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Investigation of AgGaSe_2 as a wide band gap solar cell absorber

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Motivation

Why AgGaSe₂?

- Wide band gap (1.75 - 1.8 eV)
- Potential tandem top cell absorber
- Good band alignment with CdS¹
- Not widely studied

Is Ag the new Cu?

Questions addressed here

- Which secondary phases can form during co-evaporation?
- Detection of secondary phases?
- Solar cell behaviour with presence of secondary phases?

1. Keller, et al. *Progress in Photovoltaics: Research and Applications* 28, no. 4 (April 2020): 237–50.

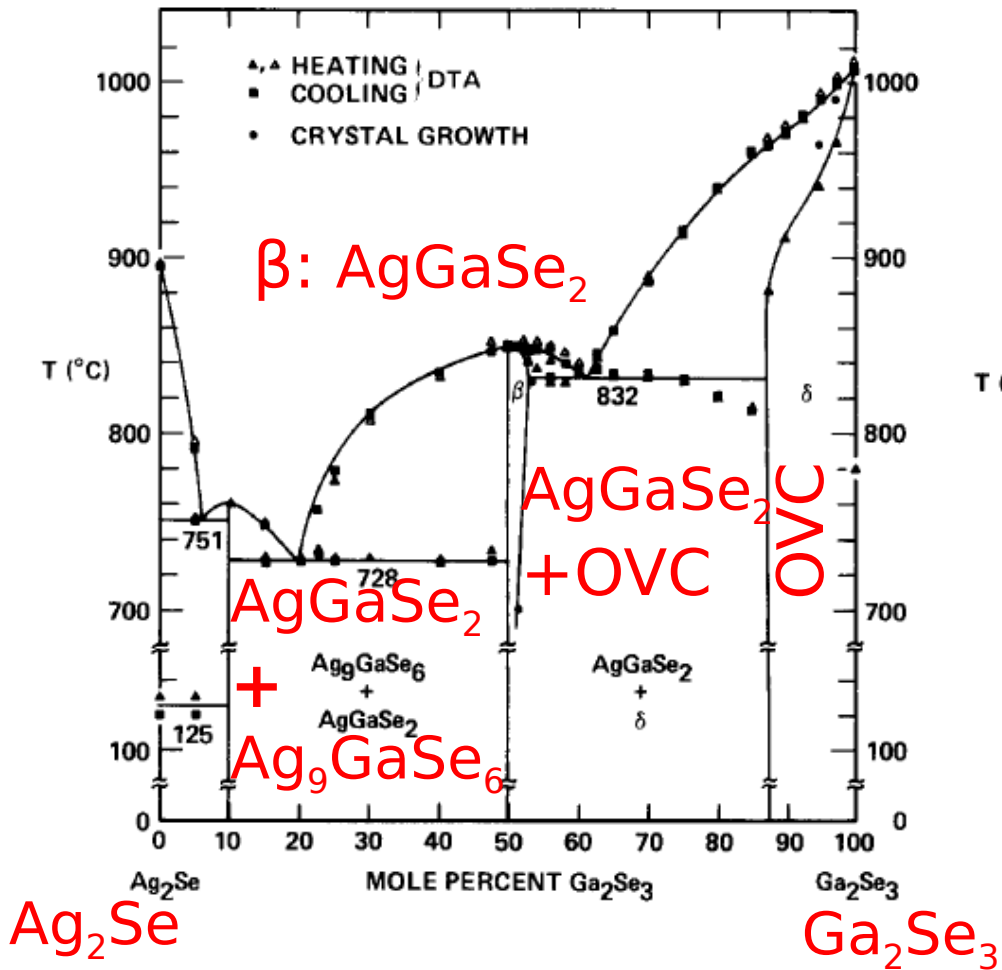


FIG. 1a

Ag₂Se-Ga₂Se₃ Pseudobinary Phase Diagram

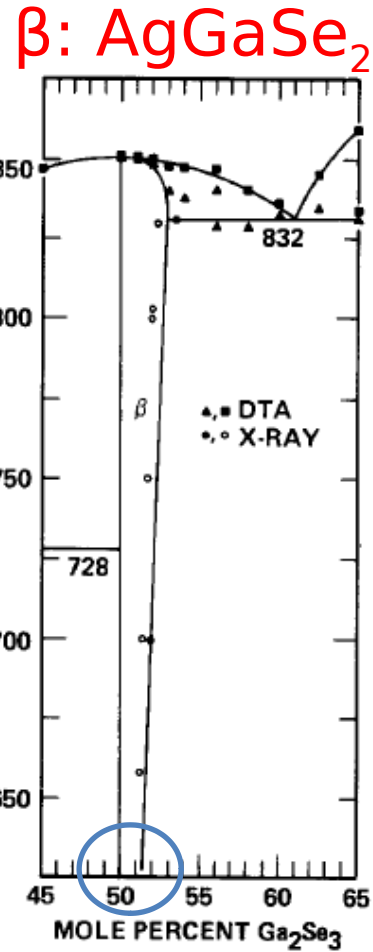



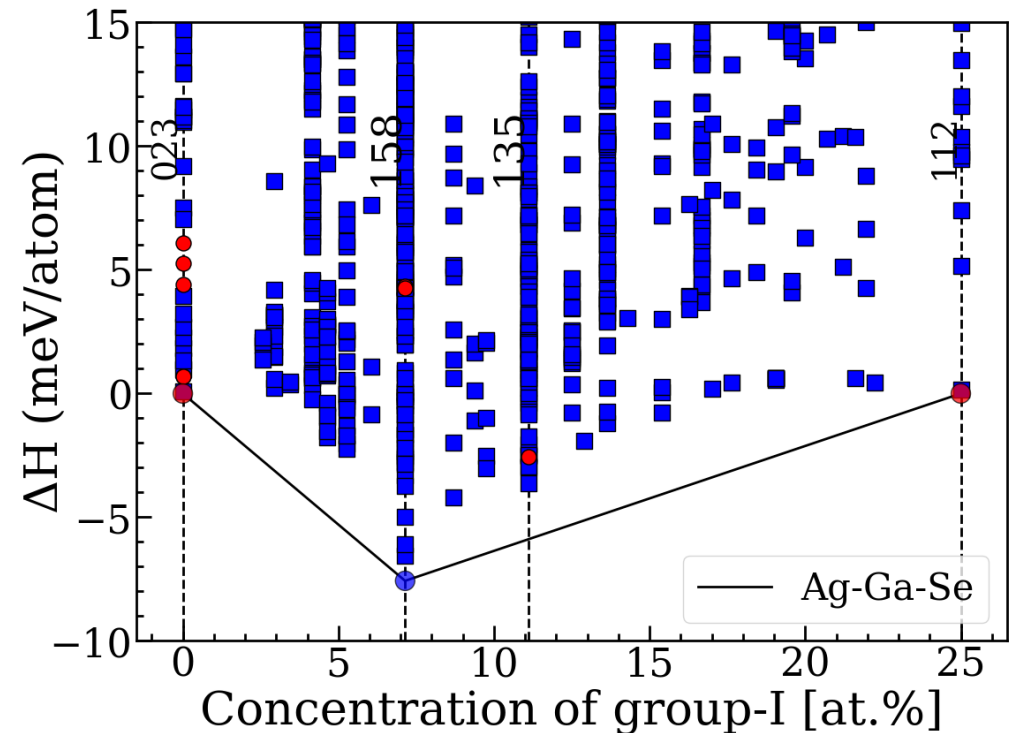
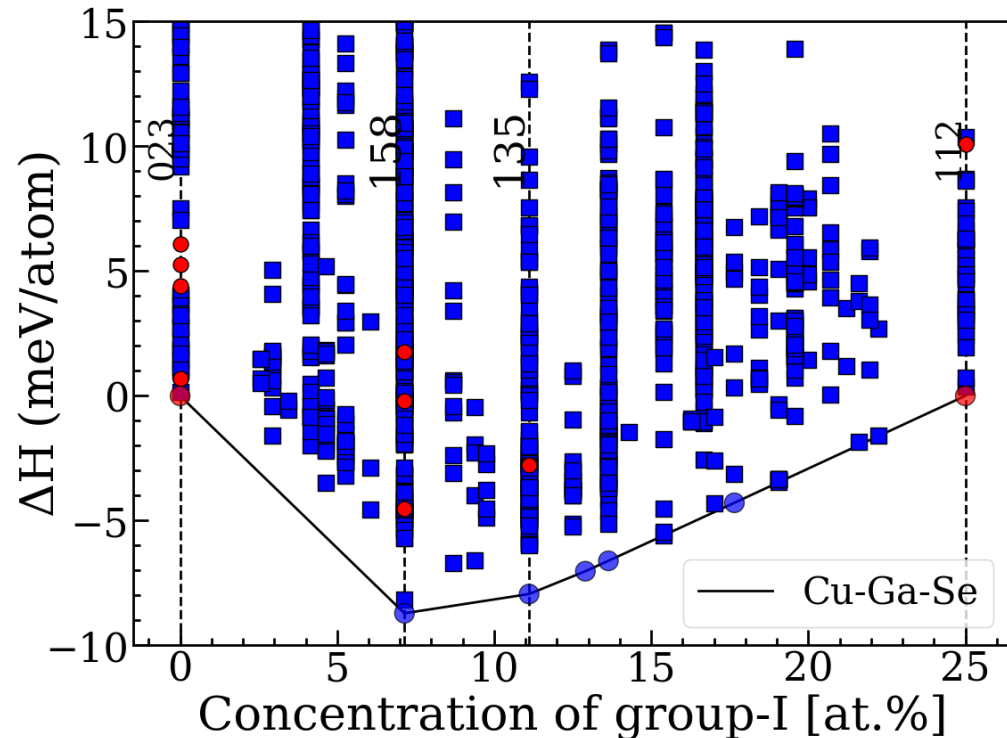
FIG. 1b

