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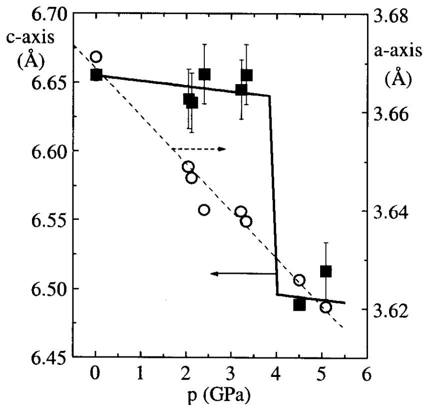
Report:

The measurements proved to be vital for a further understanding of the switchable mirror materials [1]. However, some experimental complications led to a far from optimal result.

A 1000 nm thick polycrystalline yttrium film covered by a 30 nm Pd caplayer is evaporated under UHV conditions on the culet (-500 mm diameter) of one of two diamonds in a Diamond Anvil Cell (DAC) setup. The rhenium gasket is filled with solid hydrogen. After pressurisation of the DAC, temperature is raised to -240 K, where the yttrium film absorbs a fraction of the surrounding solid hydrogen and switches to a transparent semiconducting stoichiometicYH_3 film. High pressure measurements are indispensable to test e.g. the Car-Parrinello calculations [2] since these are always made for the stoichiometric YH_3 .

Light transmission measurements up to high pressures (25 GPa) previously performed at the Vrije Universiteit in Amsterdam[3] show that, up to about 4 GPa, the semiconducting gap energy E_g hardly decreases as a function of increasing pressure. Above 4 GPa, however, E_g starts to decrease quickly (dE_g/dp = 53 meV/GPa).

Figure 1. Dependence of the c-axis lattice parameter (squares, full line and left hand scale) as a function of pressure showing a clear jump at ~ 4 GPa. At the same pressure the optical properties change too (see text). For comparison also the a-axis lattice parameter is shown (circles, dashed line and right hand scale)



Diffraction measurements are performed in a Laue Geometry with a 30 μm beam and a 30 μm final size gasket hole. Despite strong diffraction peaks originating from the rhenium gasket the (100) and the (011) reflections of the hcp YH_3 are measured, from which the a-axis and the c-axis lattice parameters shown in Fig. 1 are calculated. The a-axis lattice parameter decreases continuously, while the c-axis decreases in a steplike manner. This sudden decrease occurs at the same pressure where the change in dE_g/dp is observed. The bulk modulus of YH_3 is found to be a factor 4 to 5 higher than for the yttrium metal, just as in other transition metal-hydrides[4].

The low maximum pressure and large error bars in the present experiment are due to the small final gasket hole caused by leakage through the rhenium gasket. This problem may be avoided by using a steel gasket and we plan to apply for beam time in the future to complete these measurements.

The beam time left after the gaskets collapsed (thus preventing further high pressure work), was used to make a detailed map of the composition in a diffusion profile[5] on a similar sample and provided a wealth of information on local composition during diffusion.

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[4] B. Baranowski et al. in Molecular systems under high pressure, 139 (ed. R. Pucci and G. Piccitto), Elsevier science, 1991.
[5] F.J.A. den Broeder et al., Nature 394, 656 (1998).