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Supporting Information

Insight of the preponderant role of the lattice size in the Sn-based colusite for promoting high power factor

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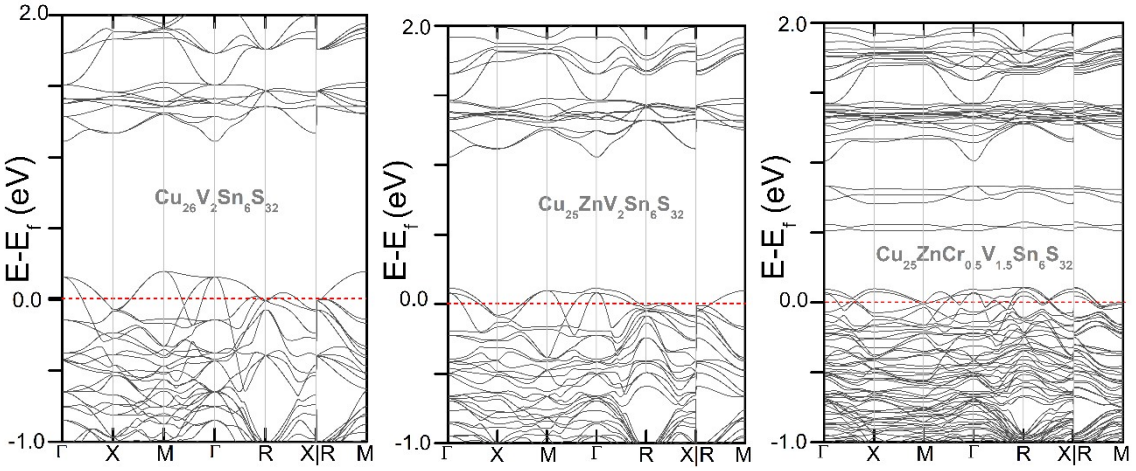


Figure S1. Electronic band structures of $Cu_{26}V_2Sn_6S_{32}$, $Cu_{25}ZnV_2Sn_6S_{32}$, and $Cu_{25}ZnCr_{0.5}V_{1.5}Sn_6S_{32}$

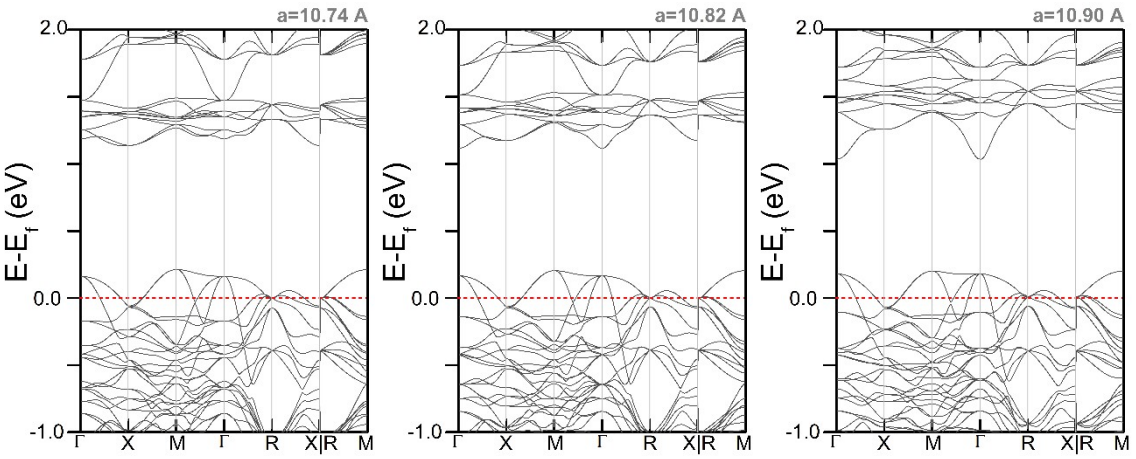


Figure S2. Electronic band structures and density of states (DOS) of $Cu_{26}V_2Sn_6S_{32}$ assuming different lattice parameters *a* (10.74 Å, 10.82 Å, and 10.90 Å)

