ESRF	**Experiment title:** **Structures and Transitions in Alkaline Metals at High Pressure**	**Experiment number**: HS-812
Beamline: ID9	**Date of experiment**: from: 1/6/99 to: 5/6/99	**Date of report**: 18/8/99
Shifts: 12	**Local contact(s)**: M. Hanfland	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Prof R.J. Nelmes*
Dr. M.I. McMahon*
Dr. S.A. Belmonte
Dr. D.R. Allan*
T. Bovornratanaraks*
C. Vanpeteghem*
M. Guthrie*

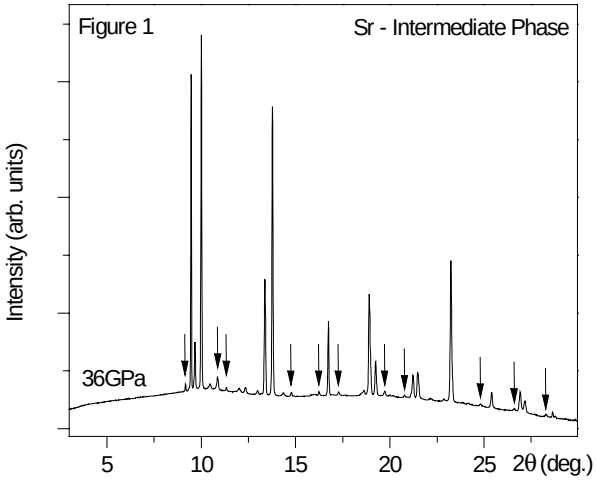
Department of Physics and Astronomy
The University of Edinburgh
Kings Buildings
Edinburgh EH9 3JZ
UK

Report:

At ambient-pressure strontium is face-centred cubic. This transforms to bcc at 3.5GPa, to the tetragonal β-tin structure at 24GPa, to phase IV at 35GPa, and to phase V at 46GPa. Sr-IV and Sr-V are complex and have resisted all previous attempts at solution. Our recent studies of Sr at SRS have confirmed the very complex nature of Sr-IV and have identified a previously unreported intermediate phase between Sr-III and Sr-IV. However, the complex nature of this phase, and the weakness of the its characteristic diffraction peaks, have prevented detailed analysis.

Our SRS studies have also revealed Sr-V to have the same incommensurate self-hosting structure we have found recently in Ba-IV. This structure comprises a tetragonal 'host' structure with channels running along the c-axis. Contained in these channels are chains of atoms from one or more 'guest' structures which are incommensurate with the host along c. In addition to a crystalline component, the guest phase contains a disordered component, giving rise to sheets of diffuse scattering perpendicular to c. In barium, we have also found a structural transition in the crystalline guest without any accompanying changes in the host.

Although we have found Sr-V to have the same incommensurate self-hosting structure as Ba-IV, our studies at SRS have not revealed the presence of diffuse scattering in Sr-V, nor any phase transitions in the guest component. The existence of both effects in Sr would greatly strengthen the similarities between the structures of Ba-IV and Sr-V. We have thus used the much higher flux obtainable at ESRF to study Sr-V in both considerably greater detail and to higher pressures than possible at SRS. We have also used the greatly-enhanced flux to make a detailed study of the intermediate phase identified between Sr-III and Sr-IV.



Powder diffraction data were collected on beamline ID9 using a wavelength of 0.4511Å. The 2-d diffraction patterns were collected on an image-plate detector and integrated using FIT2D. Figure 1 shows a diffraction pattern collected from Sr at 36GPa. The arrowed peaks identify all those diffraction peaks from the intermediate phase. Only a limited number of these peaks were visible at SRS and a considerable amount of new information has been obtained on this phase as a function of pressure. Analysis is currently in progress.

In Ba-IV, it was possible to see the diffuse scattering from the disordered guest component only because it was possible to grow sizeable single crystals – no diffuse scattering was observed from finely-powdered samples. Although Sr-V shows a propensity to recrystallise at the Sr-IV→Sr-V transition, the resulting crystallites have been too small to produce observable diffuse scattering at SRS. However, the greatly enhanced flux available at ESRF allows the diffuse scattering even from these very small crystallites to be observed. Figure 2 shows the 2-d diffraction pattern from Sr-V at 70GPa. The diffraction pattern is 'spotty' as a result of the recrystallisation, and these spots saturate the imaging plate. In addition to the powder rings, the arrows mark clear sheets of diffuse scattering from one very small single crystallite of Sr-V. This shows that, as in Ba-IV, the guest structure has some disordering of the chains along c.

The ESRF data have also revealed a 'phase' transition in the guest structure. Figure 3 shows patterns collected at 69 and 74 GPa. At 69 GPa the pattern comprises the main host-lattice reflections, and guest reflections as labelled 'a', 'b' and 'c'. At 74 GPa, the host-lattice reflections are the same, but the guest reflections have become weaker and new reflections – as marked by arrows – have appeared. The most probable interpretation is that, like Ba-IV, Sr-V shows a transformation in its guest component – at 71(1)GPa – and we provisionally label the form below 71GPa as Sr-Va, and that above 71GPa as Sr-Vb. These results and the detection of diffuse scattering have already been submitted for publication [1].

[1] M.I. McMahon, T. Bovornratanaraks, D.R. Allan, S.A. Belmonte and R.J. Nelmes, Submitted to Phys Rev B. (1999).

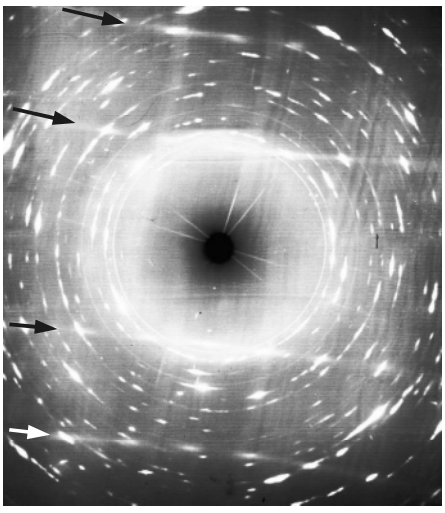


Figure 2

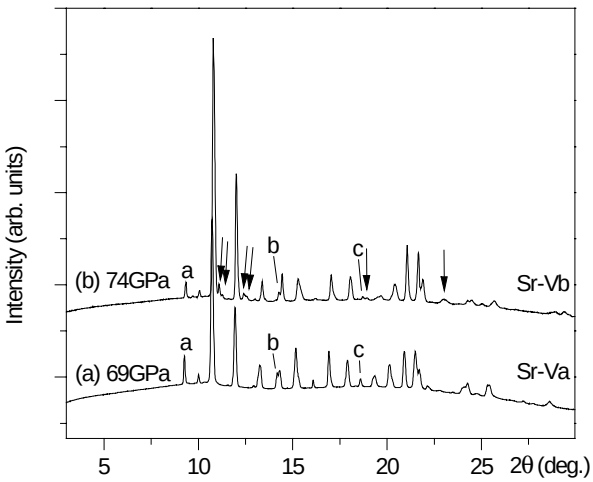


Figure 3