

Supporting information for

Flux-boostered coating of idiomorphic CuInS₂ crystal layer on Mo-coated glass

substrate

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Table S1 Fabrication conditions of CuInS₂ crystal layers on under-layer/Mo/SLG from InCl₃-NaCl flux.

Run No.	Solute Conc. (mol%)	Solute		Flux		Holding temp. / °C	Holding time / h	Under- layer
		Cu ₂ S / g	In ₂ S ₃ / g	InCl ₃ / g	NaCl / g			
1	50	0.2081	0.4261	0.2893	0.0764	550	1	none
2	70	0.2631	0.5387	0.1567	0.0414	550	1	In
3	70	0.2631	0.5387	0.1567	0.0414	550	1	Cu
4	70	0.2368	0.5387	0.1567	0.0414	550	1	In ₂ S ₃
5	70	0.2368	0.5387	0.1567	0.0414	550	1	Cu ₂ S

Table S2 Crystal Data and Structure Refinement for CuInS₂. (J. D. Burnett, et al., *Mater. Chem. Phys.*, 2014, **147**, 17).

compound	CuInS ₂
fw	242.496
T (K)	300
wavelength (Å)	1.066 or 2.665
cryst syst	tetragonal
space group	I -4 2 d
a (Å)	5.52406(9)
b (Å)	5.52406(9)
c (Å)	11.1429(2)
vol. (Å ³)	340.03
Z	4
R _{int}	0.0477

Table S3 Solubility of Cu₂S and CuInS₂ in NaCl-InCl₃ flux at 400 °C.

Entry	Sample	Solubility in NaCl-InCl ₃ (mol %)
1	In ₂ S ₃	Not determined ^a
2	Cu ₂ S	0.648
3	CuInS ₂	0.208

^a In₂S₃ block (10×10×5 mm), used as starting sample, became finely crushed through the test, indicating high solubility of In₂S₃ in NaCl-InCl₃ flux.

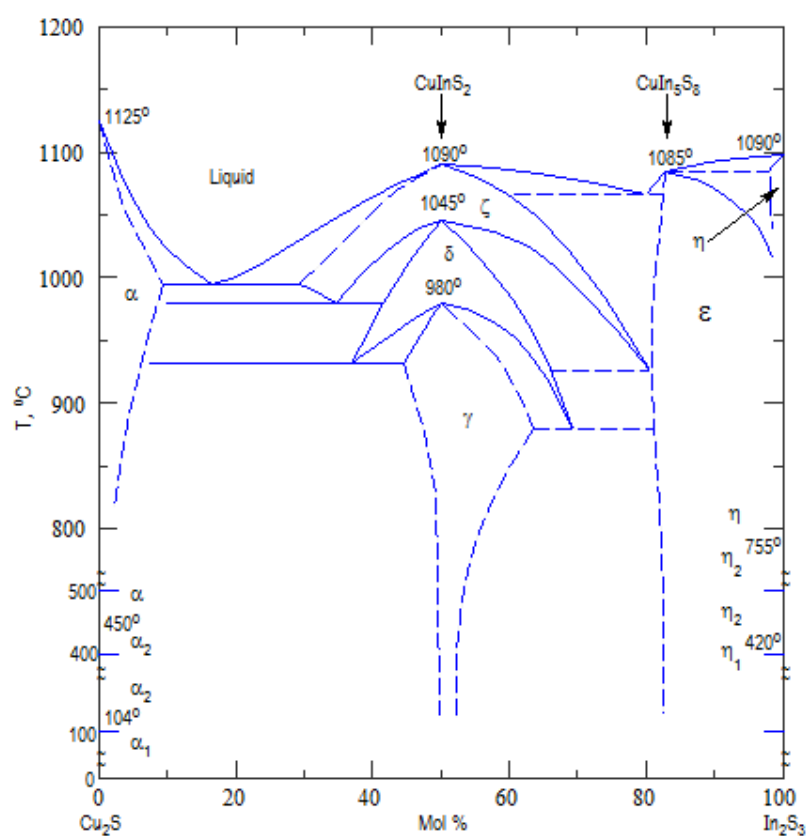


Figure S1. Phase diagram of Cu-In-S compounds (J. J. M. Binsma, L. J. Giling, and J. Bloem, *J. Cryst. Growth*, 1980, **50**, 429). γ , δ , ζ represent chalcopyrite, zincblende, and unknown structures, respectively.