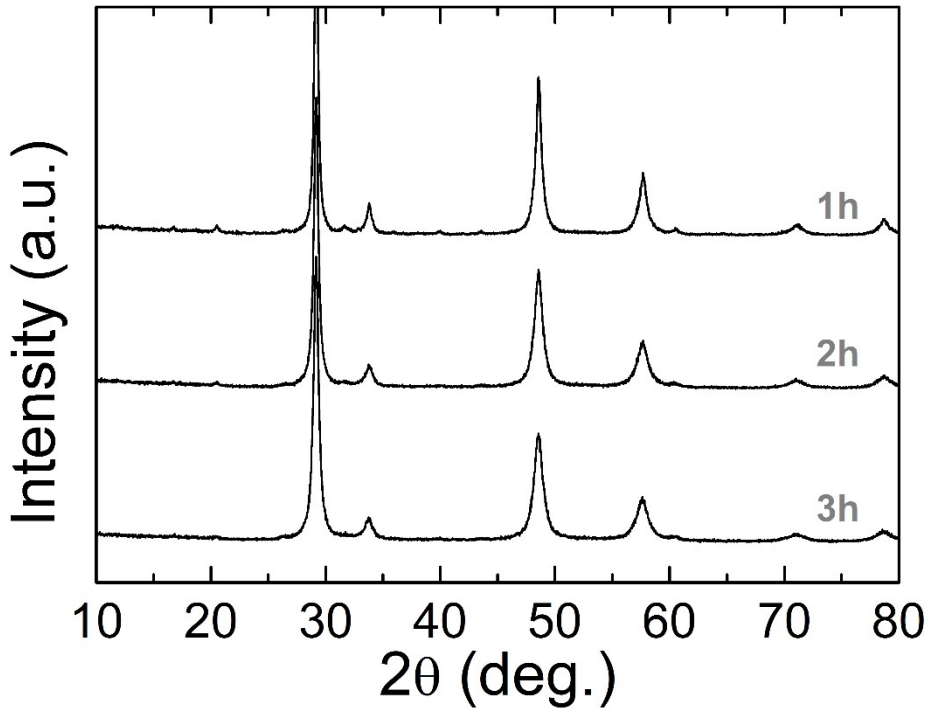
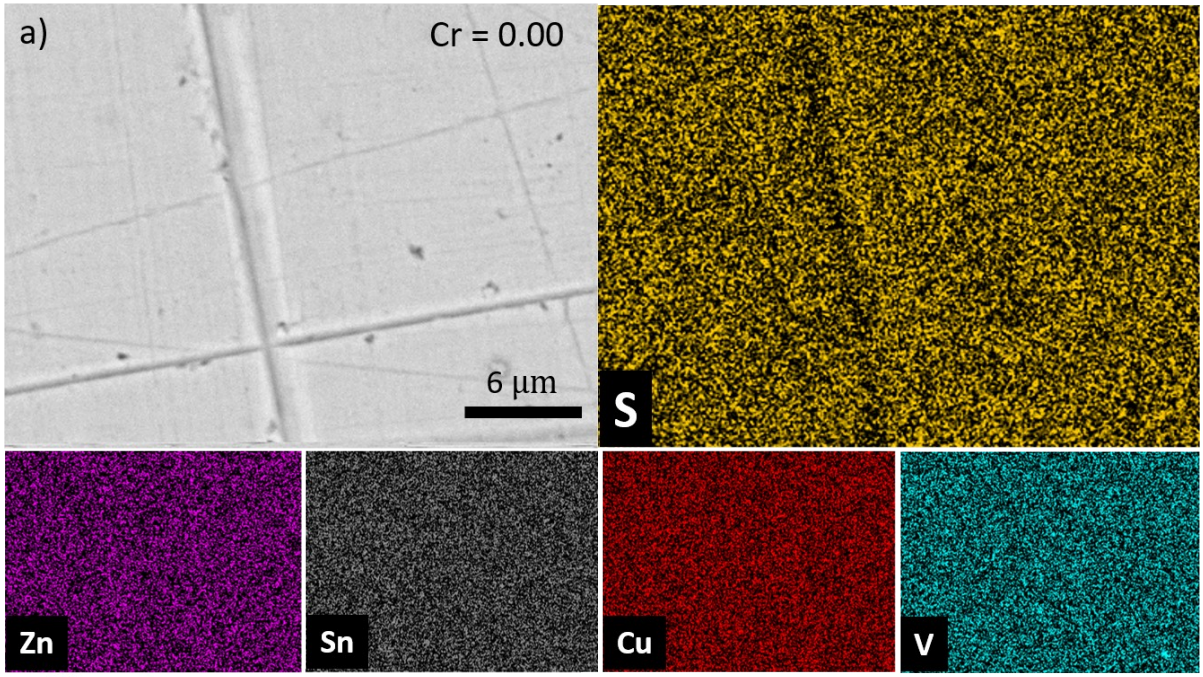
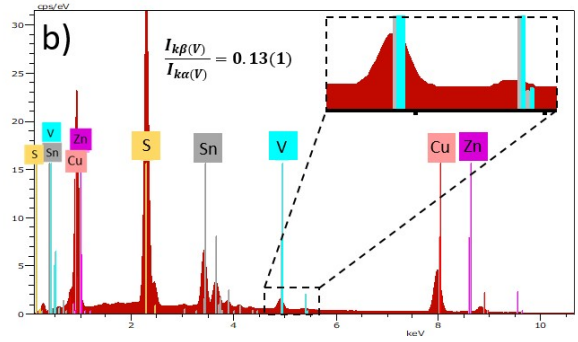


Figure S3. Powder X-ray diffraction patterns of $Cu_{25}ZnV_2Ge_6S_{32}$ compounds ball milled for a different time





