\vec{a}_o)$ plane, where the subscript "o" stands for orthorhombic. The numbers to the right in Figure 6 indicate the fractional coordinates along the $\vec{a}_o$ direction. (The figure is drawn to scale in the $\vec{b}_o,\vec{c}_o$ directions, but has been expanded along the $\vec{a}_o$ direction for the sake of clarity). In order to simplify the interpretation, we follow Lebech et al. [12] and assume that the fractional coordinates for the Yb and H atoms in the orthorhombic phase do not change with pressure up to the transition. This approximation should not change the overall picture of the transition.

Consider first the projection of the Yb atoms on the $(\vec{b}_o,\vec{c}_o)$ plane (Figure 6a). At 14.3 GPa, near the phase transition, b_o = 3.368 Å and c_o = 6.294 Å. At about the same pressure, in the hexagonal phase, a_h = 3.617 Å, where the subscript "h" stands for hexagonal. Hence, at 14.3 GPa, a_h is close to b_o and $a_h\sqrt{3}$ = 6.265 Å very close to c_o. Thus only a small dilation of b_o *) and a very small contraction of c_o are needed to place the projections of seven Yb atoms (marked B) in the corners and the centre of a regular hexagon with a_h = 3.617 Å. As a

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*) An indication of this may possibly be noticed in Figure 3.

matter of fact, in Figure 6a it is already assumed that the dilation and contraction have taken place, because on the scale of Figure 6a the difference in positions would be difficult to see. As concerns the Yb atoms marked by C, the shifts needed to place them in the centres of the triangles formed by the Yb atoms marked by B, i.e. into the correct positions in a hexagonal structure, are larger (indicated by arrows).

As can be seen from Figure 6b, the shifts (in fractional coordinates) of the Yb atoms in the $(\vec{b}_o,\vec{a}_o)$ plane are small. However, one must assume large collective shifts along the $\vec{a}_o$ axis of all atoms located on partly distorted $(\vec{b}_o,\vec{c}_o)$ planes leading to the large contraction of a_o to c_h (from 5.434 A to 4.839 A) at the structural transition.

In order to try to understand the large contraction of a_o, we now turn to the hydrogen atoms. From Figure 6 it is seen that there are two types of hydrogen atoms, H' and H''. In the projection on the $(\vec{b}_o,\vec{c}_o)$ plane the H'' atoms (marked by A and D) lie in the corners and centre of two irregular hexagons (indicated by the dot-dashed triangles in Figure 6a) displaced by $b_o/2$ with respect to the hexagons formed by the Yb atoms marked by B. The irregular H'' hexagons are nearly planar (see Figure 6b), and hence the packing of the H'' atoms in the $(\vec{b}_o,\vec{c}_o)$ "planes" is as dense as the packing of the Yb atoms in these "planes". In the projection on the $(\vec{b}_o,\vec{a}_o)$ plane, the H'' atoms are displaced by $\sim a_o/4$ above and below the projection of the Yb atoms.

For the H' atoms, the situation is different. In the orthorhombic phase the projections of H' atoms on the $(\vec{b}_o,\vec{c}_o)$ plane are almost the same as the projections of the Yb atoms. However, in the projection on the $(\vec{b}_o,\vec{a}_o)$ plane, half of the H' atoms is displaced $\sim a_o/9$ above the corresponding Yb atoms; the other half is displaced $\sim a_o/9$ below the Yb atoms. Hence, the packing of H' atoms in the $(\vec{b}_o,\vec{c}_o)$ planes is only half as dense as the packing in $(\vec{b}_o,\vec{c}_o)$ "planes" of the Yb and H'' atoms.