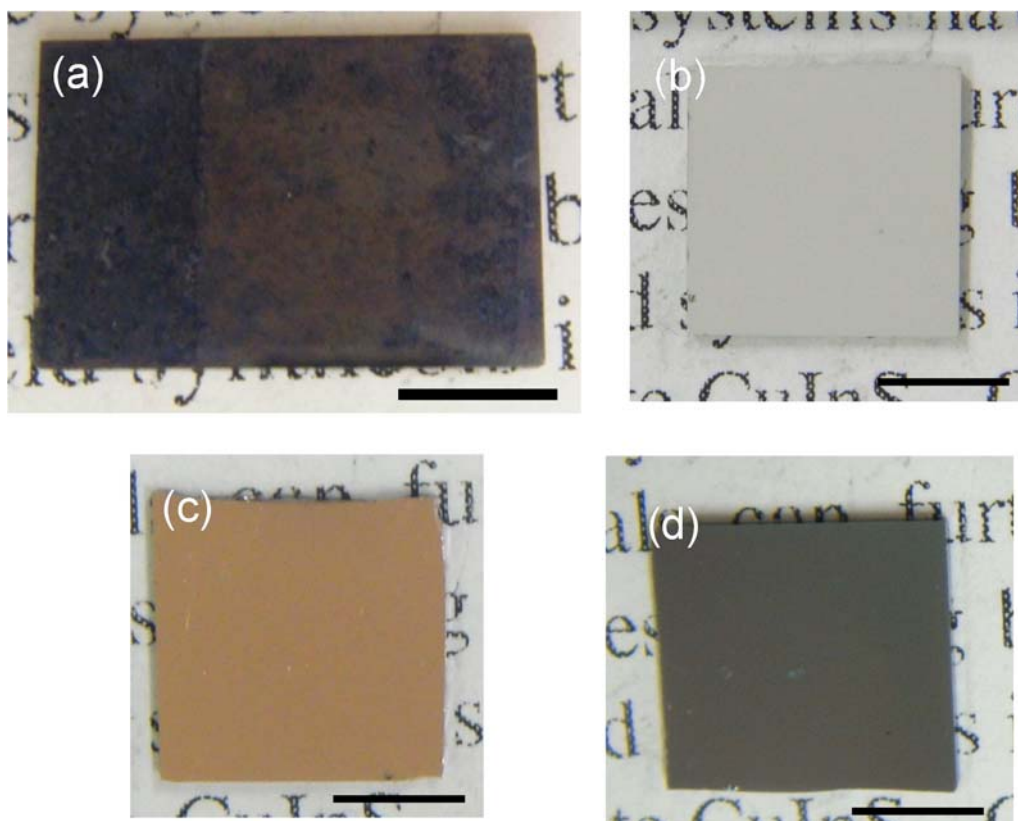


Figure S2. Optical images of (a) Mo/SLG, (b) In/Mo/SLG, (c) Cu/Mo/SLG, (d) Cu₂S/Mo/SLG. All scale bars represent 5 mm in length.