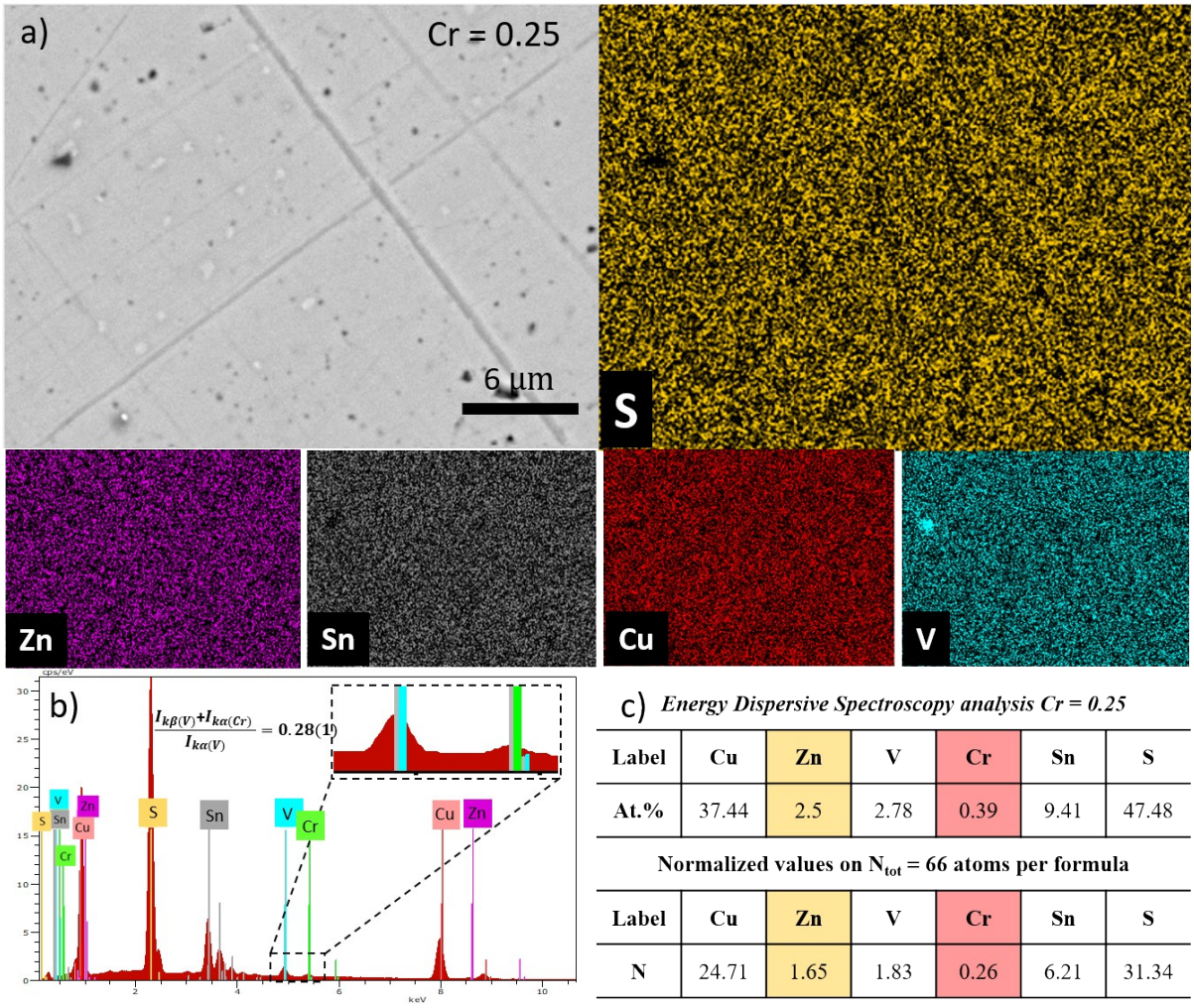
c) *Energy Dispersive Spectroscopy analysis Cr = 0*

Label	Cu	Zn	V	Cr	Sn	S
At.%	37.22	2.45	3.16	0	9.5	47.67

Normalized values on N_{tot} = 66 atoms per formula

Label	Cu	Zn	V	Cr	Sn	S
N	24.57	1.62	2.09	0	6.27	31.46

Figure S4. Energy dispersive spectroscopy analysis results on the polished surface of the $Cu_{25}ZnV_2Sn_6S_{32}$ sample sintered by SPS with a) EDS mapping b) its corresponding spectrum, and c) calculated atomic compositions