Phase diagram

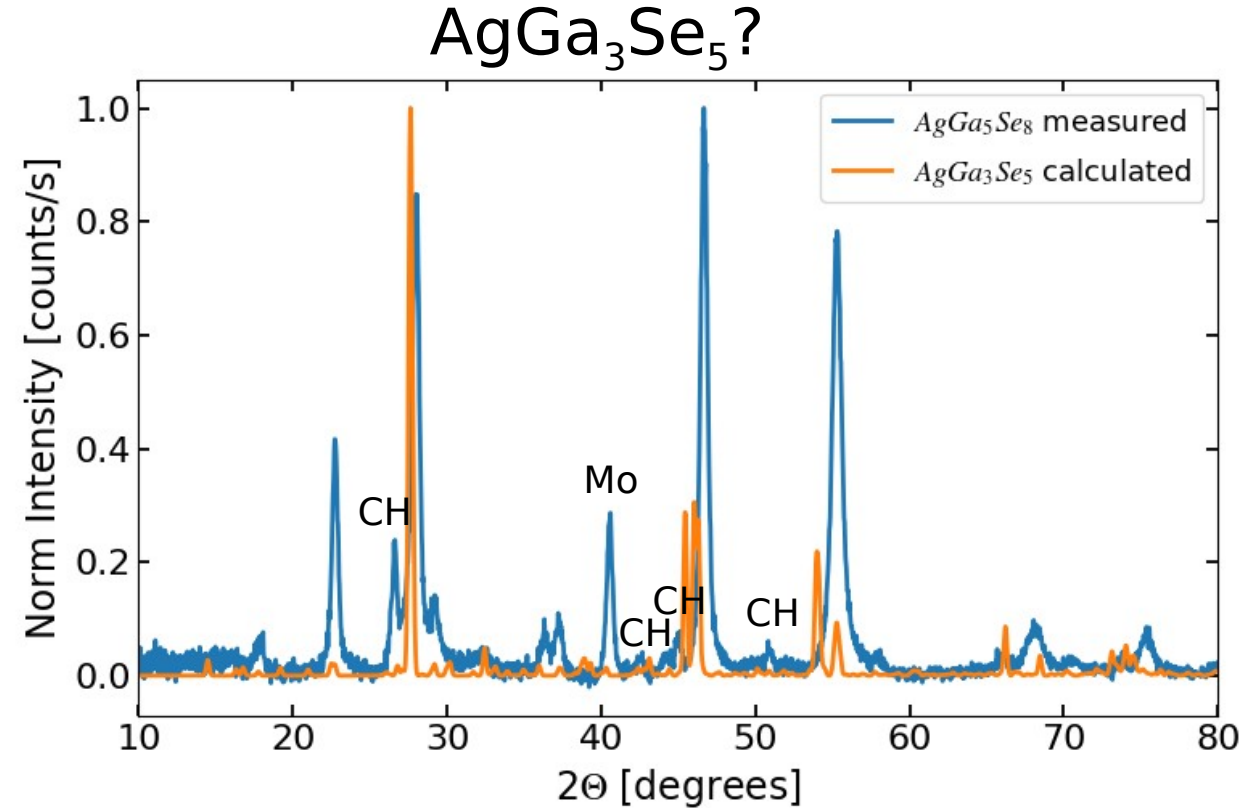
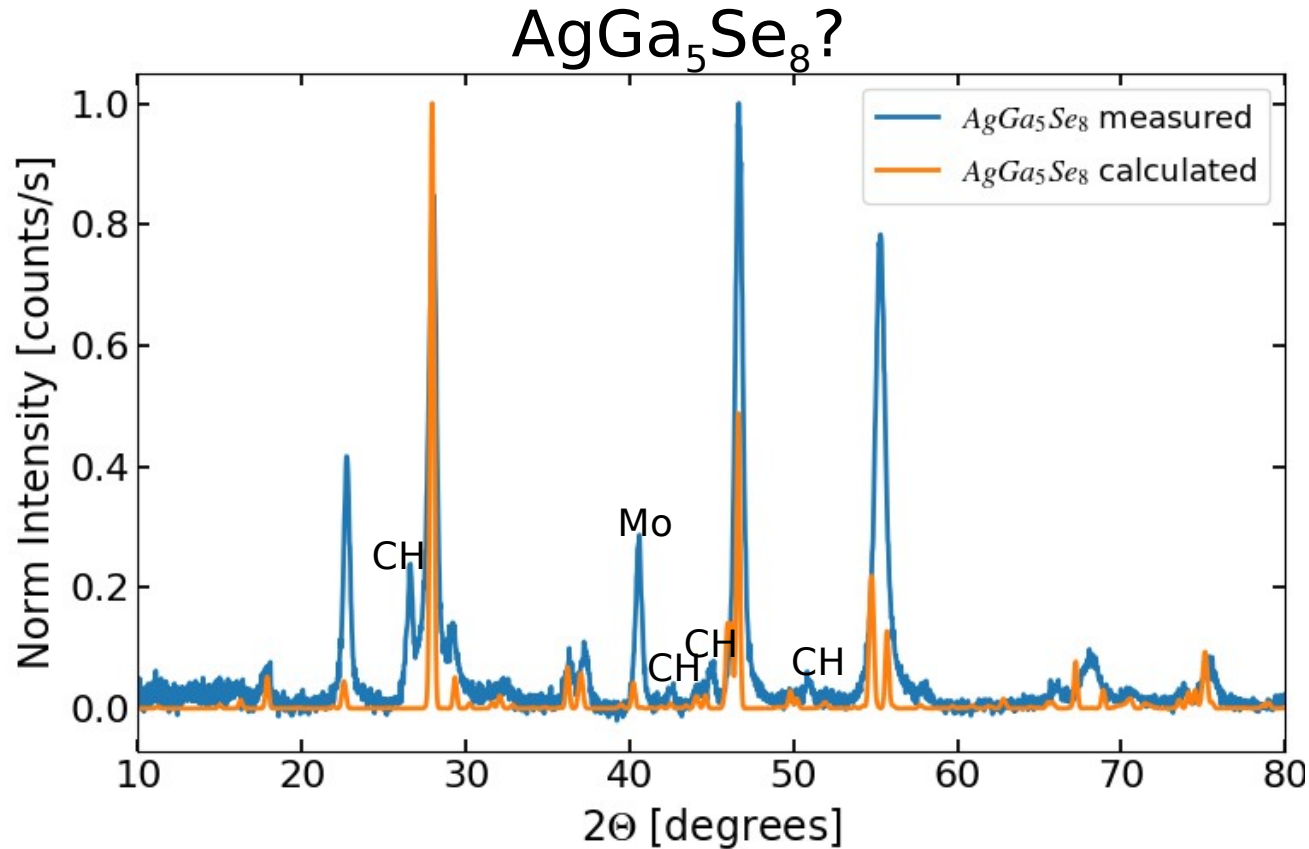
- AgGaSe₂ single phase region: [Ag]/[Ga] = 0.95 - 1 
- Valid for thin film by co-evaporation?
- What is the ordered vacancy compound (OVC)?

What is the OVC phase?

- Enthalpy of formation from DFT calculation
- AgGaSe_2 has low tolerance to off-stoichiometry
- AgGa_5Se_8 is the most stable OVC



AgGa₅Se₈ or AgGa₃Se₅?

