Monocrystalline CdSe for Si-based tandem applications: its potential and challenges

Yong-Hang Zhang[1]

Other Contributors: Zheng Ju,[2] Xin Qi,[1] Stephen Schaefer,[1] Martha McCartney,[2] David Smith,[2] Allison McMinn,[1] Andrew Chizmeshya,[3] and Sachit Grover[4]

[1]School of Electrical, Computer, and Energy Engineering,

[2]Department of Physics,

[3]School of Molecular Science,

Arizona State University, Tempe, AZ 85281, USA

[4]California Technology Center, First Solar Inc., Santa Clara, CA, 95050, USA

This work is supported by the NSF I/UCRC SPF2050 and First Solar Inc.

SPF2050

SOLAR POWERED FUTURE

NSF

First Solar.

ASU

MBE Optoelectronics Group

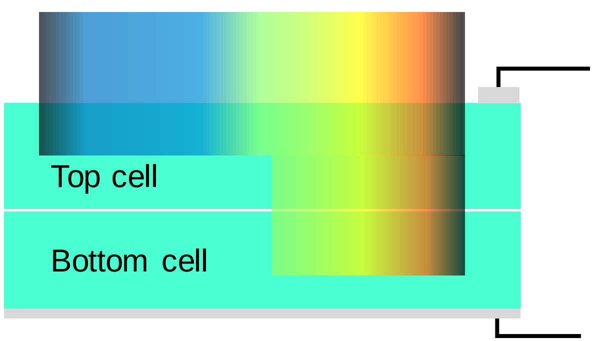
Motivation: CdSe/Si tandem solar cells

Overview:

- CdSe with a bandgap of 1.72 eV is ideal for Si based tandem cell.
- Theoretical power conversion efficiency of the tandem cell is ~40%.
- The predicted achievable tandem-cell efficiency may exceed 30% even with a minority carrier lifetimes as short as 1 ns in the CdSe cell

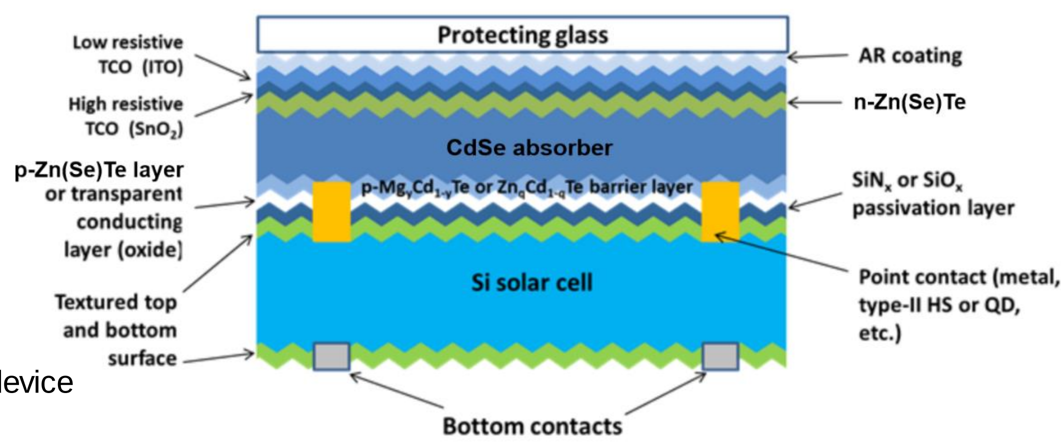
Goal:

Study MBE-grown CdSe double-heterostructures (DHs) and its potnetial application in solar cells.



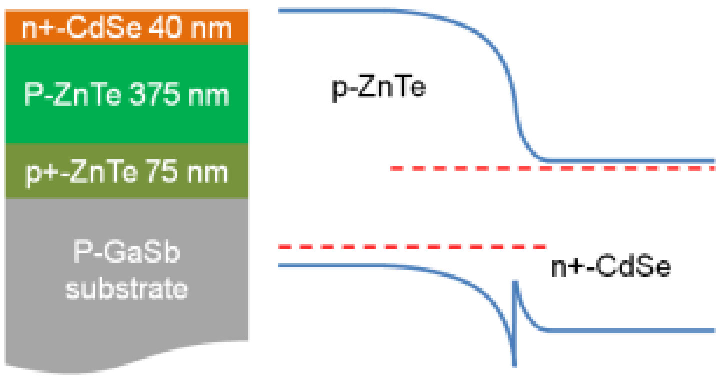
Schematic of a two-junction 1.7 eV/ 1.1 eV tandem device

