THE UNIVERSITY
of EDINBURGH

Dynamic and Static Compression of Antimony

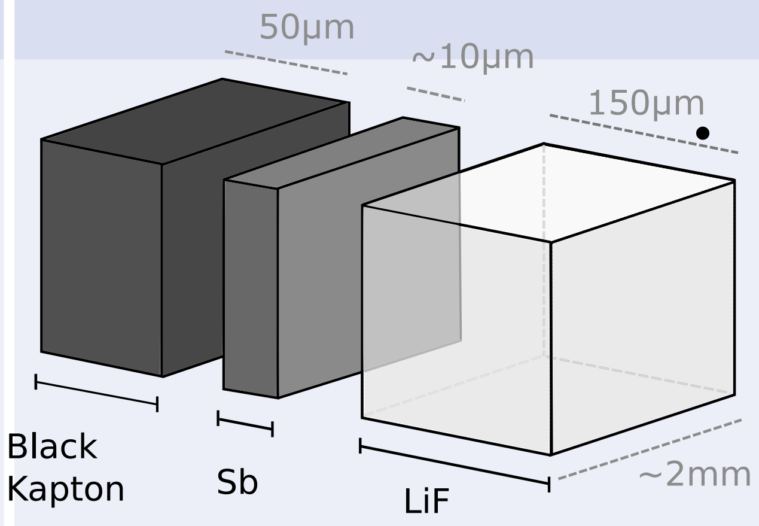
A. L. Coleman,[1] M. G. Gorman,[1,2] R. Briggs,[1,2] R. S. McWilliams,[1] D. McGonegle,[3] M. Stevenson,[1] C. A. Bolme,[4] A. E. Gleason,[4,5] D. E. Fratanduono,[2] R. F. Smith,[2] E. Galtier,[6] H. J. Lee,[6] B. Nagler,[6] E. Granados,[6] S.G. Macleod,[1,7] G. W. Collins,[8] J. H. Eggert,[2] J. S. Wark,[3] and M. I. McMahon[1]

[1]SUPA, The University of Edinburgh, [2]Lawrence Livermore National Laboratory, [3]University of Oxford, [4]Los Alamos National Laboratory,, [5]Stanford University, [6]Linac Coherent Light Source, [7]Atomic Weapons Establishment, [8]University of Rochester

Motivation

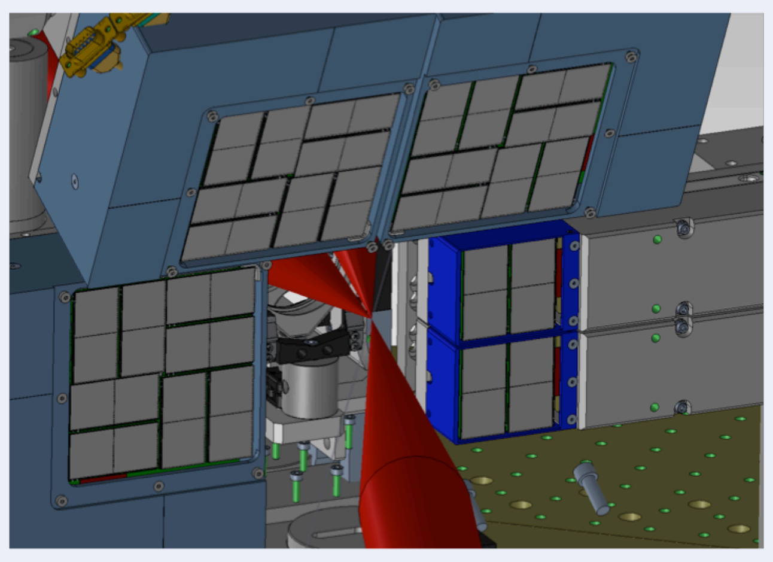
- XFELS are revolutionising the field of dynamic, high-pressure physics by allowing x-ray diffraction data to be obtained on the nanosecond timescales of dynamic compression experiments.
- As our ability to access more extreme pressure-temperature states increases, we are faced with fundamental questions such as **can highly-complex structures predicted in these extreme states form on the timescales of dynamic experiments?** And if so, **do we have the capability to resolve such structures?**
- Antimony is known to adopt an incommensurate host-guest structure under static compression at easily-accessible pressures. This is one of the most complex structures a single element can exhibit. This makes it an ideal candidate for investigating the capabilities of materials to form low-symmetry structures on nanosecond timescales as well as testing the capability of our current diagnostics to resolve such structures.

