

SUPPLEMENTARY INFORMATION

Growth of bismuth and antimony-based chalcogenide single crystals by physical vapor transport method

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1. Single crystal growth

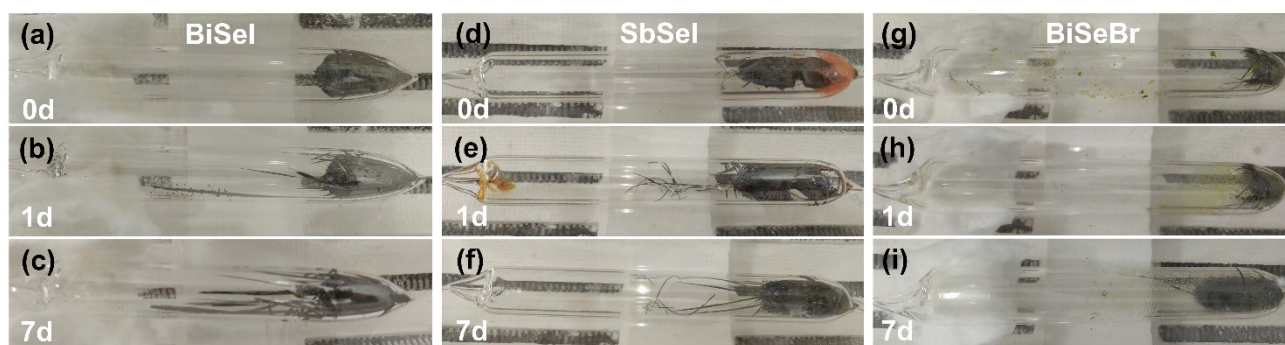


Fig. S1. BiSel in growth process (a) to (c) growth for 0 (as-synthesized), 1 and 7 days, SbSel in growth process (d) to (f) growth for 0 (as-synthesized), 1 and 7 days, BiSeBr in growth process (g) to (i) growth for 0 (as-synthesized), 1 and 7 days.

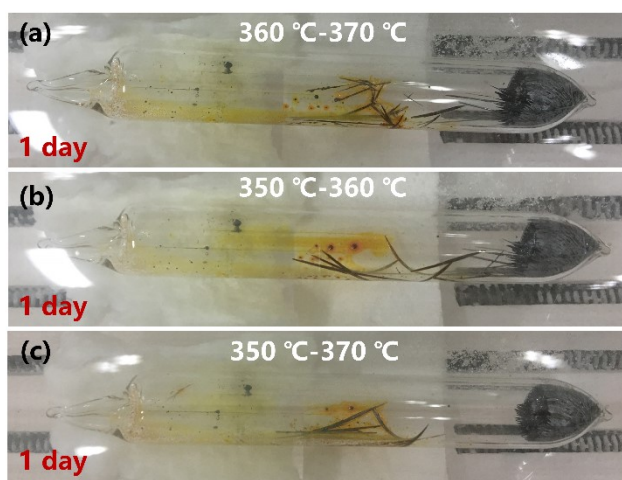


Fig. S2. SbSel single crystals grew in different temperature gradients for 1 day, 350 °C to 370 °C was chosen as optimal temperature gradient.