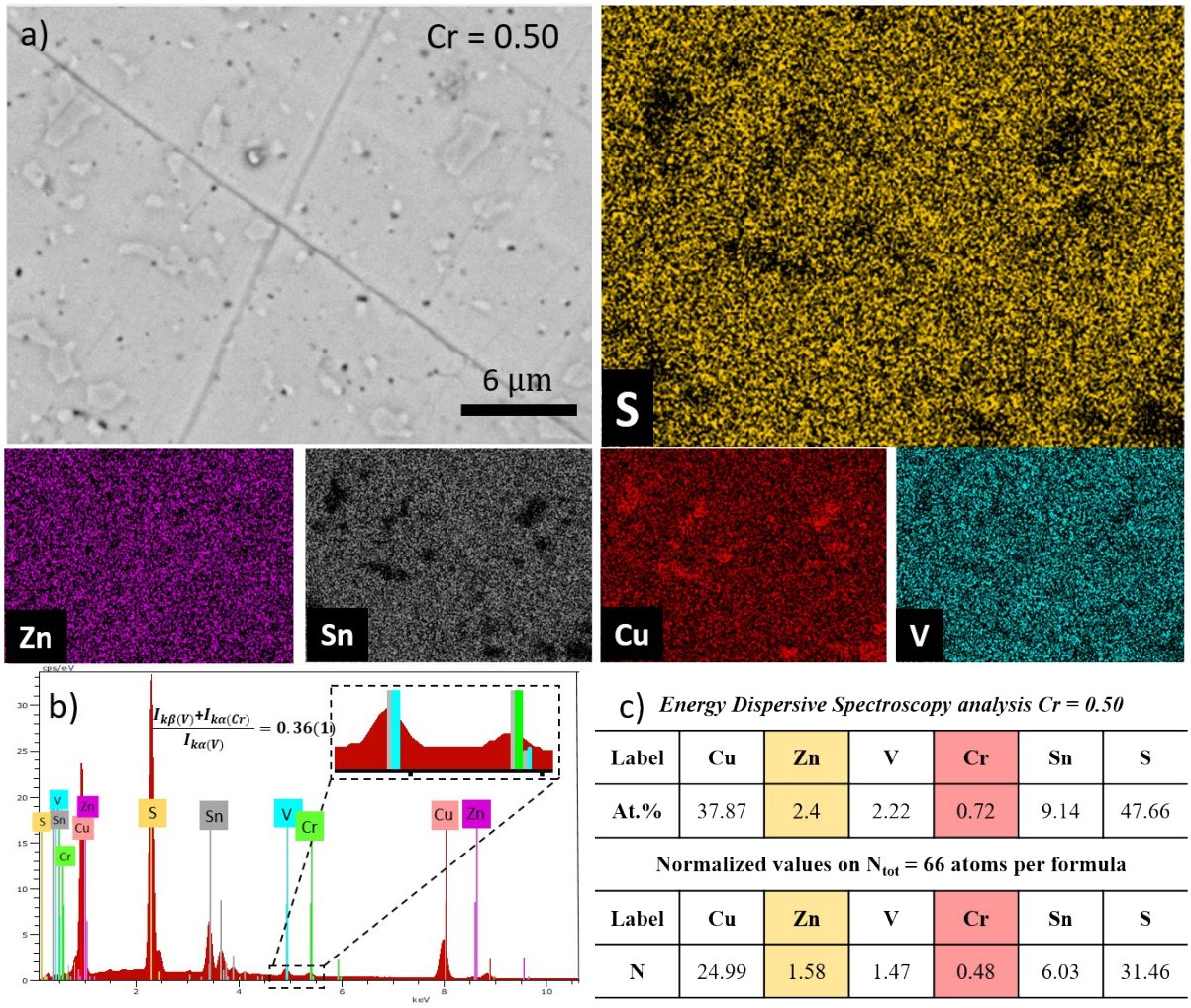
c) *Energy Dispersive Spectroscopy analysis Cr = 0.25*

Label	Cu	Zn	V	Cr	Sn	S
At.%	37.44	2.5	2.78	0.39	9.41	47.48

Normalized values on N_{tot} = 66 atoms per formula

Label	Cu	Zn	V	Cr	Sn	S
N	24.71	1.65	1.83	0.26	6.21	31.34

Figure S5. Energy dispersive spectroscopy analysis results on the polished surface of the $Cu_{25}ZnV_{1.75}Cr_{0.25}Sn_6S_{32}$ sample sintered by SPS with a) EDS mapping b) its corresponding spectrum, and c) calculated atomic compositions



c) *Energy Dispersive Spectroscopy analysis Cr = 0.50*

Label	Cu	Zn	V	Cr	Sn	S
At.%	37.87	2.4	2.22	0.72	9.14	47.66

Normalized values on N_{tot} = 66 atoms per formula

Label	Cu	Zn	V	Cr	Sn	S
N	24.99	1.58	1.47	0.48	6.03	31.46

Figure S6. Energy dispersive spectroscopy analysis results on the polished surface of the $Cu_{25}ZnV_{1.5}Cr_{0.5}Sn_6S_{32}$ sample sintered by SPS with a) EDS mapping b) its corresponding spectrum, and c) calculated atomic compositions