Methods



A **dynamic compression** experiment was conducted at the MEC end station of LCLS in May 2016 using targets consisting of 10 μm of Sb deposited onto a 50 μm thick polyimide ablator. Targets both without and with a LiF window, adhered using a thin glue layer, were used, as illustrated to the left. The CSPAD detectors, used to obtain the x-ray diffraction data, were arranged in a standard configuration, as shown below. The VISAR diagnostic was also used to make rear surface velocity measurements.

- In addition to the dynamic-compression experiment, a **static compression** experiment using a resistively-heated DAC was conducted at the Diamond Light Source. This experiment enabled the equilibrium phase-diagram of Sb to be established thoroughly, building on and showing excellent agreement with previous static-compression studies of Sb. This DAC experiment allowed valuable comparisons to be made between the behaviours of Sb under different pressure-loading regimes

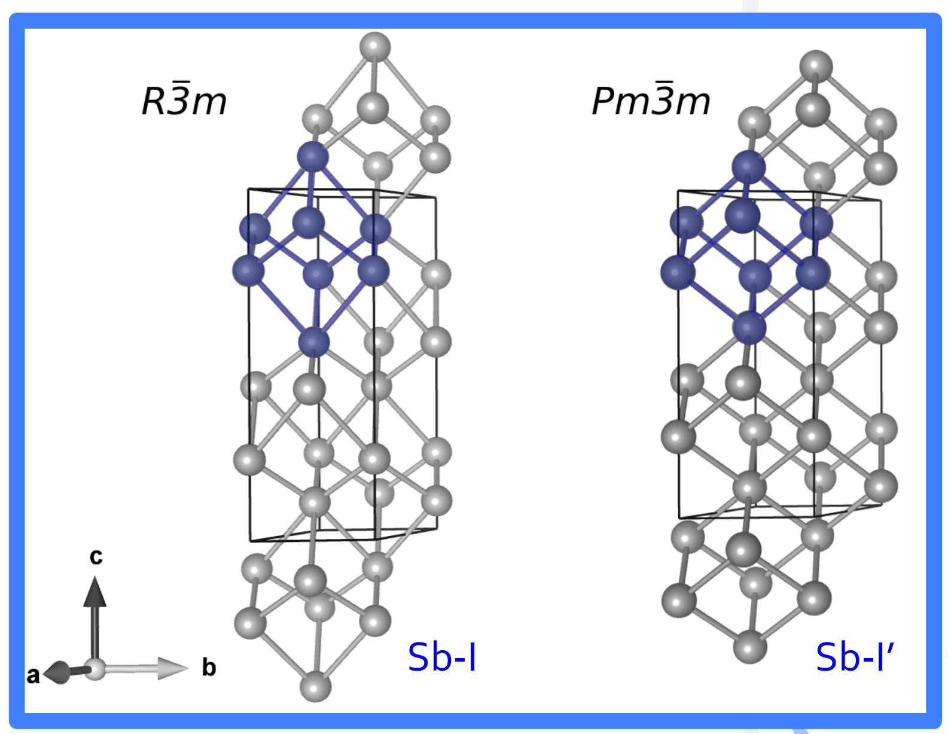


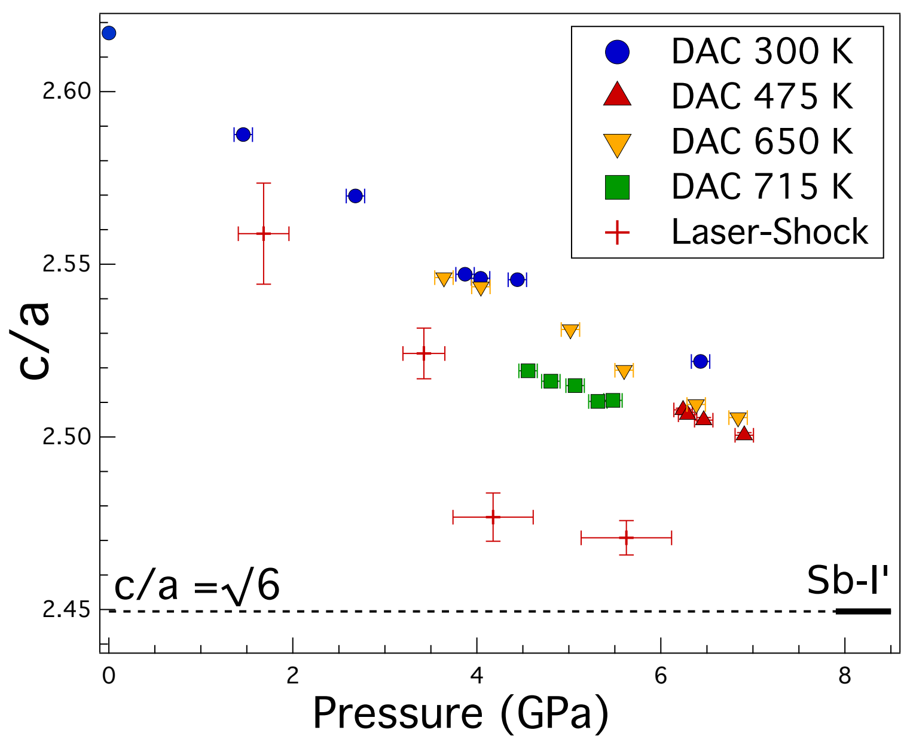
Standard configuration of detectors at LCLS.