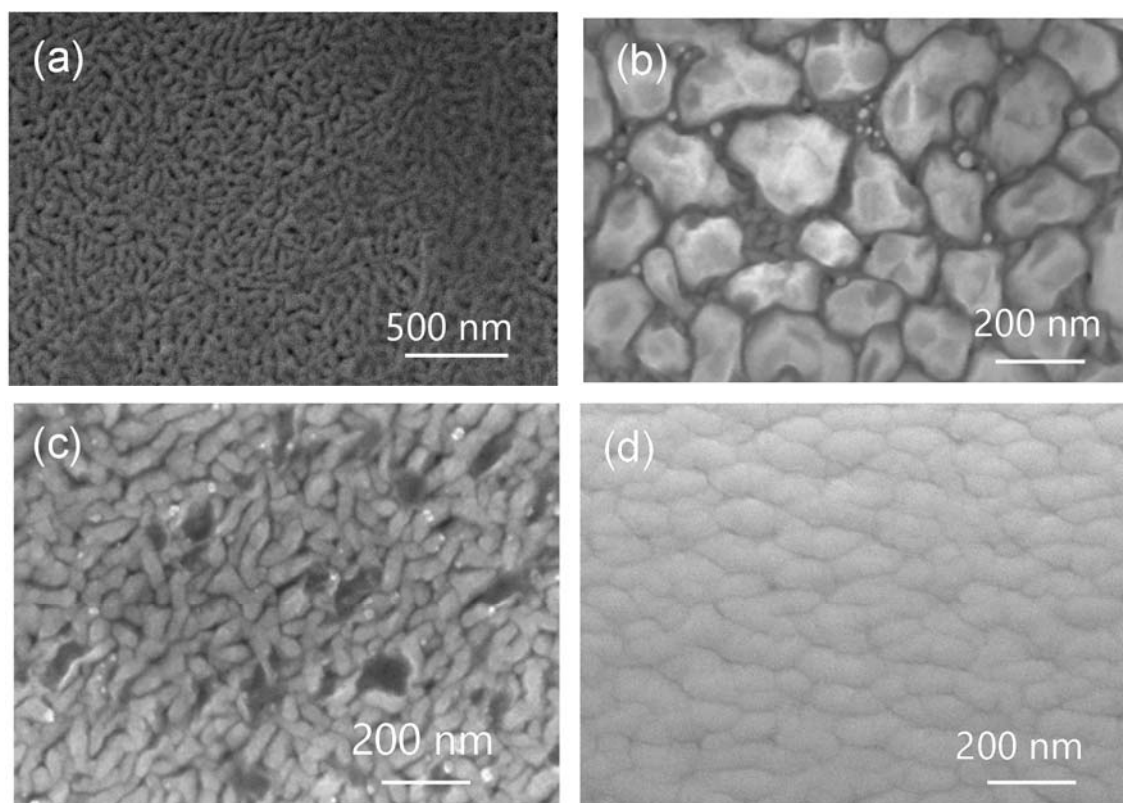


Figure S3. Top-surface FE-SEM images of (a) Mo/SLG, (b) In/Mo/SLG, (c) Cu/Mo/SLG, (d) Cu₂S/Mo/SLG.

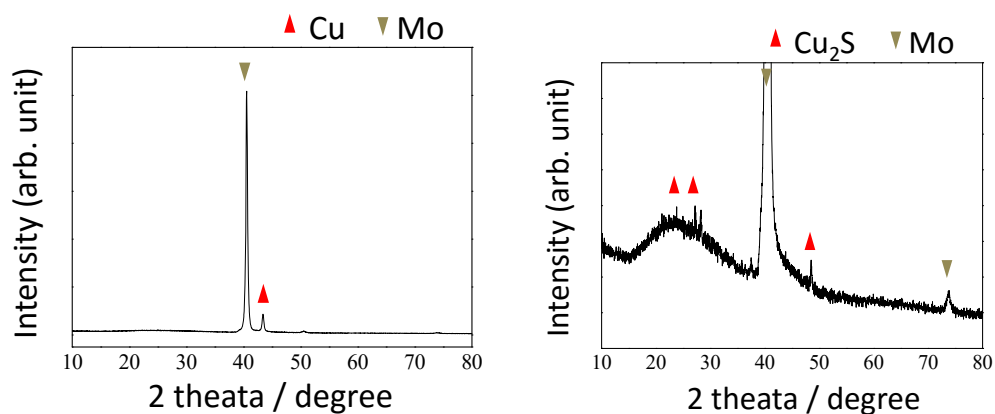


Figure S4. XRD patterns of (left) Cu/Mo/SLG and (right) Cu₂S/Mo/SLG substrate.