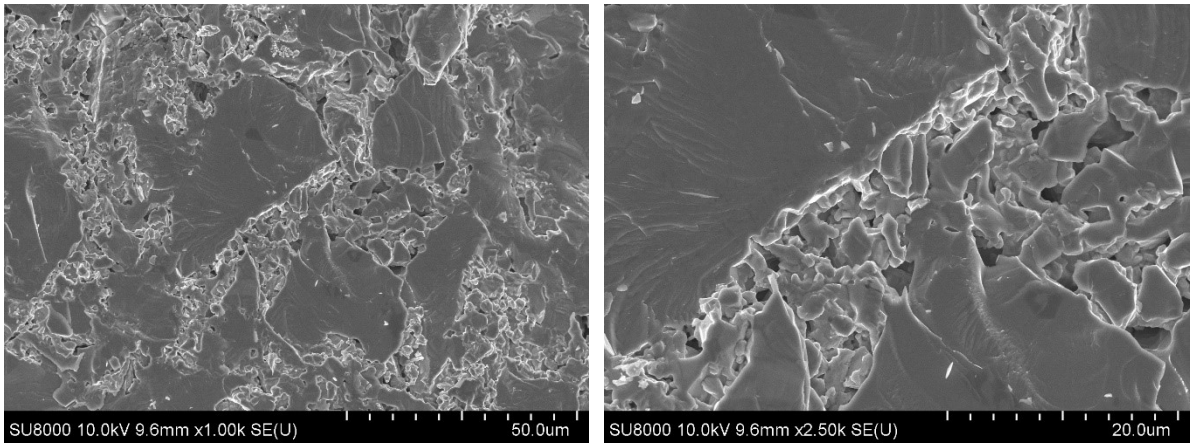


Figure S7. SEM images of a fractured surface of $Cu_{25}ZnV_2Sn_6S_3$ without ball milling step during the fabrication process

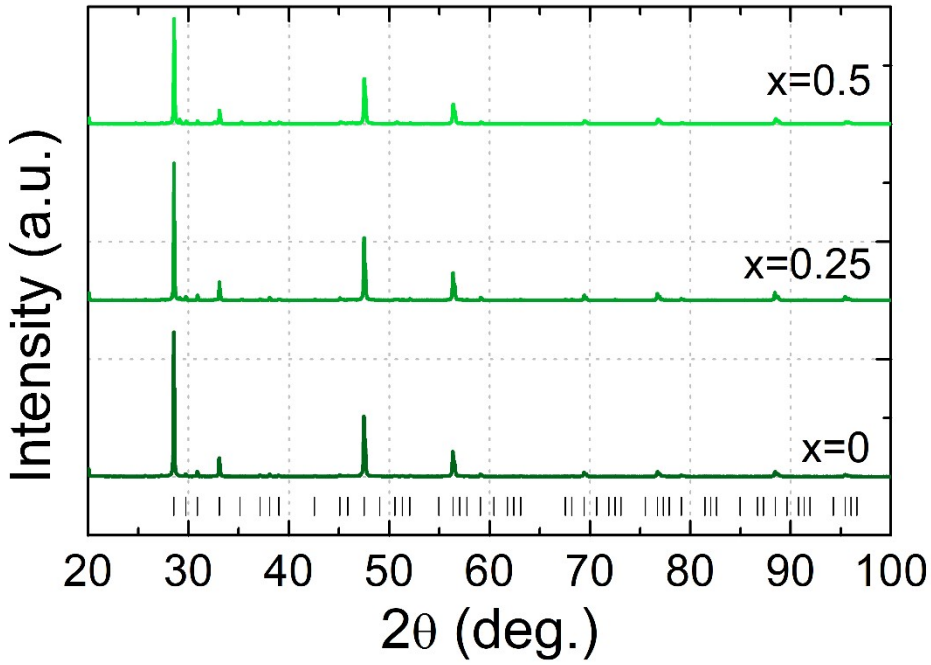
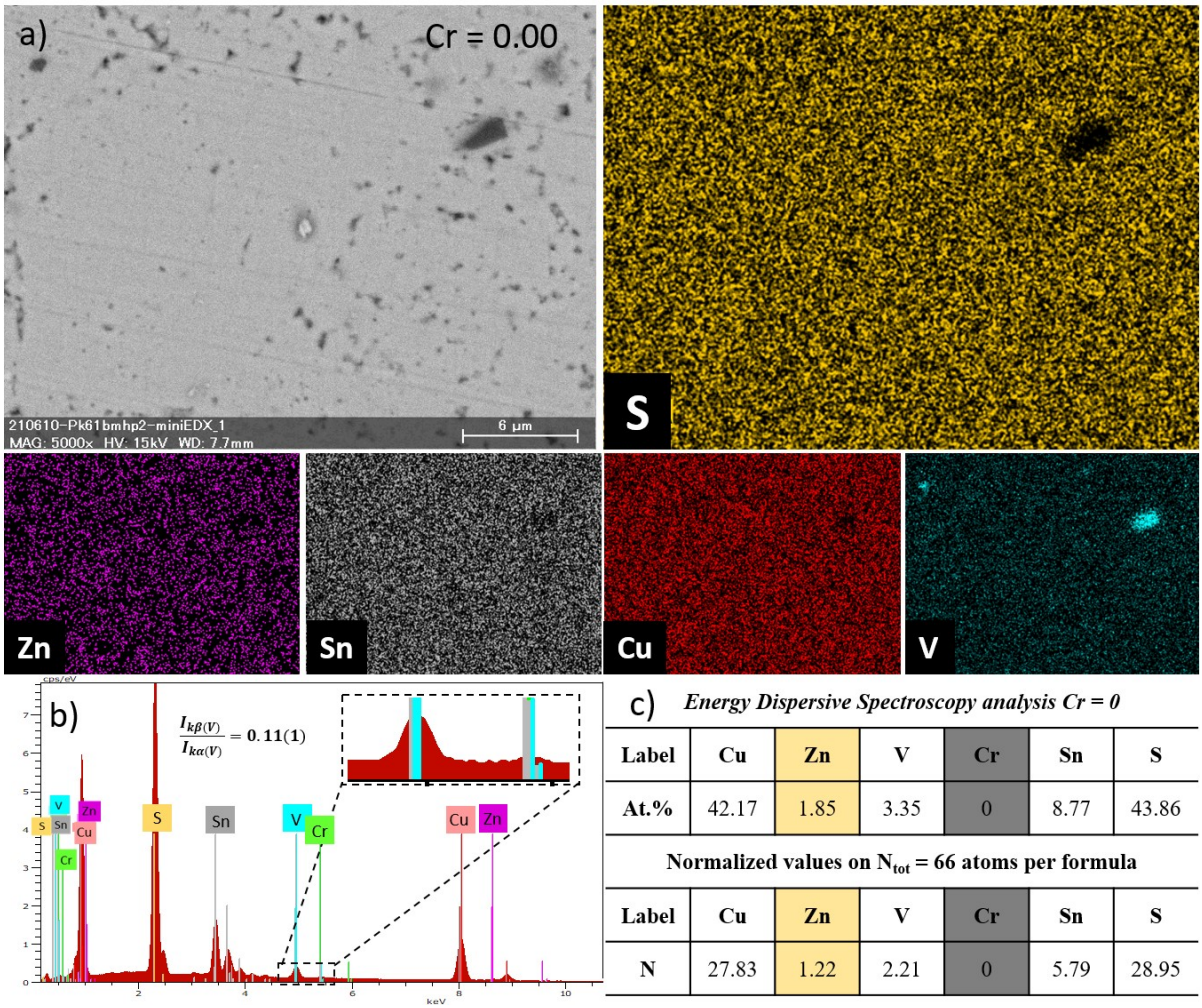