In order to form the high pressure structure suggested by Lebech et al. [12] the atoms must move as indicated by the arrows in Figure 6. It is worthwhile to notice that for a given hydrogen atom, if its shift in the $(\vec{b}_o,\vec{c}_o)$ plane is large, then its shift in the $(\vec{b}_o,\vec{a}_o)$ plane is small and vice versa. Thus, the hydrogen atoms shift along approximately straight lines, either parallel to the c_o axis (H'') or parallel to the a_o axis (H'). Using the lattice parameters of the orthorhombic and hexagonal phases at 14.3 GPa we find that apart from collective shifts of all atoms, the Yb atoms shift by $\Delta a(\text{Yb}) = -0.076$ Å, $\Delta c(\text{Yb}) = -0.014$ Å, the H' atoms shift by $\Delta a(H') = 1.18$ A, $\Delta c(H') = 0.014$ A and the H'' atoms shift (on the average) by $\Delta a(H'') = -0.23$ A, $\Delta c(H'') = 0.93$ A.

Although an experimental proof of the above picture of the structural transition does not seem possible with the presently available structural methods, we think it is plausible for the following reason: In this picture the H' atoms move to the same $(\vec{b}_0,\vec{c}_0)$ plane as the Yb atoms and end up occupying the centre of every second of the regular triangles forming the Yb hexagons. The H' atoms thus form a hexagonal lattice and it must be favourable for the H'' atoms to move to the holes of this structure. It is the combined effect of the collapse of the H' atoms into the $(\vec{b}_0,\vec{c}_0)$ planes of the Yb atoms and the shift of the H'' atoms within the neighbouring $(\vec{b}_0,\vec{c}_0)$ planes (possibly followed by a small contraction of a_0) that causes the large contraction of a_0 to c_h. Although the hydrogen atoms in the hexagonal phase supposedly occupy the fractional coordinates of a dhcp lattice, the c/a ratio of the collapsed phase is smaller than ideal. The reason is that the Yb atoms in the mixed Yb-H' hexagonal layers cause the H' atoms to be situated further apart than close packing. Hereby the H'' hexagonal layers can move closer to the H' layers than in a close packed hexagonal structure.

6. Conclusion

A structural phase transformation has been found for YbH_2 at about 15 GPa where the orthorhombic structure transforms to a hexagonal structure by a first-order transition. The phase transition is accompanied by a 5.2% decrease in volume. The phase transformation can be interpreted as a transition from a distorted hexagonal packing with $c/a \approx 1.6$ to a collapsed hexagonal structure with $c/a = 1.34$.

It has been shown that the compressibility data of the orthorhombic phase are well described by Murnaghan's equation of state. From a least squares fit we have obtained the bulk modulus $B_0 = 40.2$ GPa and its pressure derivative $B_0' = 4.75$. The bulk modulus for the hexagonal phase is 138 GPa, independent of pressure.

It is generally assumed that no valence change occurs as long as the V(P) data can be described by for example Murnaghan's equation of state with given values of B_0 and B_0'. Thus we conclude that a possible valence change from $4f^{14}(5d6s)^2$ towards $4f^{13}(5d6s)^3$ for Yb takes place either at the phase transformation or at pressures $P > 15$ GPa. The found pressure independence of the bulk modulus of the hexagonal high-pressure phase might indicate that there is an intermediate valence state. One could speculate that the unexpected hexagonal structure is connected with the non-integral valence or that the hexagonal structure is a typical high-pressure structure for the Lu-dihydrides.

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Table 1. Refined unit cell parameters of orthorhombic YbH_2. The uncertainties are the standard deviations of the least squares fit. V_{Yb} is the volume of the unit cell devided by the number of Yb atoms. The G-factor is defined in eq. (6). N is the number of diffraction peaks used for the fit.