Results

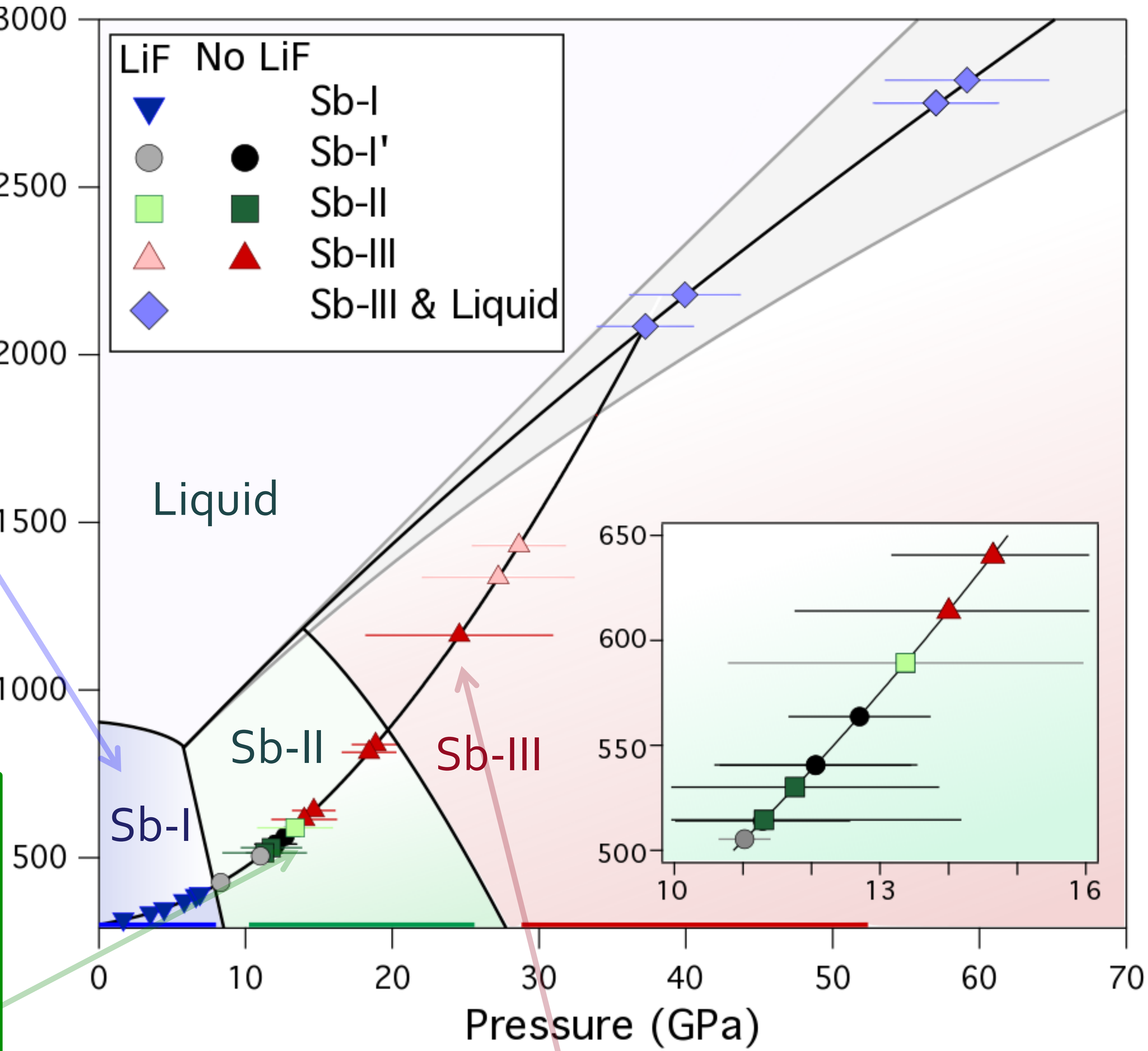
Sb-I & Sb-I′

- Under dynamic compression a **new phase (Sb-I′)** forms. This phase is not observed under static compression.
- The c/a ratio of the Sb-I phase decreases with pressure much more rapidly under dynamic compression as shown in the graph below.