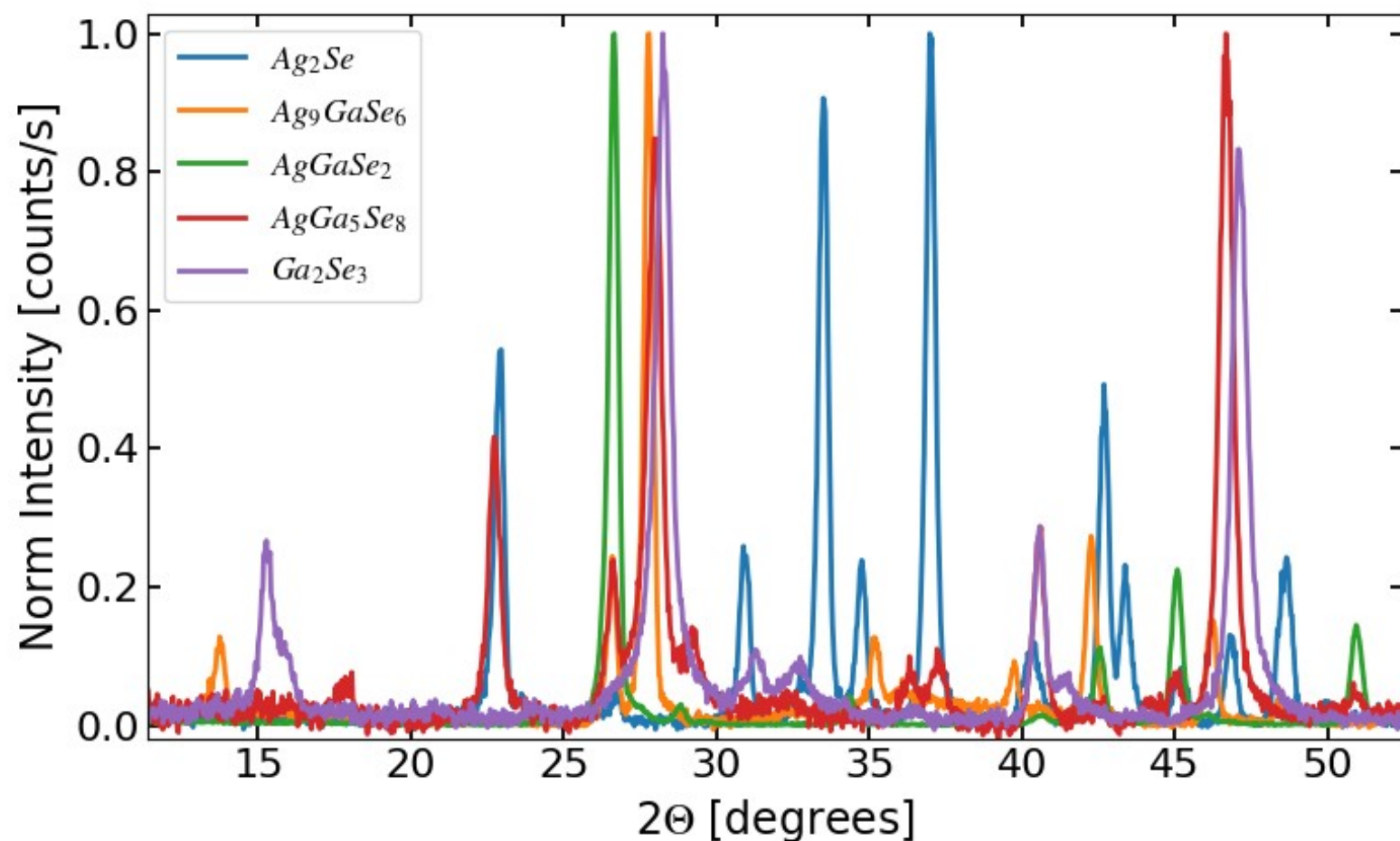


- Reference sample deposited by co-evaporation on Mo
- The predicted most stable OVC AgGa₅Se₈ matches the measured XRD pattern



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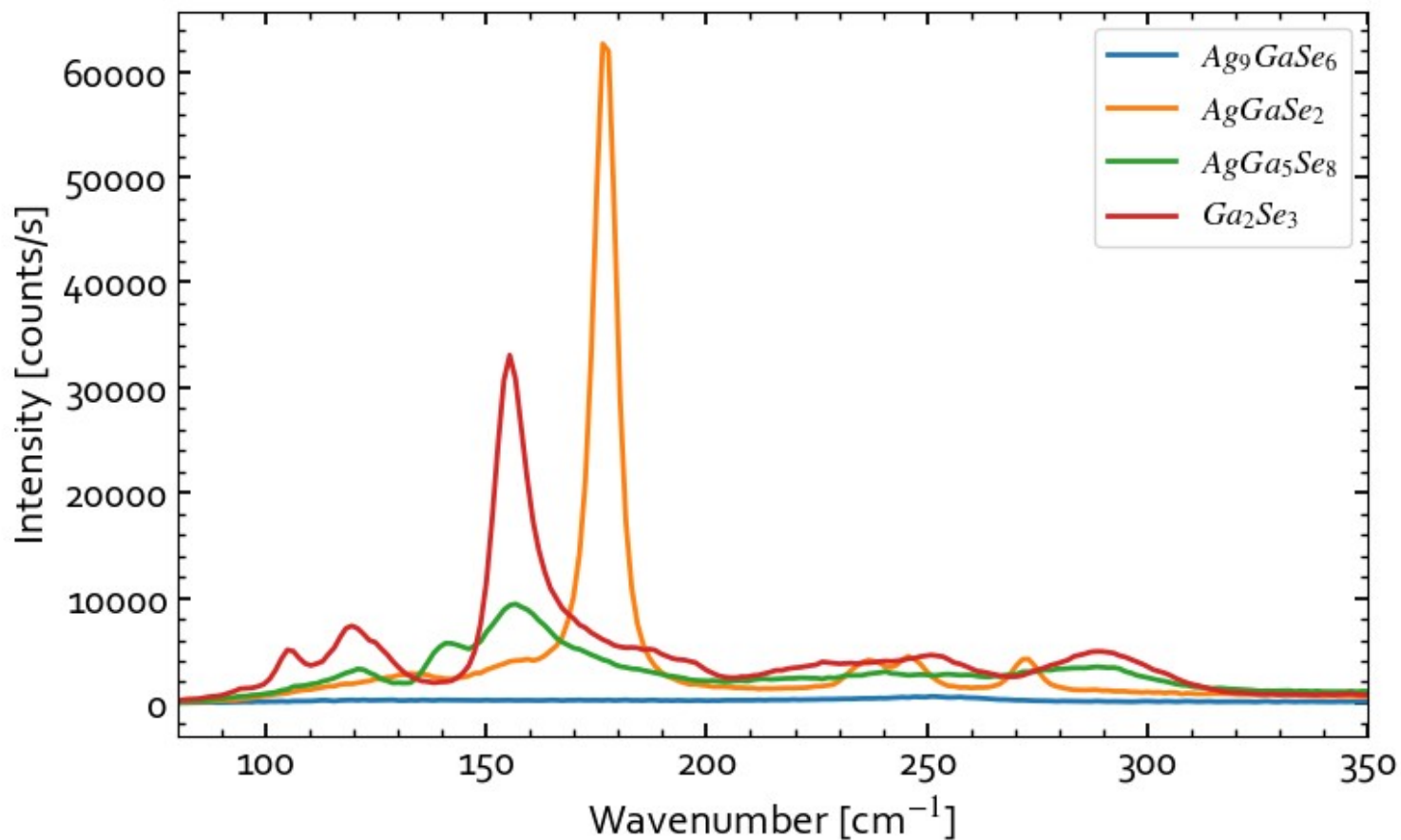
Identification by XRD



- Reference materials deposited by co-evaporation on Mo
- Substrate temperature 550°C
- Matches expected structures in literature (except $AgGa_5Se_8$)
- Unique reflections allow identification of all phases



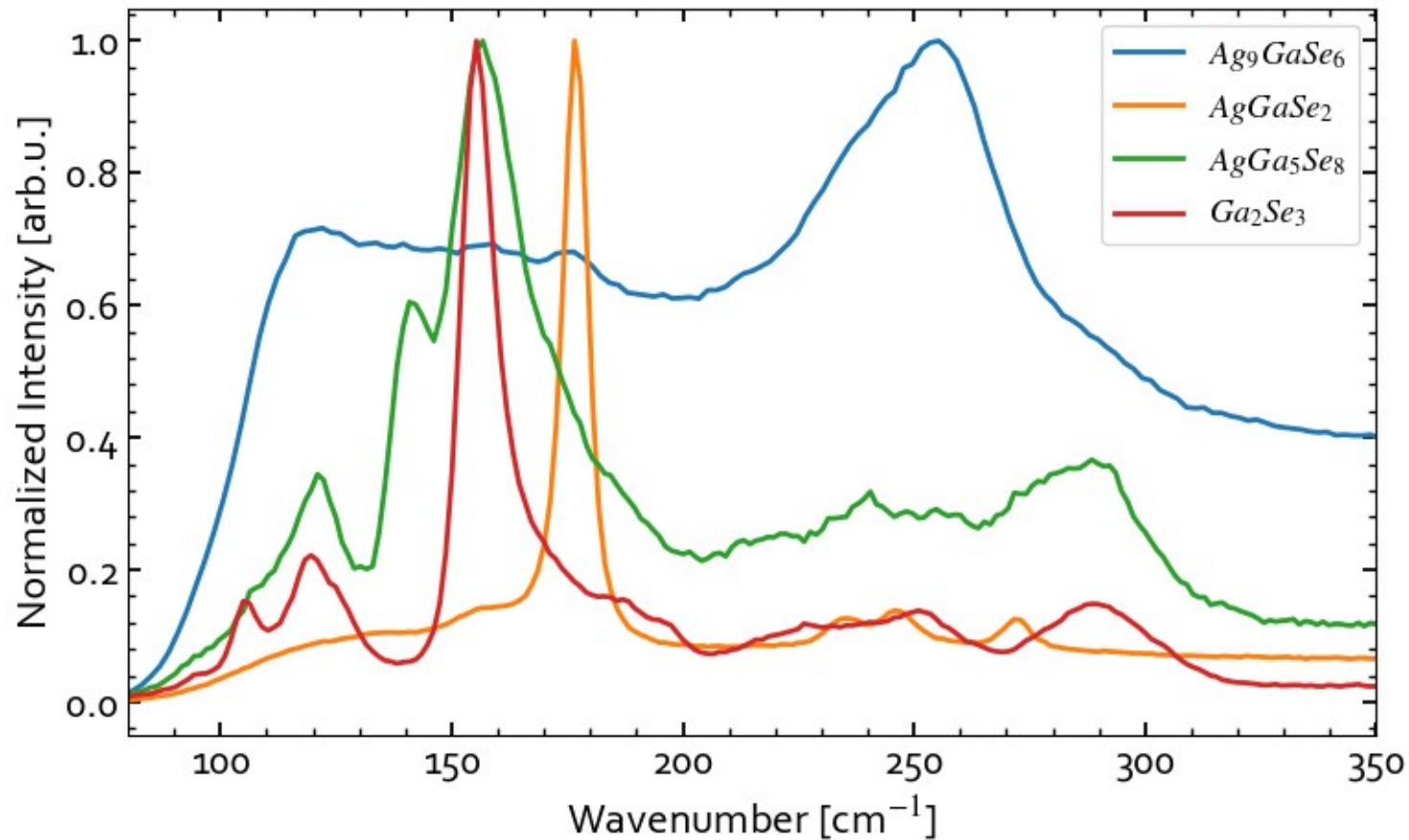
Identification by Raman



- 785 nm excitation
- Measurements with identical conditions
- Identifiable: $AgGaSe_2$, $AgGa_5Se_8$, Ga_2Se_3
- Ag_9GaSe_6 : weak signal
- Ag_2Se : no signal