Figure S8. Powder X-ray diffraction patterns of sintered $Cu_{25}ZnV_{2-x}Cr_xSn_6S_{32}$ compounds by hot-pressing



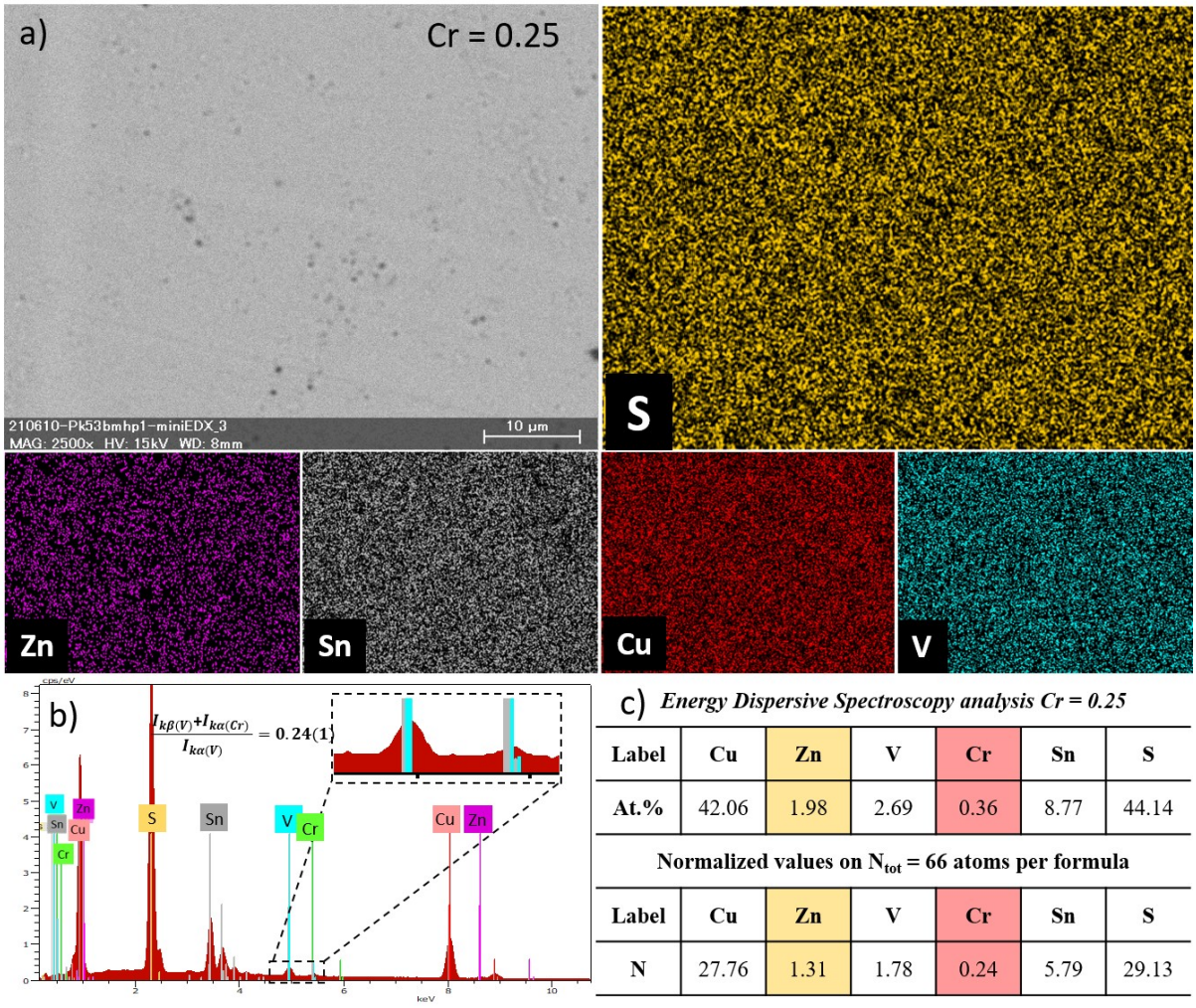
c) *Energy Dispersive Spectroscopy analysis Cr = 0*

Label	Cu	Zn	V	Cr	Sn	S
At.%	42.17	1.85	3.35	0	8.77	43.86

Normalized values on N_{tot} = 66 atoms per formula

Label	Cu	Zn	V	Cr	Sn	S