P(GPa)	a(Å)	b(Å)	c(Å)	V_{Yb}(Å^3)	G(%)	N
0	5.890 (8)	3.573 (4)	6.773 (8)	35.64 (8)	0.16	21
9.3	5.551(11)	3.419 (9)	6.438(13)	30.55(12)	0.31	21
11.53	5.501(12)	3.405(10)	6.405(16)	29.97(13)	0.34	20
14.3	5.453(14)	3.368 (9)	6.294(16)	28.90(13)	0.38	13
17.0	5.360(33)	3.404(16)	6.253(26)	28.52(25)	0.41	9
4.9	5.688(20)	3.475 (8)	6.538(12)	32.31(15)	0.26	16
1.2	5.821(14)	3.555 (6)	6.698 (8)	34.65(11)	0.17	16

Table 2. Unit cell parameters of orthorhombic YbH_2 or YbD_2 at atmospheric pressure.

Author	Sample	a(Å)	b(Å)	c(Å)
Korst and Warf [9]	YbD_2	5.871	3.561	6.763
Warf and Hardcastle [10]	YbH_2	5.905	3.570	6.792
Messer and Gianoukos [11]	$YbH_{1.78}$	5.895	3.574	6.801
Lebech et al. [12]	YbD_2	5.875	3.565	6.781
	YbH_2	5.900	3.576	6.776
This work	YbH_2	5.890	3.573	6.773

Table 3. Refined unit cell parameters of hexagonal YbH_2. The uncertainties quoted are the standard deviations of the least squares fit. V_{Yb} is the volume of the unit cell divided by the number of Yb atoms. The G-factor is defined in eq. (6). N is the number of diffraction peaks used for the fit.

P(GPa)	a(Å)	c(Å)	c/a	V_{Yb}(Å³)	G(%)	N
14.3	3.617(8)	4.839(16)	1.338(5)	27.41(15)	0.32	8
17.0	3.596(1)	4.802 (7)	1.335(2)	26.89 (4)	0.06	8
19.2	3.576(2)	4.757(10)	1.330(3)	26.34 (6)	0.09	11
21.9	3.564(3)	4.718(13)	1.324(4)	25.95 (8)	0.16	11
24.5	3.544(2)	4.680(12)	1.321(3)	25.45 (7)	0.13	11
25.8	3.536(1)	4.657 (3)	1.317(1)	25.21 (2)	0.04	10
27.5	3.524(1)	4.634 (5)	1.315(1)	24.92 (3)	0.06	8
28.2	3.520(2)	4.616 (9)	1.311(3)	24.77 (6)	0.09	8
17.95	3.586(1)	4.780 (7)	1.333(2)	26.62 (4)	0.04	7
15.4	3.609(1)	4.834(11)	1.339(3)	27.26 (6)	0.02	5

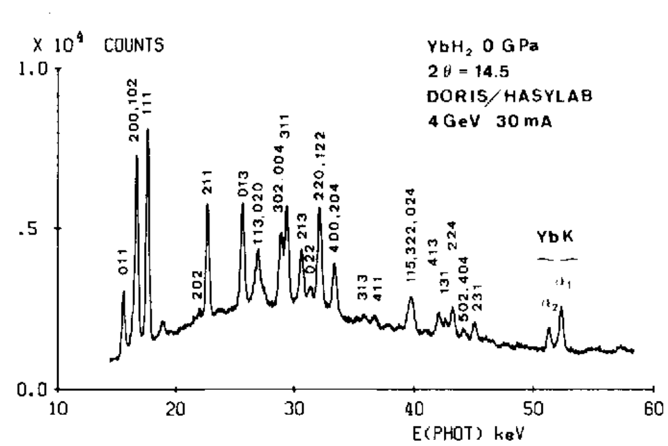

Fig. 1. X-ray energy-dispersive diffraction spectrum of orthorhombic YbH_2 at atmospheric pressure. Counting time 500 s.