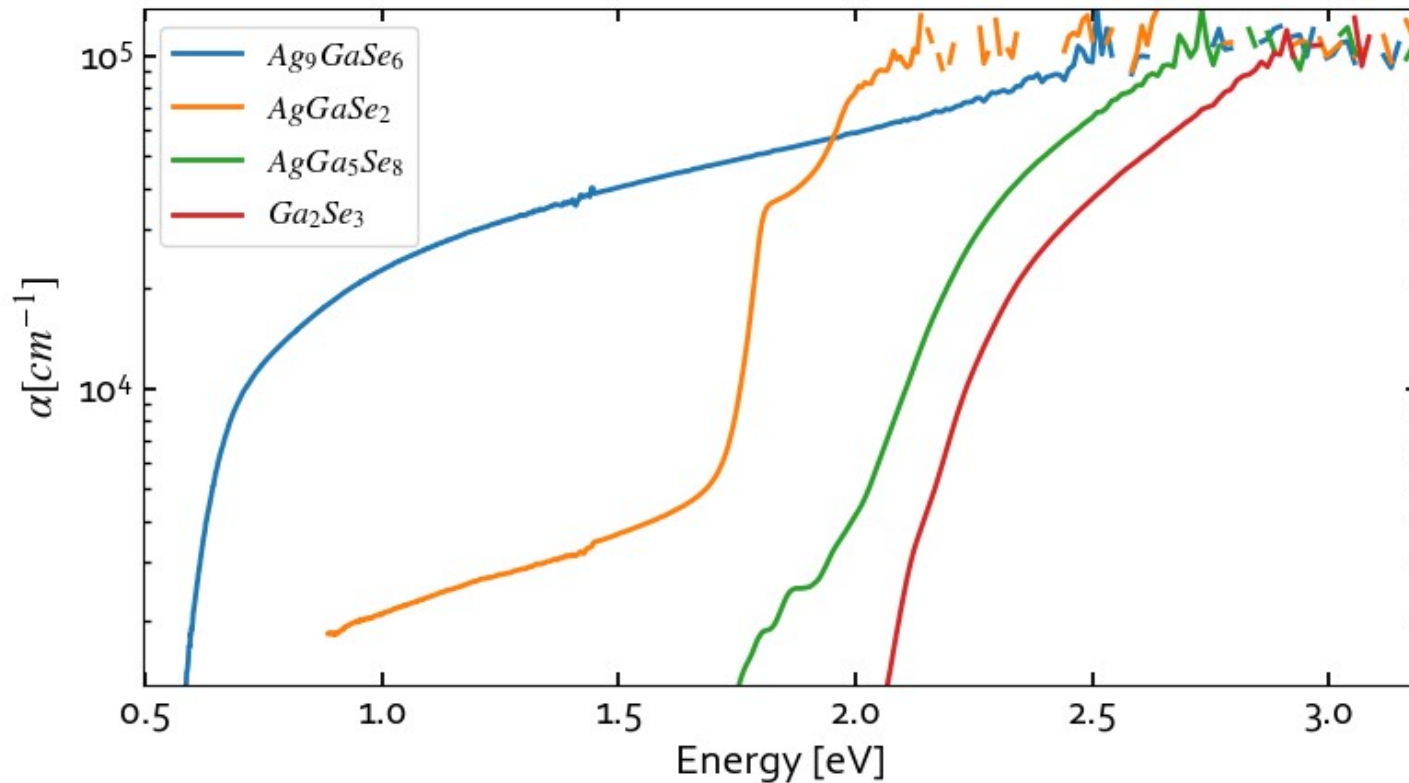
Identification by Raman



- Normalized Raman
- Ag_9GaSe_6 (10 x laser power)
- $AgGa_5Se_8$ and Ga_2Se_3 are very similar
- Raman not ideal to identify all phases in system



Band gaps of phases



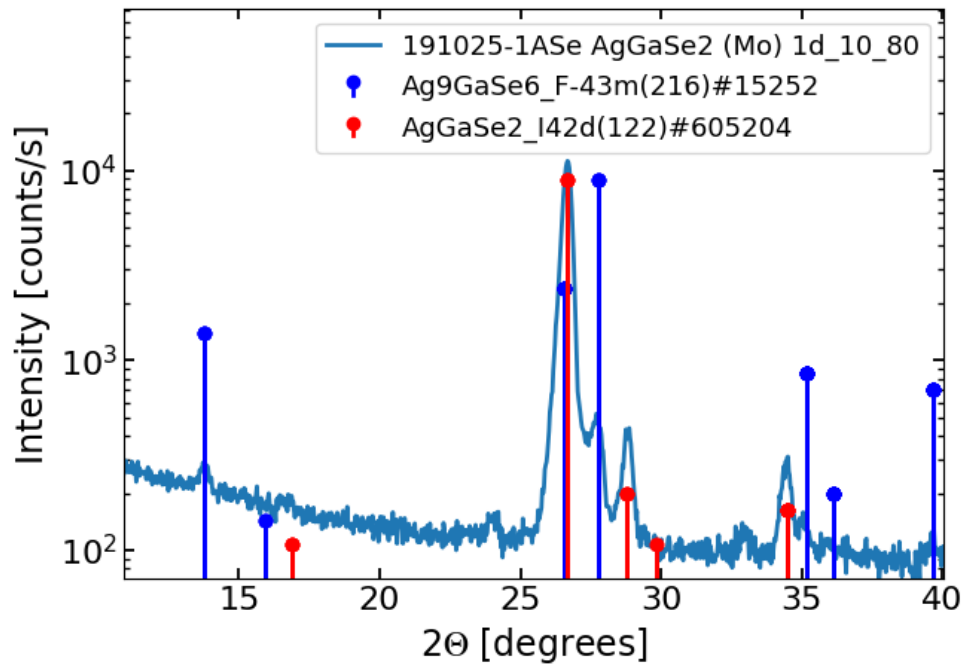
- Reference material on glass
- Spectrophotometry (T-R)

Phase	Estimated band gap [eV]
Ga_2Se_3	2.21
AgGa_5Se_8	2.11
AgGaSe_2	1.78
Ag_9GaSe_6	0.6
Ag_2Se	-