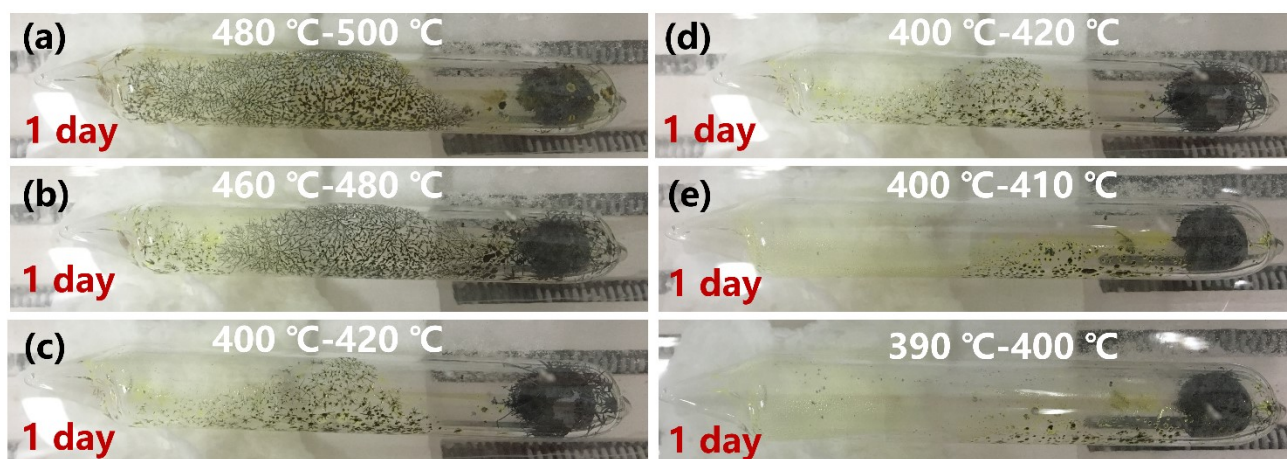


Fig. S3. BiSeBr single crystals grew in different temperature gradients for 1 day, 390 °C to 400 °C was chosen as optimal temperature gradient.

2. XRD measurement

Table S1 The lattice constants of BiSeI, SbSeI and BiSeBr.

	Lattice constants (\AA)			R_{wp} (%)	R_p (%)
	a	b	c		
BiSeI	8.7074	4.2202	10.5837	15.24	11.70
SbSeI	8.7080	4.1314	10.4223	17.86	13.47
BiSeBr	8.2138	4.1081	10.4773	20.95	14.21

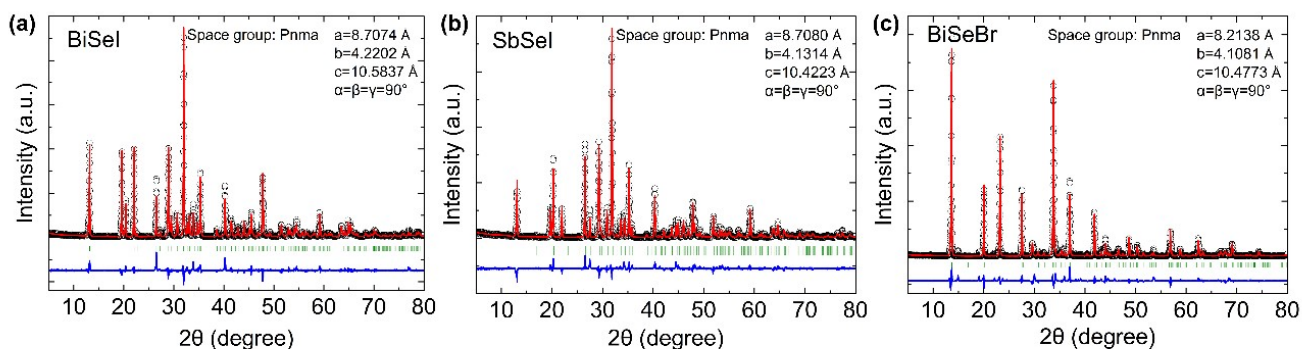


Fig. S4 The Rietveld refinement of the powder XRD data of (a) BiSeI, (b) SbSeI and (c) BiSeBr by GSAS-EXPGUI. Circles are the experimental data and red line is the refinement result. The blue line indicated the difference between the experimental and calculated results. And the expected Bragg peak positions for $A^{\text{VI}}B^{\text{VI}}C^{\text{VII}}$ phase is shown by the green tick marks.