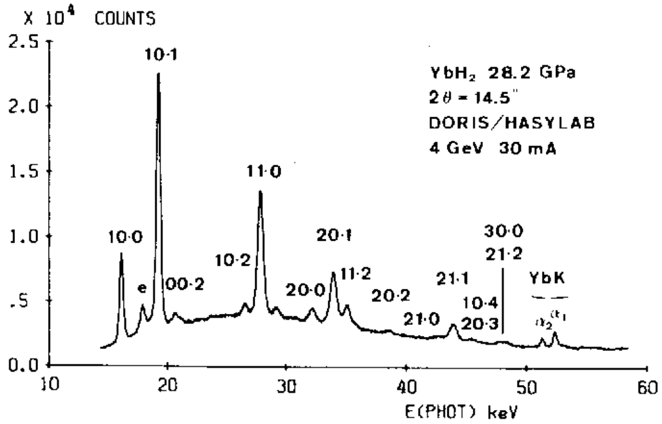

Fig. 2. X-ray energy-dispersive diffraction spectrum of hexagonal YbH_2 at 28.2 GPa. Counting time 500 s. The peaks are indexed using the three-indices notation.

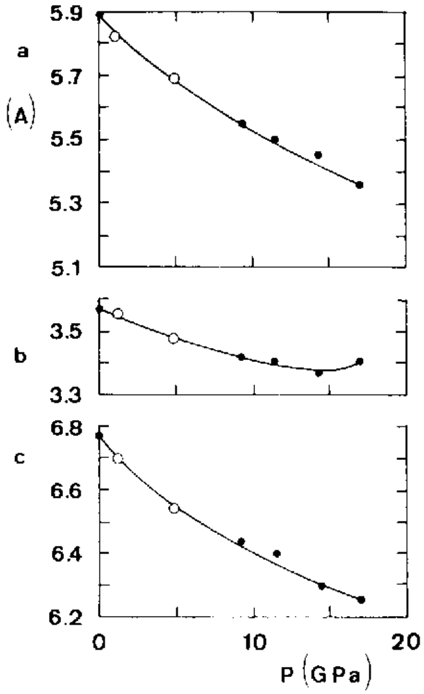

Fig. 3. Pressure dependence of the unit cell parameters for orthorhombic YbH_2. Open circles denote measurements for decreasing pressure.

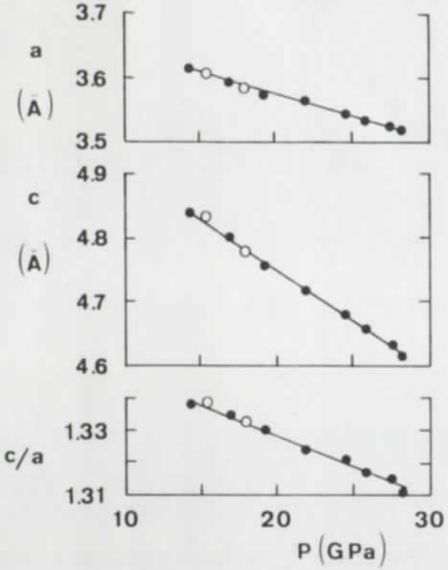

Fig. 4. Pressure dependence of the unit cell parameters and the c/a ratio for hcp YbH_2. Open circles denote measurements for decreasing pressure.

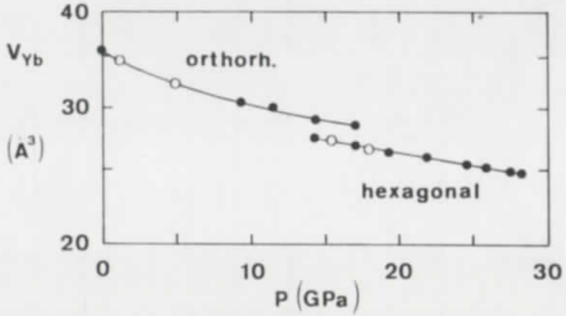

Fig. 5. Pressure dependence of the volume per Yb atom in the unit cell. Open circles denote measurements for decreasing pressure. The curve for the orthorhombic phase has been calculated from Murnaghan's equation of state using B_0 = 40.2 GPa and B_0' = 4.75.