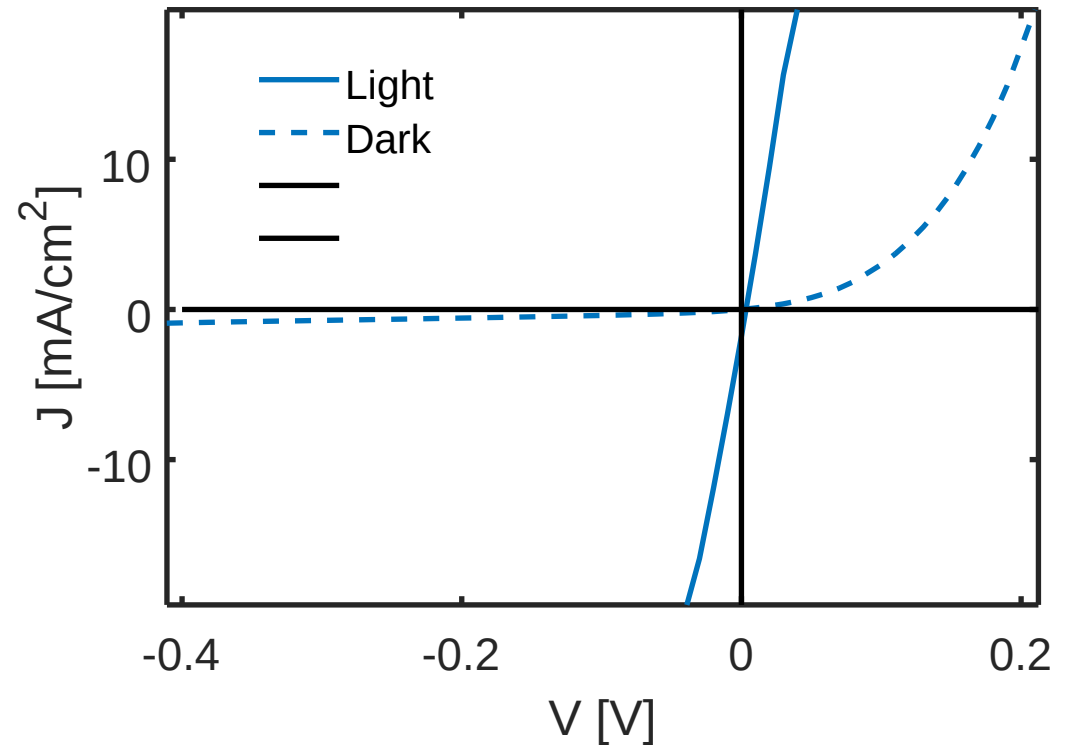
Impact of Ag_9GaSe_6 on device

$[\text{Ag}]/[\text{Ga}] = 1.16$

Ag_9GaSe_6 not etched by KCN



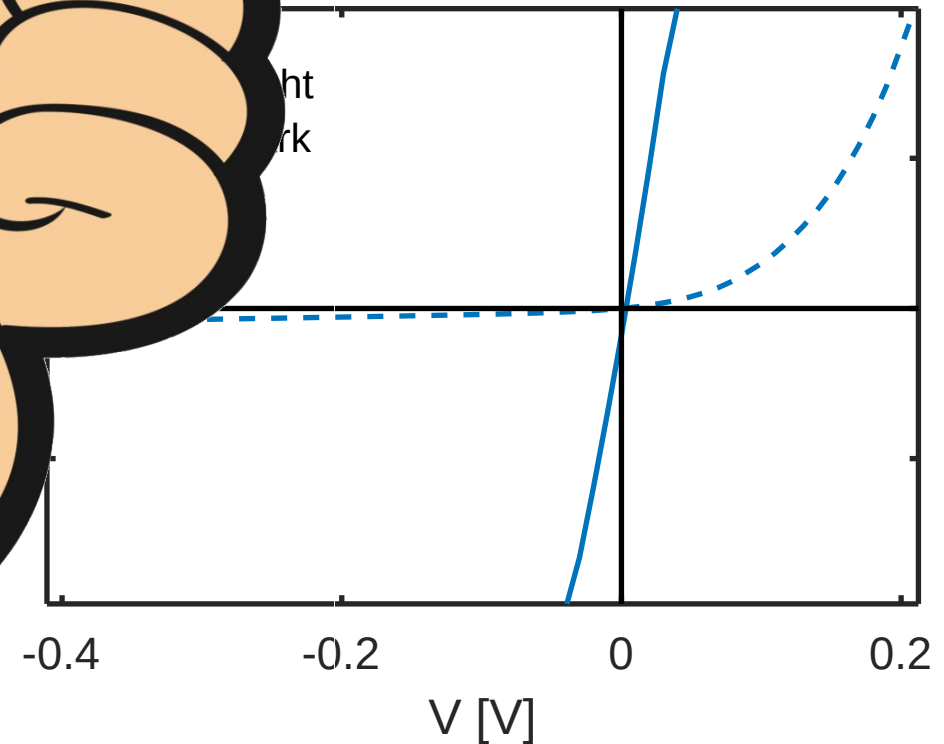
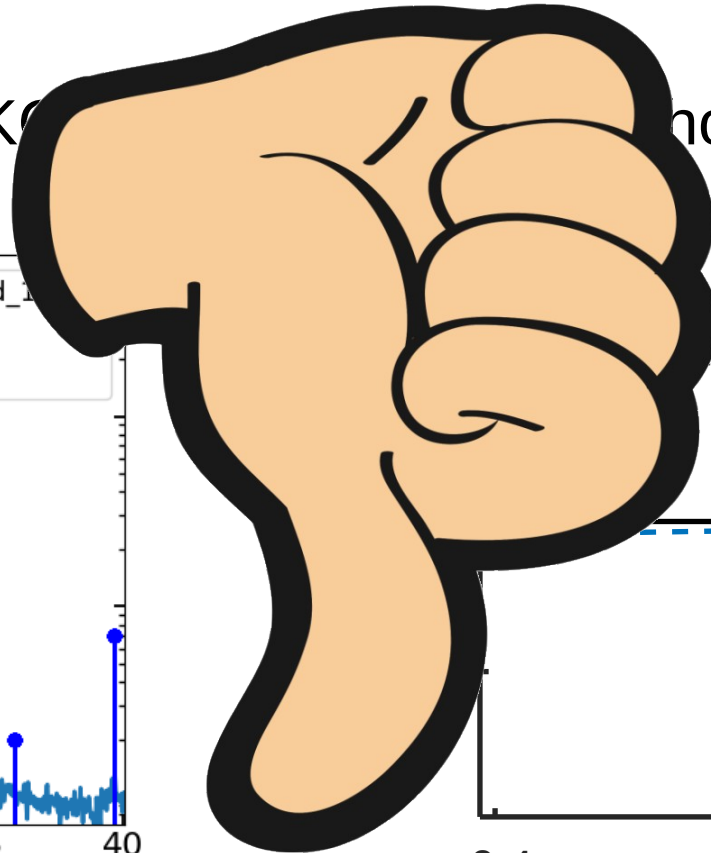
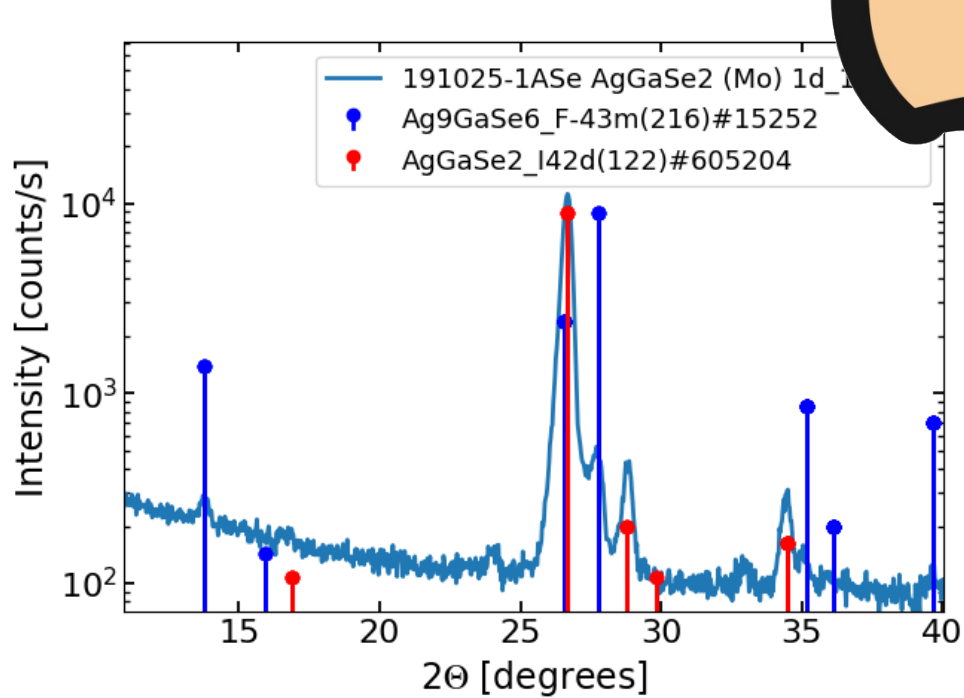
High photoconductivity?