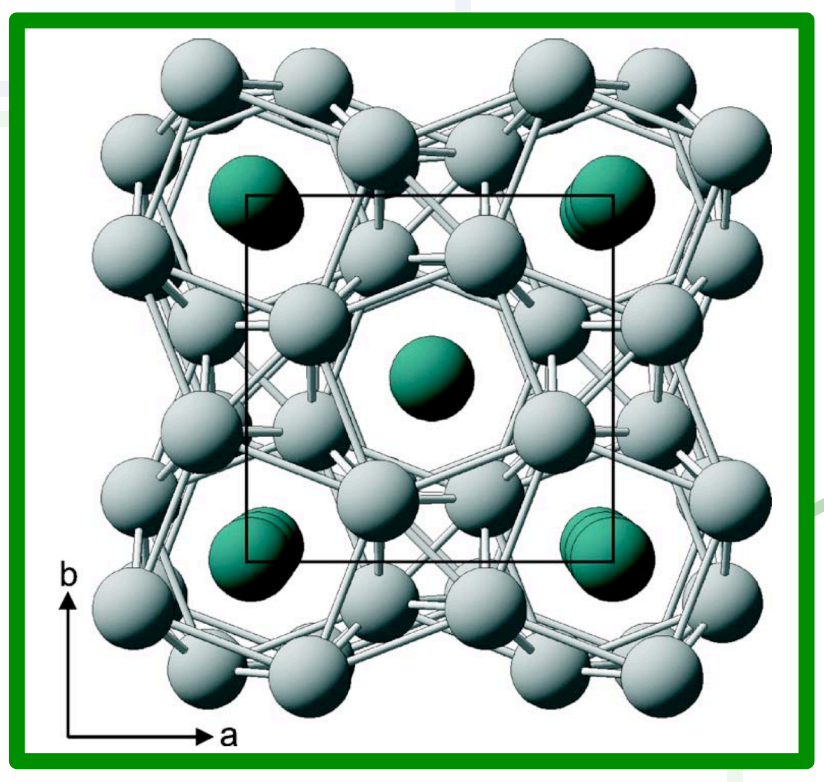
- Under dynamic compression the c/a ratio of Sb-I decreases until a value of √6 is achieved, at which point the structure is cubic, marking the new Sb-I′ phase.

