EUROPEAN SYNCHROTRON RADIATION FACILITY
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Experiment Report Form

	Experiment title: Investigating Phase Changes in the Sc-II Guest-Structure as Predicted by a Global Neural Network	**Experiment number**: HC-5278
Beamline: ID27	**Date of experiment**: from: 21 Apr 2023 to: 24 Apr 2023	**Date of report**: 2023-09-15
Shifts: 9	**Local contact(s)**: G. Garbarino, T. Poreba	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

School of Physics and Astronomy, The University of Edinburgh, Peter Guthrie Tait Road, EH9 3FD Edinburgh, UK:

C. Storm*, M. McMahon*, J. McHardy, M. Duff

Report:

The aim of this experiment was to investigate the structure of Sc-II, III, and IV phases, which despite previous investigations[1–3] have not yet been solved, but have attracted significant interest, particularly by theoretical investigators[4].

For a representative Sc-III pattern, see Fig. 1 which shows a moderately single-crystal diffraction pattern at 115GPa, as measured from the Cu pressure marker and its equation of state[5]. We had difficulties obtaining gasket-free diffraction patterns, due to the samples being about 10 microns in diameter (Fig. 2). Nonetheless, careful analysis and judicious masking of the diffraction pattern should enable us to solve the crystal structure. This work is currently ongoing.

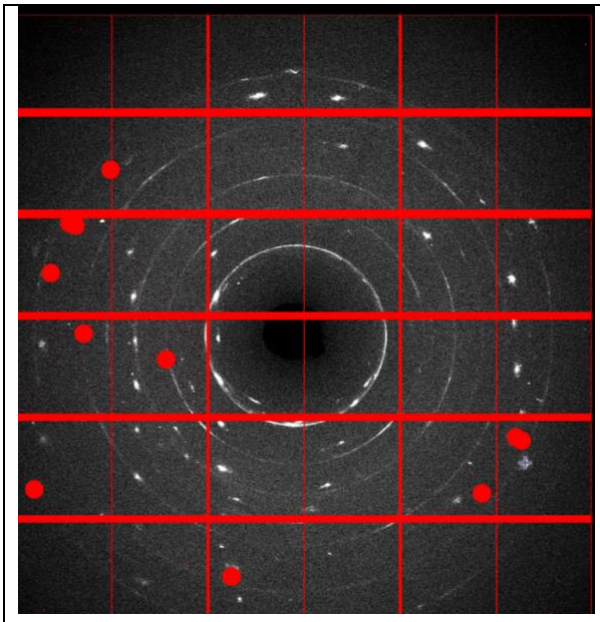

Fig 1: Debye-Sherrer rings from Sc-III at 114GPa, showing a poor powder pattern. Diffraction peaks from the diamond anvils have been masked.

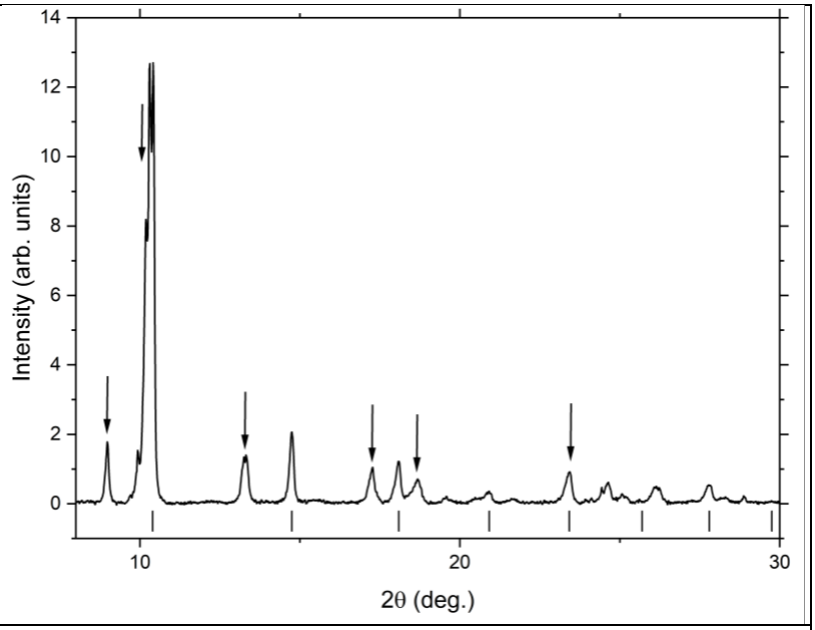

Fig 2: The diffraction pattern of Fig. 1 integrated and background-subtracted, with gasket (W) peaks marked with ticks below the pattern. Arrows indicate Sc diffraction peaks.

References:

1. Akahama, Y., Fujihisa, H. & Kawamura, H. New helical chain structure for scandium at 240 GPa. *Phys Rev Lett* **94**, 195503 (2005).
2. Fujihisa, H. *et al.* Incommensurate composite crystal structure of scandium-II. *Phys Rev B* **72**, 132103 (2005).
3. McMahon, M. I., Lundegaard, L. F., Hejny, C., Falconi, S. & Nelmes, R. J. Different incommensurate composite crystal structure for Sc-II. *Phys Rev B* **73**, 134102 (2006).
4. Zhu, S., Huang, Z., Hu, Q. & Xu, L. Pressure tuned incommensurability and guest structure transition in compressed scandium from machine learning atomic simulation. *Physical Chemistry Chemical Physics* **24**, 7007–7013 (2022).
5. Fratanduono, D. E. *et al.* Probing the Solid Phase of Noble Metal Copper at Terapascal Conditions. *Phys Rev Lett* **124**, 015701 (2020).