Impact of Ag_9GaSe_6 on device

$[\text{Ag}]/[\text{Ga}] = 1.16$

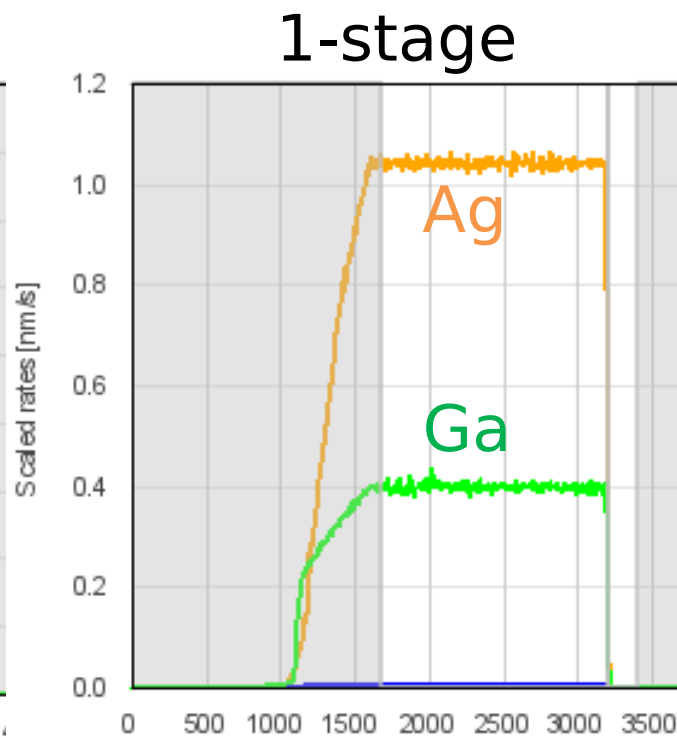
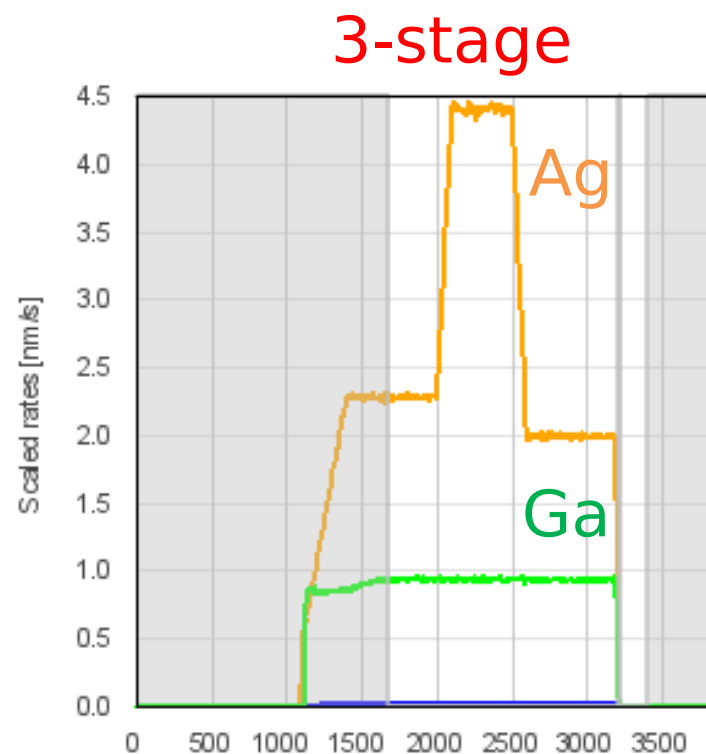
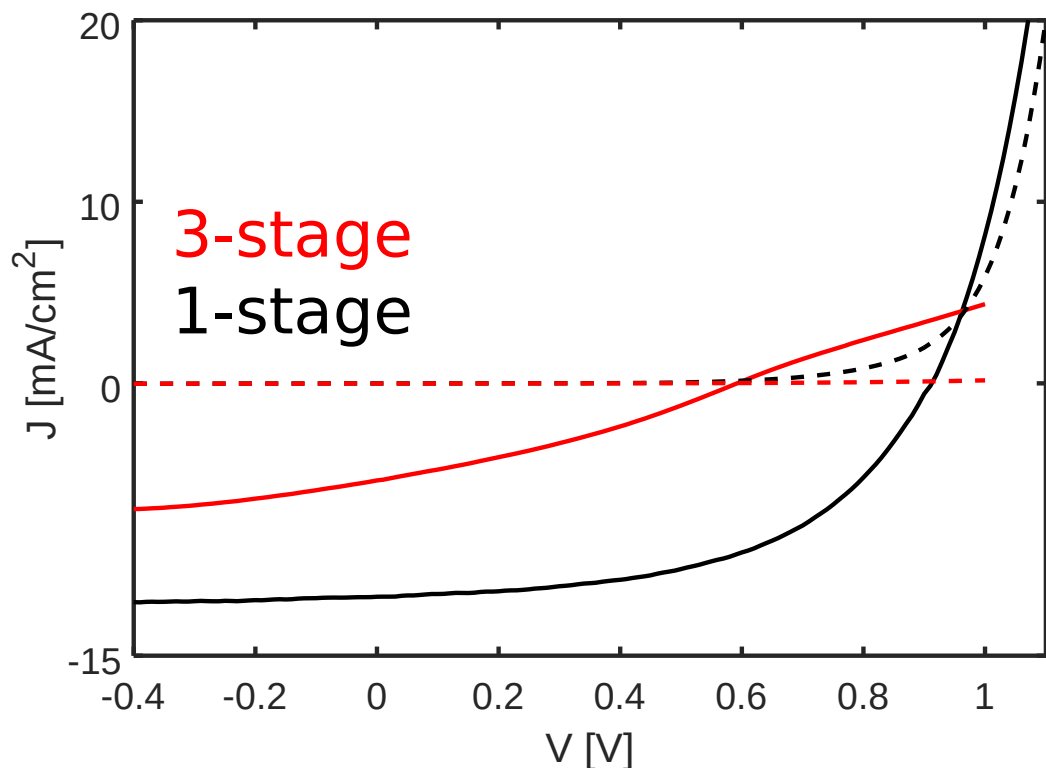
Ag_9GaSe_6 not etched by KOH photoconductivity?





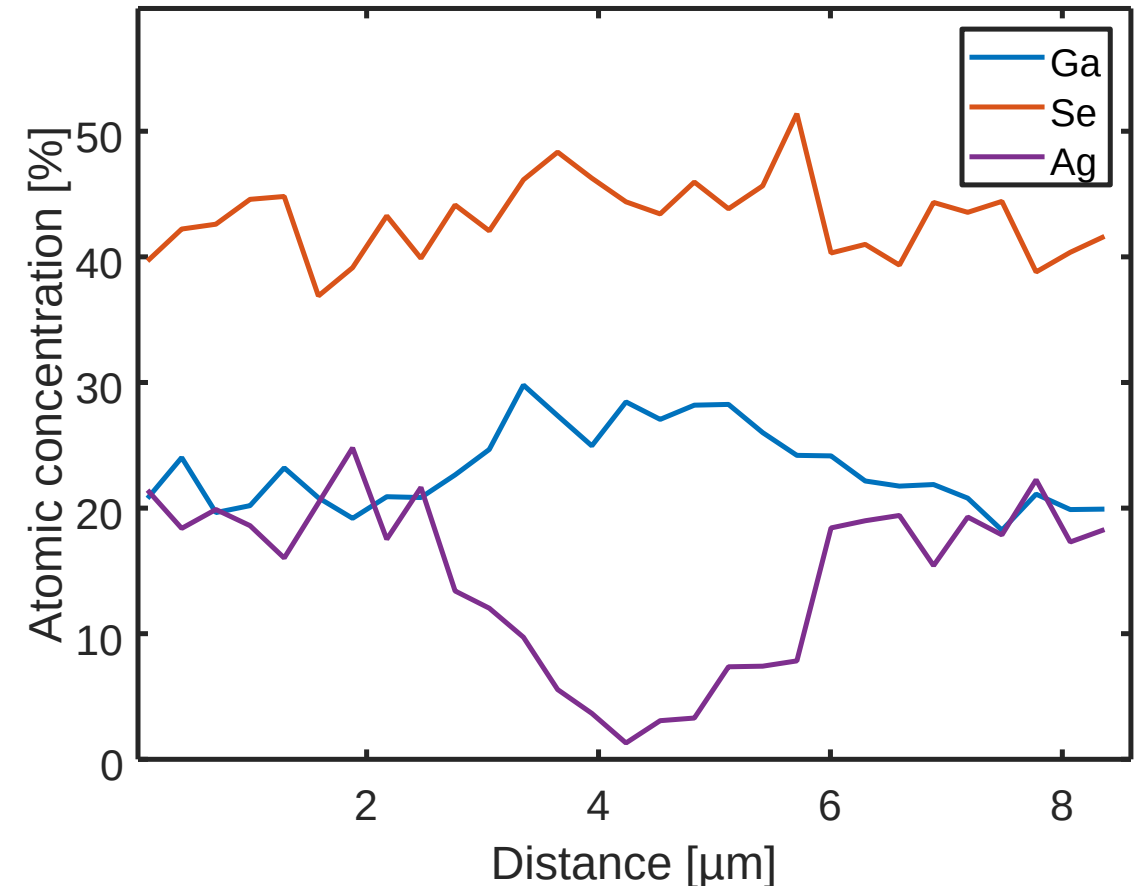
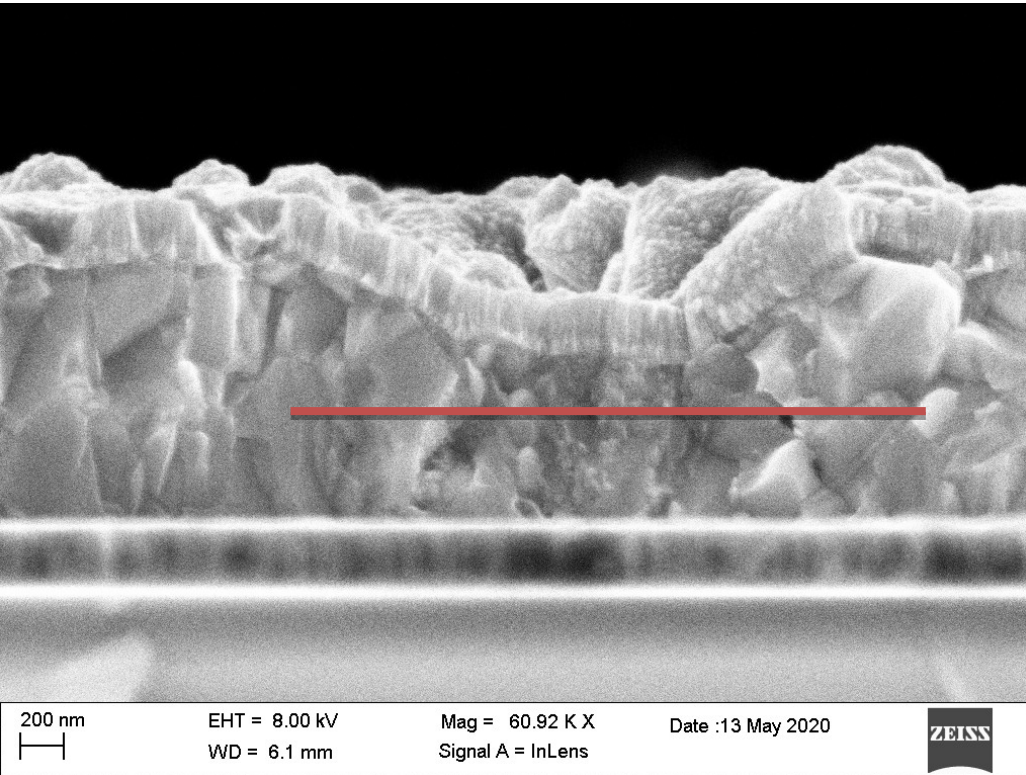
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Impact of AgGa_5Se_8 on device