3. SEM results

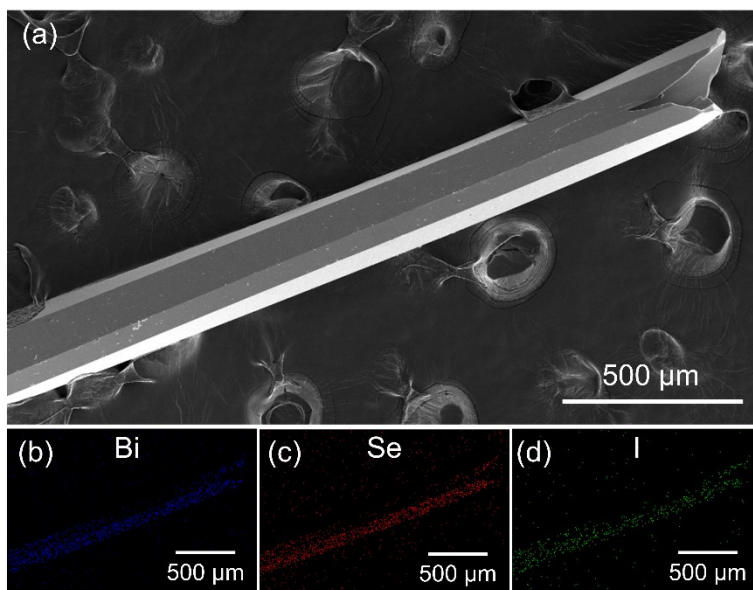


Fig. S5. (a) a typical SEM image of the BiSeI single crystal; (b) to (d) corresponding EDS mapping images of the grown BiSeI crystal.

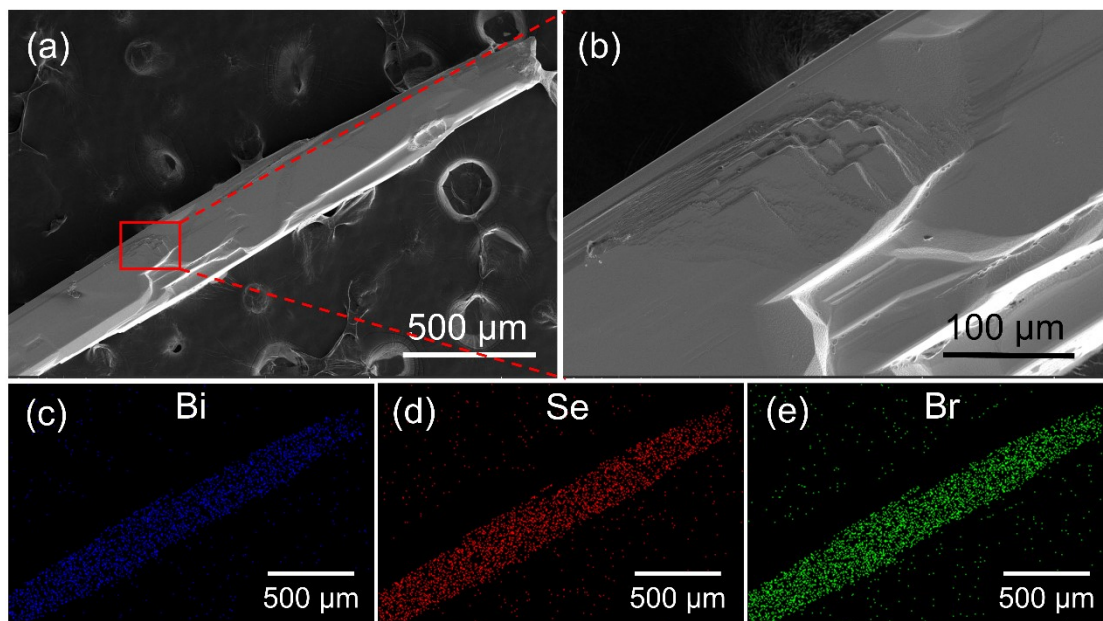


Fig. S6. (a) a typical SEM image of the BiSeBr single crystal and (b) SEM image of the tail of the one-dimensional BiSeBr crystal, (c) to (f) corresponding EDS mapping images of the grown BiSeBr crystal.