N	27.83	1.22	2.21	0	5.79	28.95

Figure S9. Energy dispersive spectroscopy analysis results on the polished surface of the $Cu_{25}ZnV2Sn_6S_{32}$ sample sintered by hot-pressing with a) EDS mapping b) its corresponding spectrum, and c) calculated atomic compositions



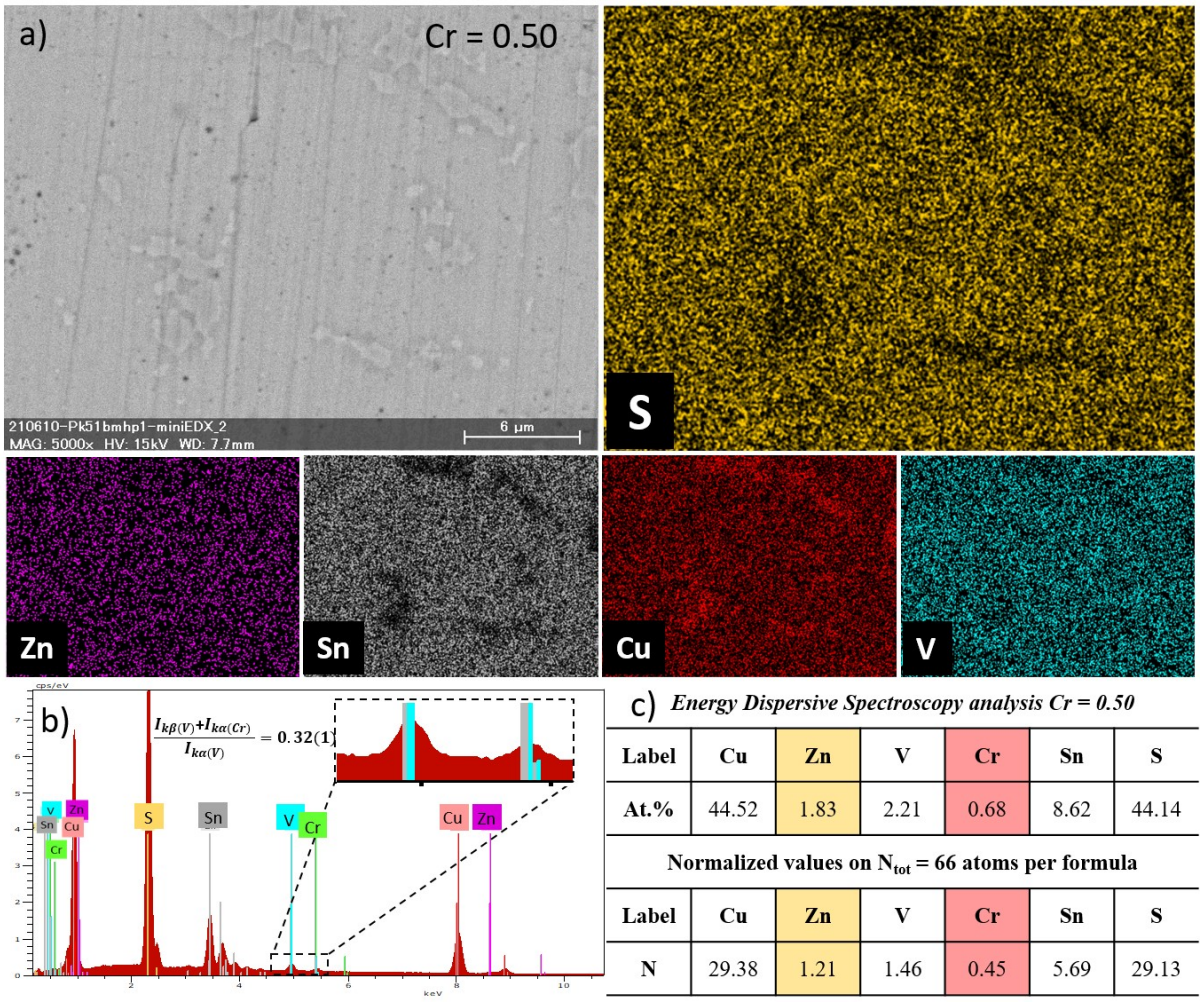
c) *Energy Dispersive Spectroscopy analysis Cr = 0.25*