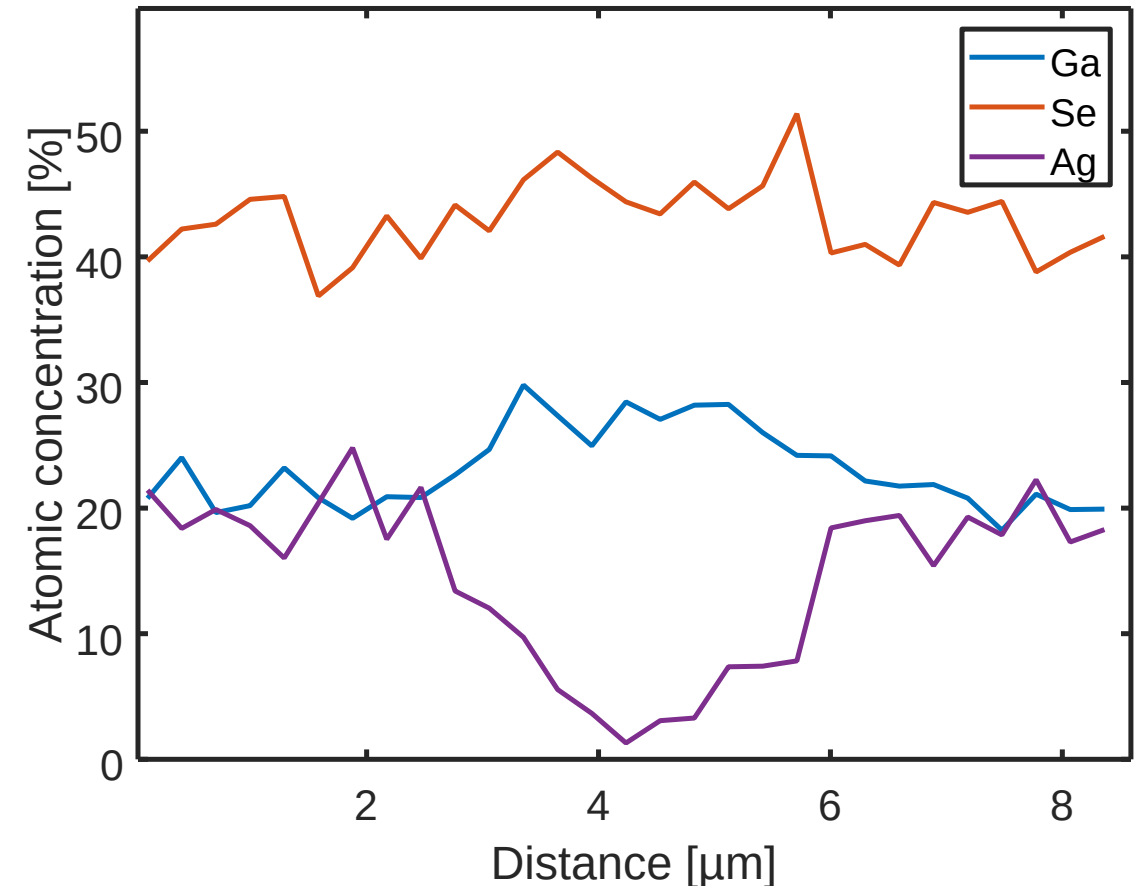
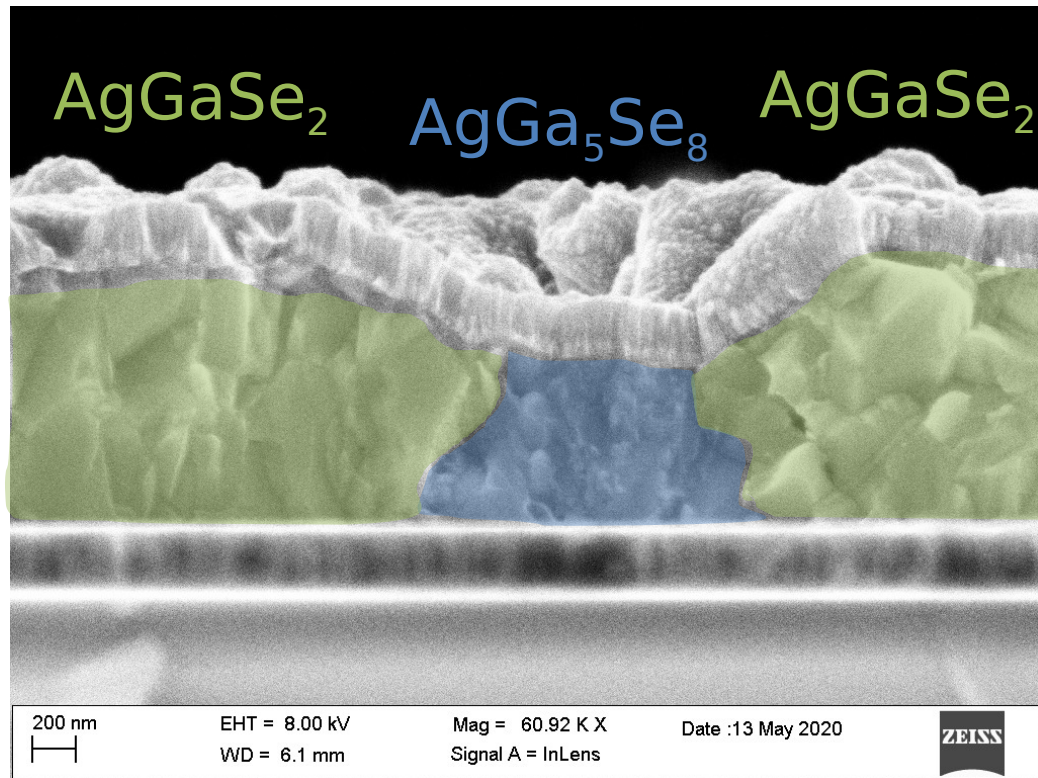


	[Ag]/[Ga]	V_{oc} [mV]	J_{sc} [mA/cm ²]	FF [%]	Efficiency [%]
1-stage	0.86	911 (833)	12.2 (11.7)	53 (52)	5.8 (5.1)
3-stage	0.87	592 (590)	5.3 (2.1)	32 (34)	1 (0.4)