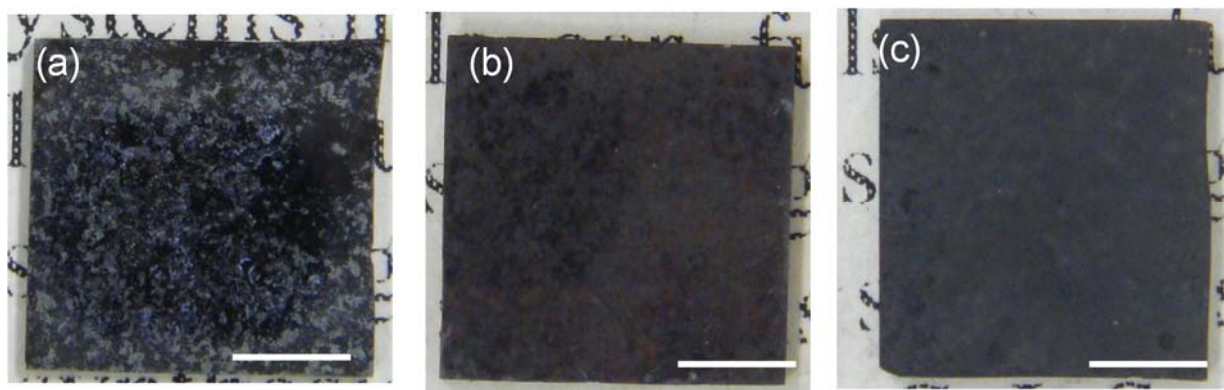


Figure S5. Optical images of CuInS₂ crystals grown on (a) In/Mo/SLG, (b) Cu/Mo/SLG, and (c) Cu₂S/Mo/SLG. All scale bars represent 5 mm in length.

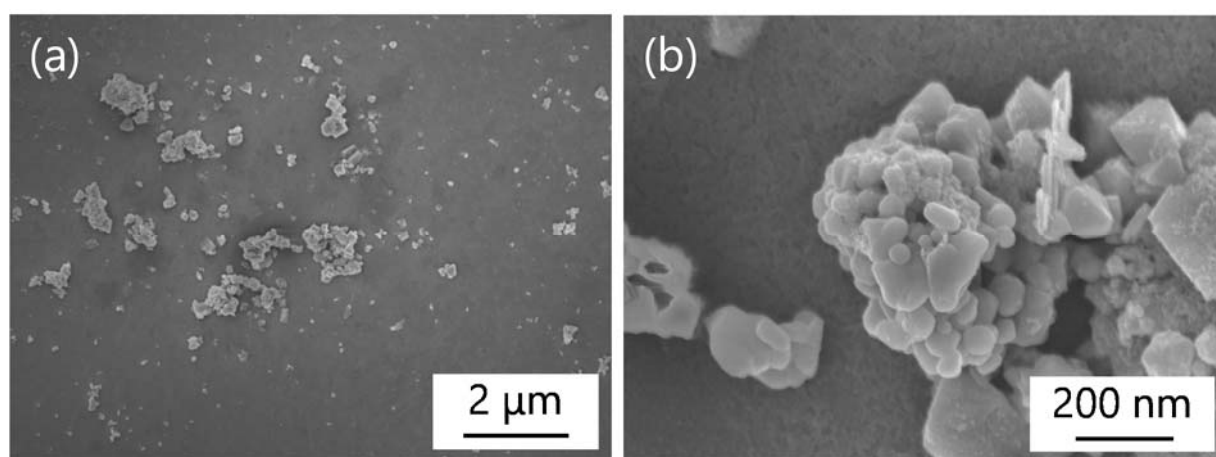


Figure S6. Top-surface FE-SEM images of CuInS₂ crystals grown on In₂S₃/Mo/SLG substrate.