Label	Cu	Zn	V	Cr	Sn	S
At.%	42.06	1.98	2.69	0.36	8.77	44.14

Normalized values on N_{tot} = 66 atoms per formula

Label	Cu	Zn	V	Cr	Sn	S
N	27.76	1.31	1.78	0.24	5.79	29.13

Figure S10. Energy dispersive spectroscopy analysis results on the polished surface of the $Cu_{25}ZnV_{1.75}Cr_{0.25}Sn_6S_{32}$ sample sintered by hot-pressing with a) EDS mapping b) its corresponding spectrum, and c) calculated atomic compositions



c) *Energy Dispersive Spectroscopy analysis Cr = 0.50*

Label	Cu	Zn	V	Cr	Sn	S
At.%	44.52	1.83	2.21	0.68	8.62	44.14

Normalized values on N_{tot} = 66 atoms per formula

Label	Cu	Zn	V	Cr	Sn	S
N	29.38	1.21	1.46	0.45	5.69	29.13

Figure S11. Energy dispersive spectroscopy analysis results on the polished surface of the $Cu_{25}ZnV_{1.75}Cr_{0.25}Sn_6S_{32}$ sample sintered by SPS with a) EDS mapping b) its corresponding spectrum, and c) calculated atomic compositions

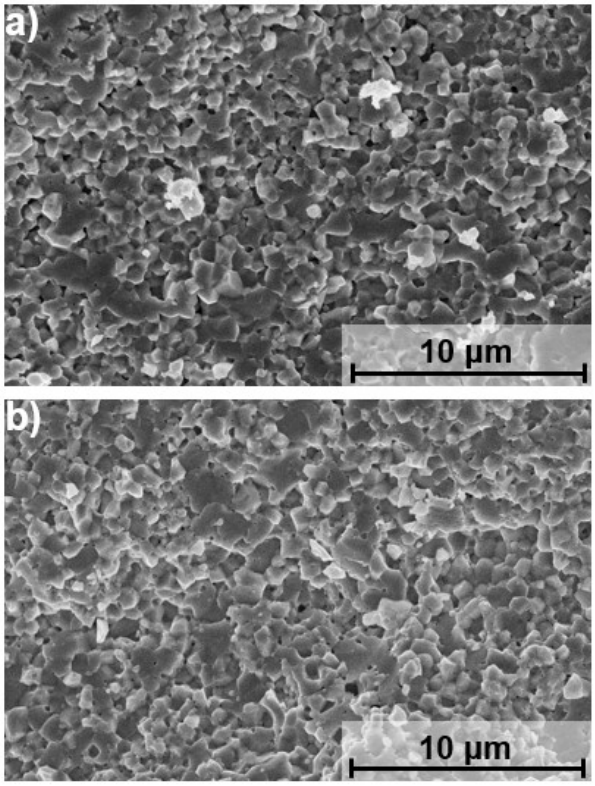


Figure S12. SEM images of a fractured surface of the hot-pressed $Cu_{25}ZnV_{2-x}Cr_xSn_6S_{32}$ (a) $x = 0$, (b) $x = 0.5$.