AgGa₅Se₈ distribution in 1-stage device

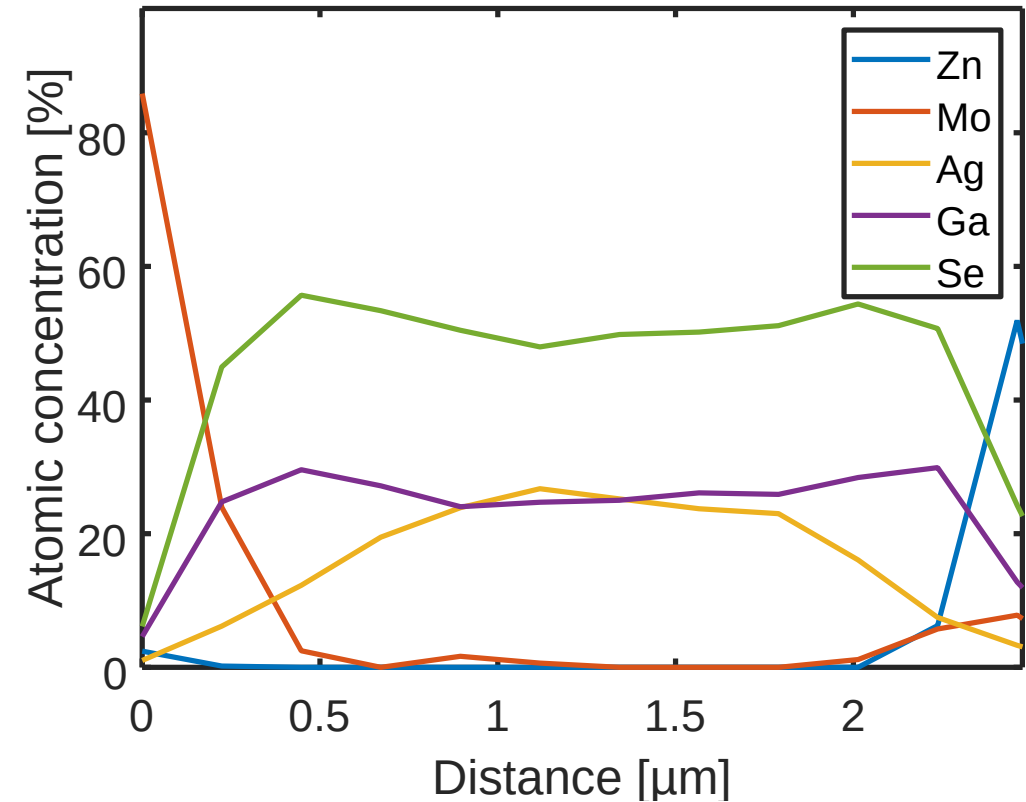
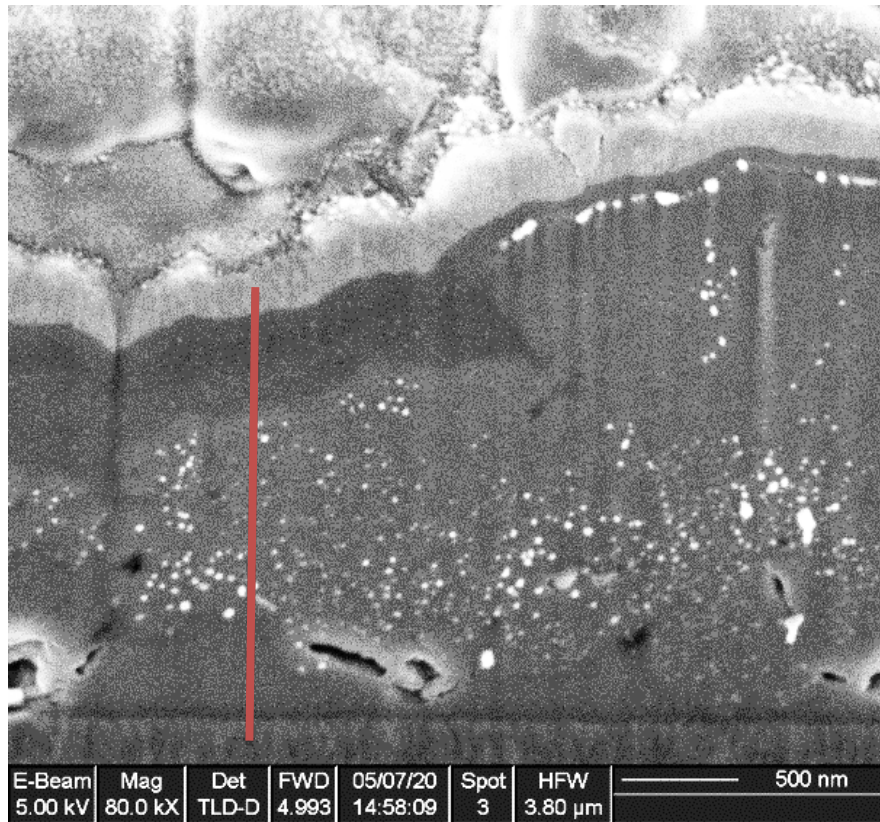


AgGa₅Se₈ distribution in 1-stage device

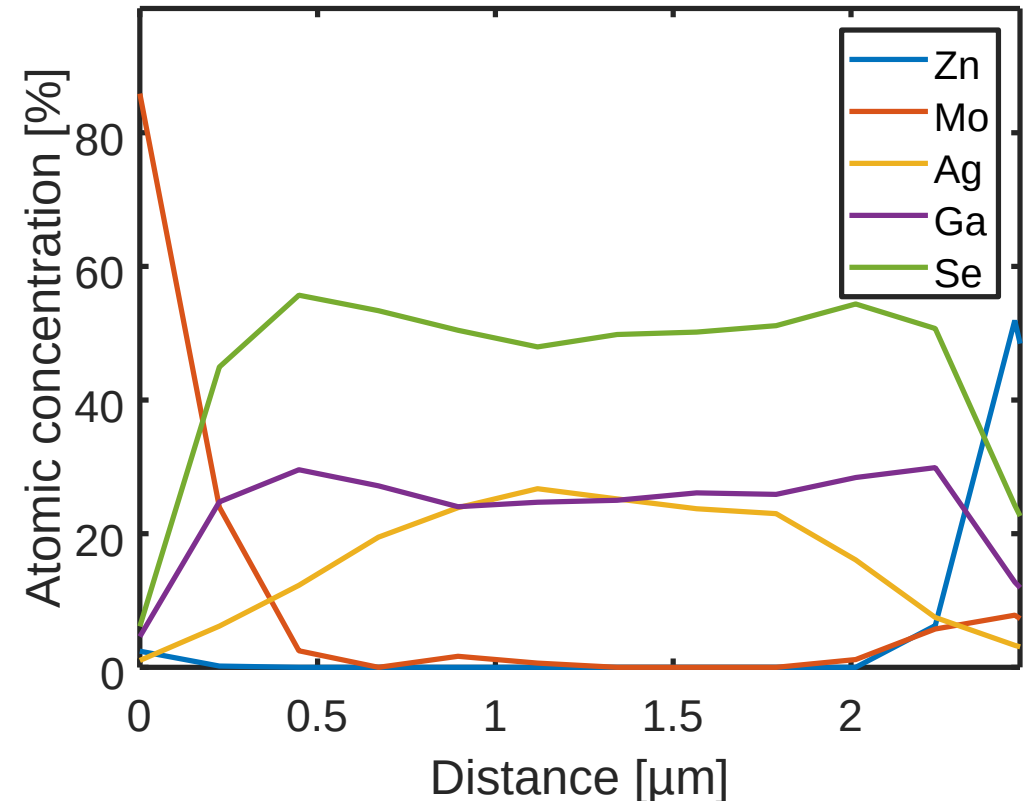
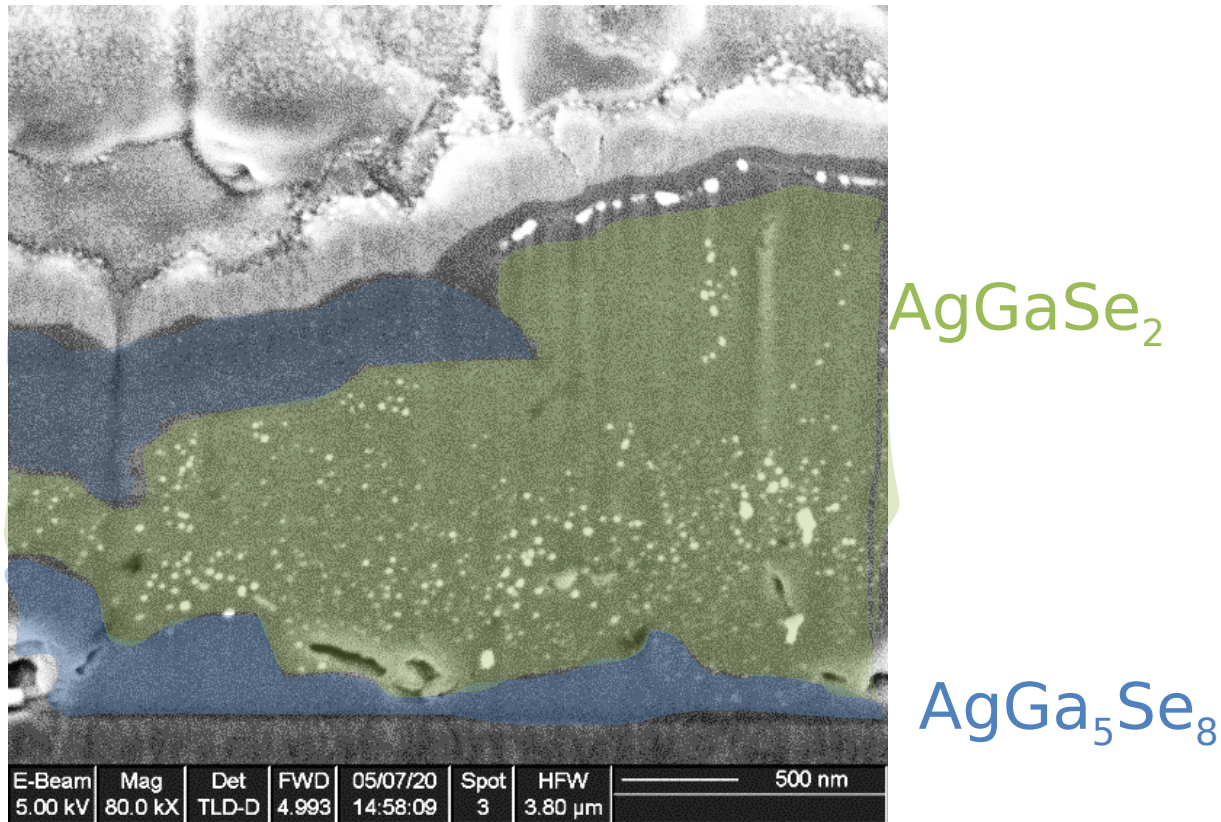


1-stage: AgGa₅Se₈ located in spots and extend through film

AgGa₅Se₈ distribution in 3-stage device



AgGa₅Se₈ distribution in 3-stage device



3-stage: AgGa₅Se₈ located front and back surface



Summary

- Narrow single phase region ($0.9 < [\text{Ag}]/[\text{Ga}] < 1$)
- Phases identifiable in XRD, (Raman)
- Presence of Ag_9GaSe_6 ($E_g = 0.6$ eV) detrimental
- Device may work with inclusions of AgGa_5Se_8 ($E_g = 2.11$ eV), but distribution of phase important



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Acknowledgements

