EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON



Experiment Report Form

ESRF	Experiment title: Structure Determination of Simple Metals at Unprecedented Compressions	Experiment number: HC-4887
Beamline: ID27	Date of experiment:from: 26 April 2022to:30 April 2022	Date of report : 2022-09-12
Shifts: 9	Local contact(s): T. Poreba, M. Mezouar	Received at ESRF:

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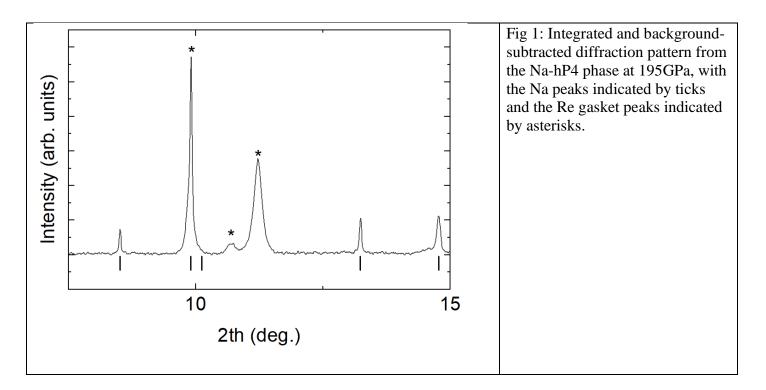
Report:

The aim of this report was to investigate the phase transitions of sodium (Na) metal up to the hP4 phase, with a view of (a) resolving discrepancies between shock and static high-pressure data and (b) searching for the (002) peak which should become visible in Na in the hP4 electride phase.

The experiment itself went very well, with all samples achieving pressures above 200GPa and transforming to the hP4 phase. We observed the transparency of this phase as reported by Ma et al. [1] and have collected data from the first single crystal sample of this phase. The high brilliance of ID27 was extremely useful, particularly due to the low scattering strength of Na (Z=11) (see Fig. 1); despite the Re gasket peaks being significant, the Na peaks are well-resolved and sharp. We were very pleased with the quality of the diffraction pattern, which has allowed us to reliably refine lattice parameters and atomic coordinates.

The discrepancy between results from shock and DAC experiments remains difficult to explain, but the high quality of our data has given us renewed confidence in the results from static high-pressure experiments. The (002) peak was not seen, and we are currently working to explain this in the framework of the electride-nature of the hP4 phase. It is possible that this peak's intensity, though non-zero, remains too weak to be observed directly. We have however seen indirect proof of the electride-nature of the phase and are our paper detailing

these results is currently in the late stages of preparation. We anticipate submitting to a high-impact journal, and we would be very pleased to return to ID27 for experiments in the future.



References:

[1] Y. Ma, M. Eremets, A. R. Oganov, Y. Xie, I. Trojan, S. Medvedev, A. O. Lyakhov, M. Valle, and V. Prakapenka, Nature **458**, 182 (2009).