

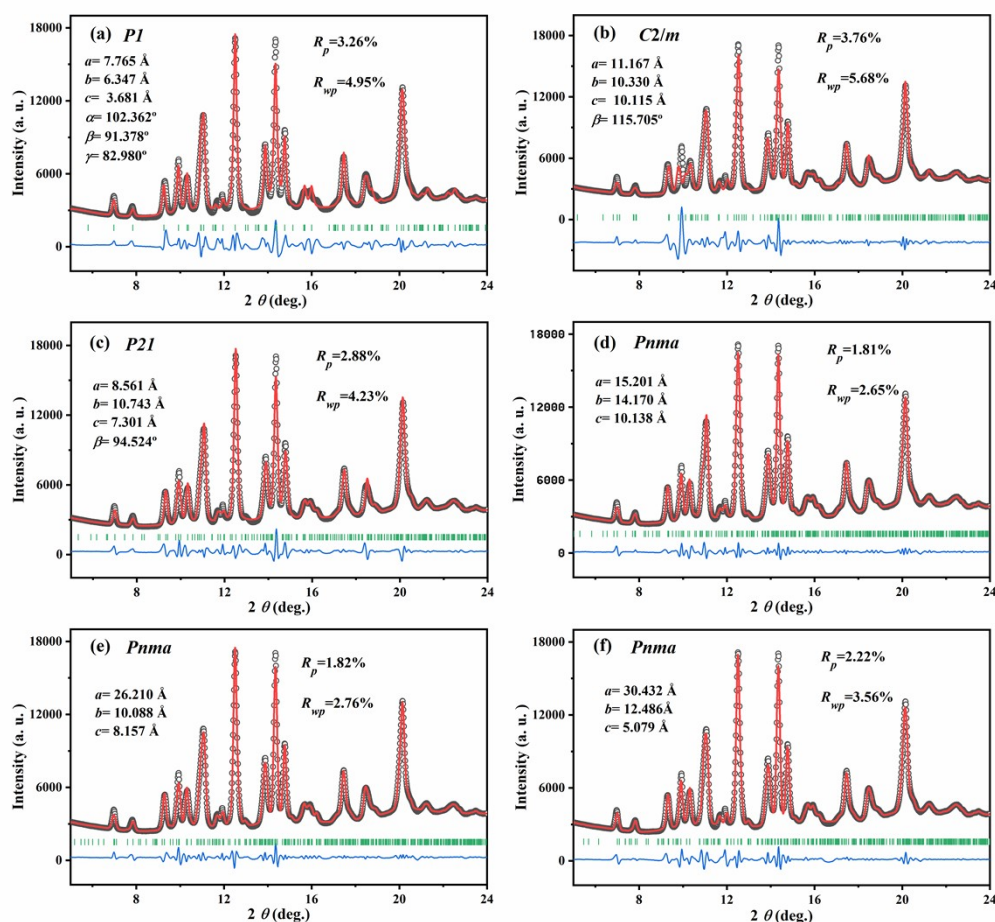
Pressure-induced phase transitions, amorphization and alloying in Sb_2S_3

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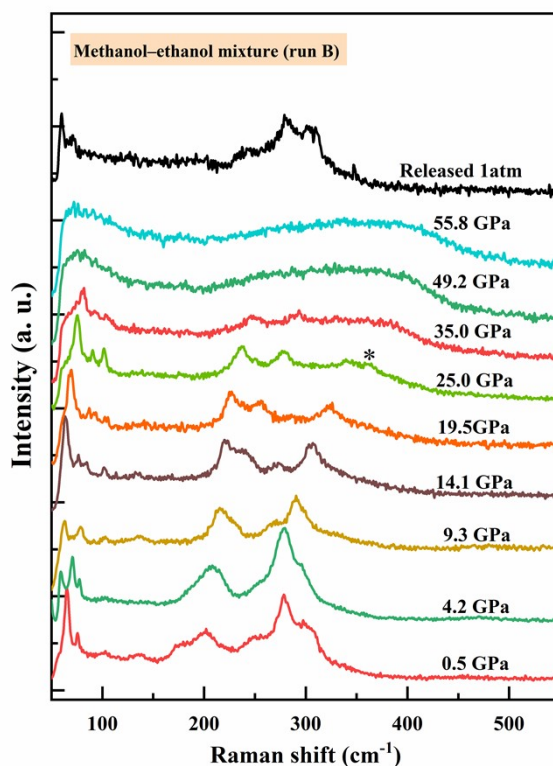
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Fig. S1 Le Bail refinement results of Sb_2S_3 at 18.2 GPa (run 1) with different structures. The black open circles and red solid line represent the experimental and simulated data, respectively, and the blue solid lines at the bottom are the residual intensities. The solid short vertical bars indicate the peak positions.



Here, the XRD patterns of Sb_2S_3 was treated as a single phase (phase II) above 8.2 GPa (run 1). Due to the pronounced broadening and overlapping of Bragg peaks, it is found that the experimental XRD patterns at 18.2 GPa can be indexed to several structures, *i.e.* $P1$, $C2/m$, $P21$ and at least three $Pnma$, respectively. Their fitting results are good, but none of them can conduct Rietveld refinement, which makes the structure determination of phase II is impossible.

Fig. S2 Raman spectra of Sb_2S_3 versus pressure during compression and decompression at room temperature with the methanol-ethanol (4:1) mixture as the PTM (run B). excitation wavelength was 532 nm.



As we can see, the Raman spectrum obtained in run A with no PTM was of higher quality than that obtained in this run. Nevertheless, a new Raman mode was also observed at about 25 GPa which should be assigned to M15. Above 35.0 GPa, the Raman spectra become rather featureless. After full decompression, the Raman modes show pronounced broadening accompanied by a few features of phase I, which is good consistent with the results in run A.