Fig. 6. The projections of the atoms in the orthorhombic phase of YbH_2 at 14.3 GPa on the $(\vec{b}_0,\vec{c}_0)$ plane (Fig. 6a) and $(\vec{b}_0,\vec{a}_0)$ plane (Fig. 6b). The thin full lines in (a) connect Yb atoms (circles) in almost the same $(\vec{b}_0,\vec{c}_0)$ plane. The dot-dashed lines connect H'' atoms (open squares) in almost the same $(\vec{b}_0,\vec{c}_0)$ plane. The thick broken lines indicate the orthorhombic unit cell. Note that in (b) the figure has been expanded along the $\vec{a}_0$ direction. The numbers to the right indicate the fractional coordinates along the $\vec{a}_0$ direction.

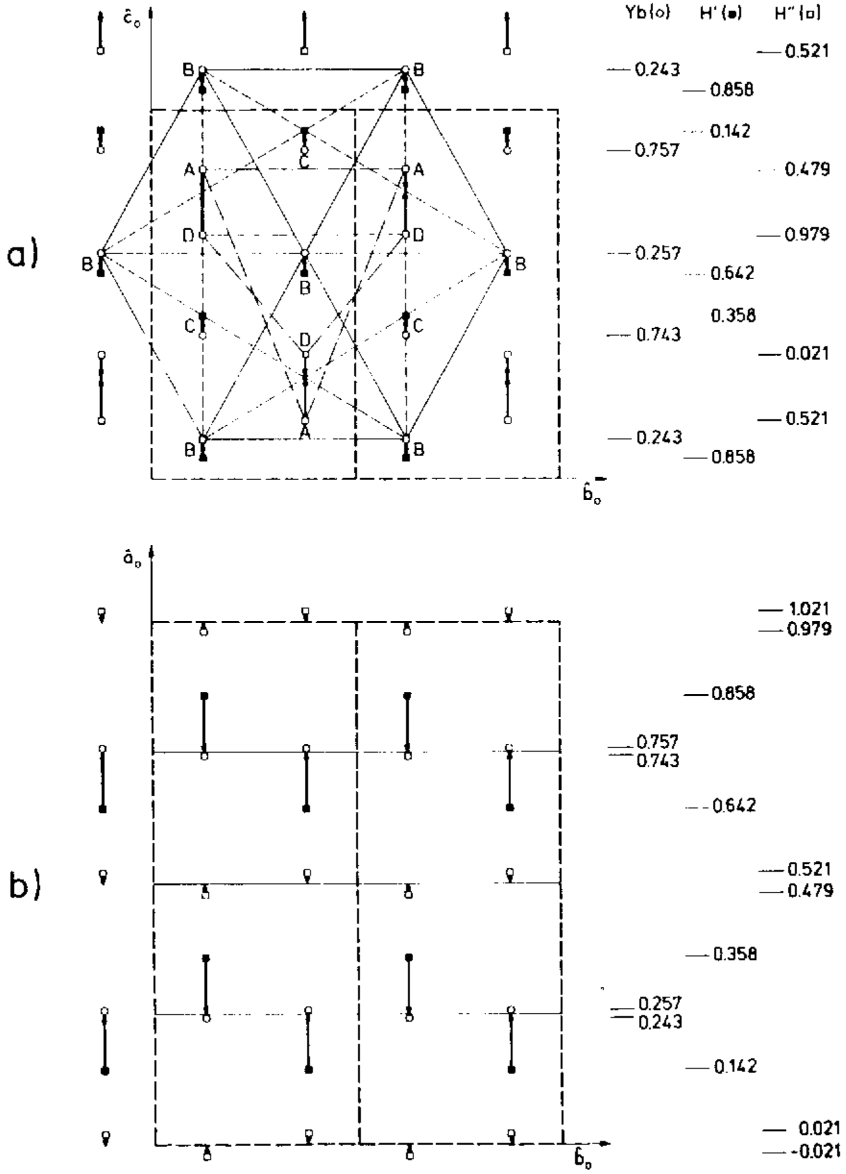

Fig. 6