ESRF	**Experiment title:** Structural Studies on ScII	**Experiment number:** HS-180
Beamline: ID09	**Date of experiment:** from: 17-Apr-97 7:00 to: 19-Apr-97 7 : 00	**Date of report:** 9-oct-97
Shifts: 6	**Local contact(s):** Hanfland, Michael	*Received at ESRF':*

Names and affiliations of applicants (* indicates experimentalists):

H. J. Hesse, M. Winzenick, W. B. Holzapfel,
Universität-Gesamthochschule Paderborn, 33095 Paderborn, Germany

M. Hanfland,
ESRF, BP 220,38043 Grenoble-Cedex, France

Report:

Conventionally Sc, Y and the Lanthanide-metals (Ln) are labelled as the Rare Earths (RE) due to their similarity of the physical and chemical properties'. The trivalent RE-metals and Y show under pressure a common sequence of different structural transitions with decreasing atomic number: hcp(hP2) - Sm-type(hR9) - dhcp(hP4) - fcc(cF4) - distorted-fcc(hR24?)[2]. The symbols in parentheses represent the Pearson's notation. In contrast to this general behaviour Sc shows a completely different pressure driven transition from Sc(I) to Sc(II). At ambient conditions Sc is characterised by a hcp(hP2)-structure (Sc(I)). Around 20 GPa Sc shows a structural transition into the Sc(II)-phase. First attempts to describe the Sc(II) structure, based on diffraction data taken from conventional x-ray sources, suggest a possible tetragonal lattice with a primitive unit-cell. Using synchrotron radiation for x-ray diffraction experiments operating in an energy dispersive mode more recently, the diffraction pattern of Sc(I1) was described by our group established as a pseudo-body-centred-cubic structure (cI24) using a unit-cell with 24 atoms with a = 741.2(l) pm at 3 1 GPa where each lattice point is suggested to be occupied with an icosahedral cluster[3].

Figure 1 shows typical diffraction spectra of Sc measured within a pressure range up to 40 GPa. These spectra were taken at the ESRF in the angle dispersive mode with monochromised synchrotron radiation having a wavelength of λ = 419.46 pm. The diffracted intensity was collected by an imaging-plate. The spectra up to 20 GPa were measured with a membrane-diamond-anvil-cell. At pressures above 20 GPa we used a diamond-anvil-cell of Syassen-Holzapfel-type with B.&-backing-plate allowing for a larger diffraction angle. Liquid nitrogen or mineral oil were used in these experiments as pressure transmitting medium. For pressure determination the ruby luminescence method was applied.

Fig. la shows typical spectra of Sc(I) at different pressures. All diffraction lines can be attributed to the hP2-structure of Sc(I). Fig. lb displays typical diffraction spectra of Sc(I1) above 20 GPa. In agreement with the former work the observed diffraction lines can be attributed to a pseudo-body-centred-cubic structure giving

clear evidence for the distinctly different pressure dependant behaviour of Sc in comparison to the usual trivalent RE-metals. The Sc(II)-phase seems to be a new prototype structure since the arrangement of icosahedral clusters in a bee-lattice under pressure is quite unique. Within the next future additional energy-dispersive high pressure studies are planned since effects of texture do not yet allow for a determination of atomic position parameters.

References:

[I] U. Benedict, W.B. Holzapfel, ***in Handbook on the Physics and Chemistry of Rare Earths,*** Vol. 17, K. A. Gschneidner, Jr., L. Eyring, G. h. Lander, G. R. Choppin (eds.), (North Holland, Amsterdam 1993) p. 245.

[2] Y. K. Vohra, W. A. Grosshans, W. B. Holzapfel, Phys. Rev. B 25, 6019 (1982).

[3] Y. C. Zhao, F.Porsch, W. B. Holzapfel, Phys. Rev. B 54, 9715 (1996)

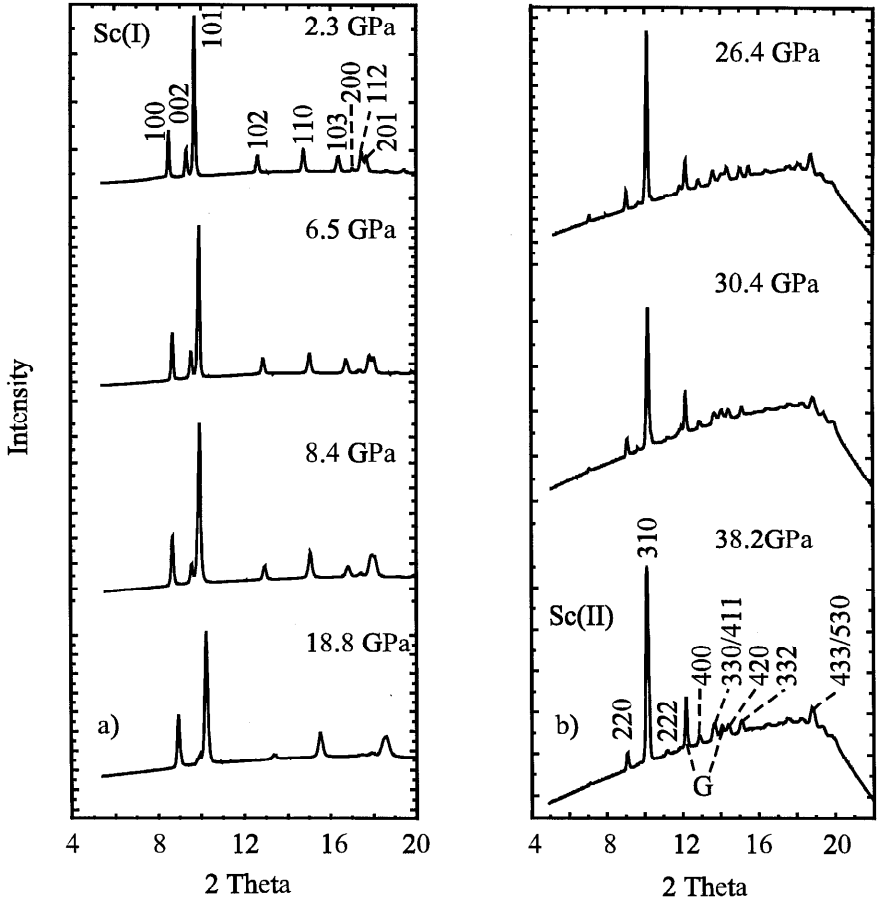

Fig. 1: X-ray diffraction spectra of Sc(I) and SC(I1) at different pressures. The spectra shown in a) are measured with a membrane-DAC whereas the data from b) are measured in Syassen-Holzapfel cell using a B_4C-backing-plate. The lines indicated by the letter G arise from the gasket material Inconel.