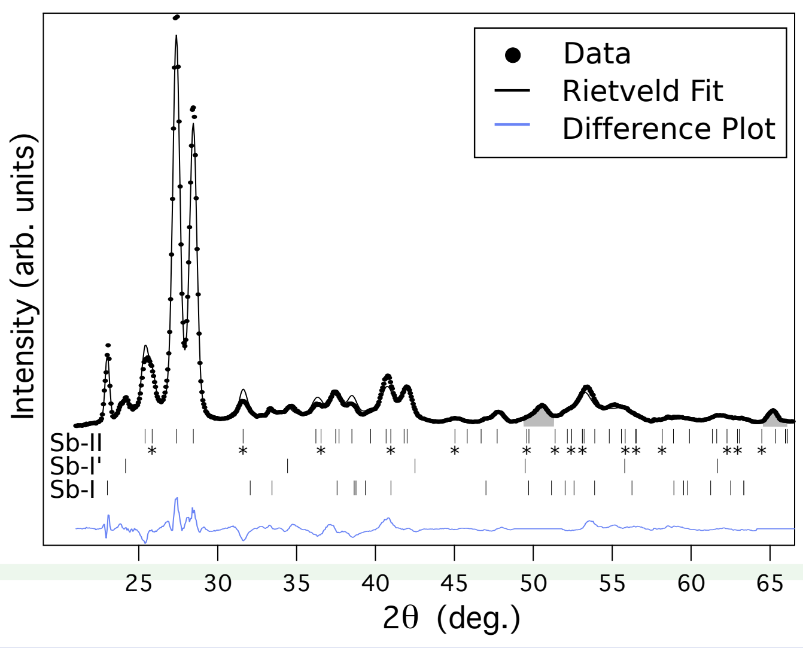


The phase diagram of Sb as established in the resistively-heated DAC experiment to 31 Gpa and 835 K [1]. The bars at 300 K show the phase boundaries determined in previous room-temperature DAC studies [2]. The data points on the Hugoniot-curve were obtained at the dynamic compression experiment at LCLS. The melt curve is extrapolated from pre-existing melt-curve data to ~ 9 GPa [3] to the first data point at which liquid diffraction signal is observed in the shock-compression experiment. The grey error bars surrounding the melt curve represent the uncertainty in this melt curve extrapolation.

Sb-II

- This work presents the **first observation of the complete formation of an incommensurate host-guest structure under dynamic compression.**
- The quality of the diffraction data from LCLS is such that Rietveld refinements may be used to obtain lattice parameters and atomic positions for this complex structure as shown below.

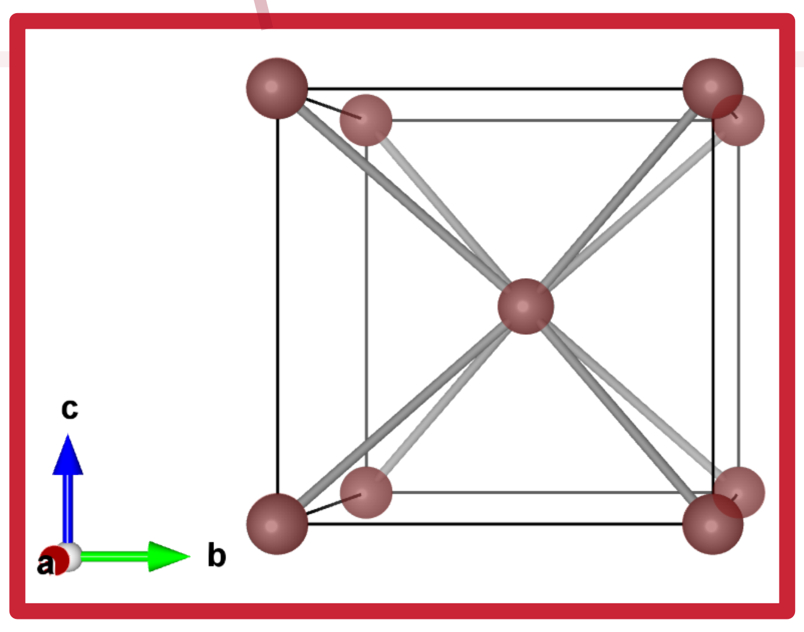




- There are differences between Sb-II phase formed under static and dynamic compression. As shown on the phase diagram, the Sb-II phase exists over a very small pressure region under shock compression (on-Hugoniot) in comparison to the equilibrium phase diagram.

Sb-III

- The Sb-III (bcc) phase forms at a much lower pressure under shock compression (as shown on the phase diagram) than under static compression.



- Under shock compression, liquid diffraction is observed in coexistence with Sb-III signal, indicating the Hugoniot coincides with the melt curve

Conclusions

- This work has shown conclusively that highly-complex structures **can** form fully on the nanosecond timescales of dynamic compression and that we now have the capability to resolve these structures!
- An interesting result has been found in the marked difference between the phase behaviour of Sb under different pressure loading regimes. Under dynamic compression the formation of cubic structures appears to be more energetically favourable. It is interesting to consider how the phase boundaries of Sb differ under intermediate pressure loading regimes (such as dynamic DAC or ramp-compression) and how these effects could be simulated in a meaningful way.
- It would certainly be interesting to explore whether the differences observed between Sb under different pressure loading regimes are mirrored in other elements that are known to exhibit complex structures.

References

[1] A. L. Coleman, M. G. Gorman, R. Briggs *et al.*, *Phys. Rev. B*, (2018)
[2] O. Degtyareva, M.I. McMahon, R.J. Nelmes, *High Pressure Research*, **24**, *319-256 (2004)*
[3] S. M. Stishov and N. A. Tikhomirova, Sov Phys JETP **48**, 1215 (1965)
[4] W. Klement, A. Jayaraman, and G. C. Kennedy, Physical Review **131**, 632 (1963)

Acknowledgements

EPSRC
Engineering and Physical Sciences Research Council
CSEC
SLAC NATIONAL ACCELERATOR LABORATORY
diamond
AWE
Lawrence Livermore National Laboratory