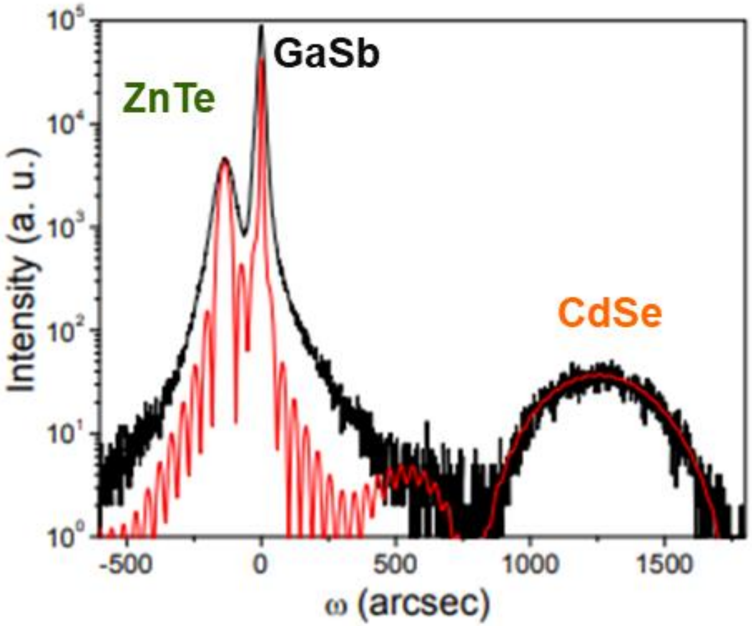
CdSe/Si tandem cell concept

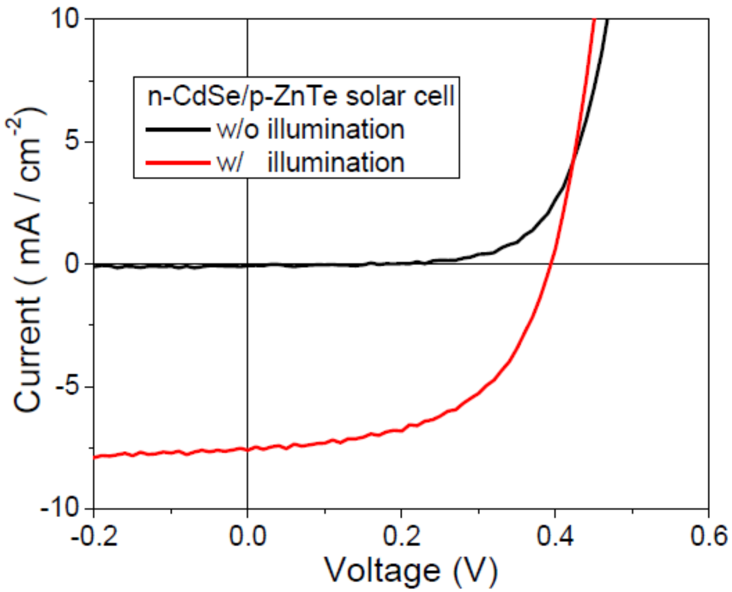


Our previous work on CdSe thin films

- Most existing research focuses on poly CdSe using non-epitaxial methods: closed-space sublimation, thermal evaporation, electrodeposition
- We demonstration of single-crystal CdSe for n^+-CdSe/p-ZnTe solar cells in 2009.

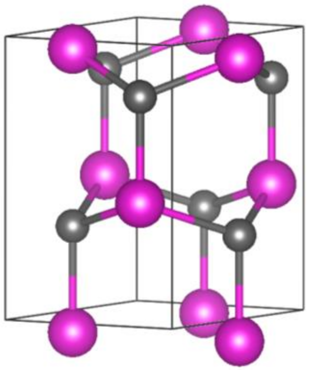




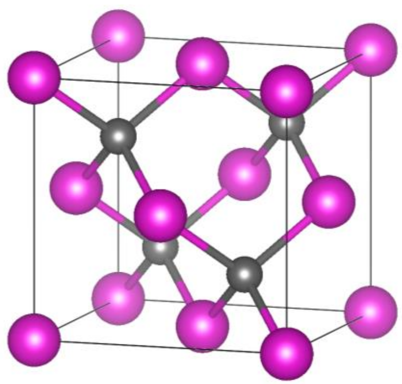


Our previous work: S. Wang *et al*, "CdSe/ZnTe Heterojunction Solar Cells Grown on GaSb", PVSC 2009.

Phases of CdSe



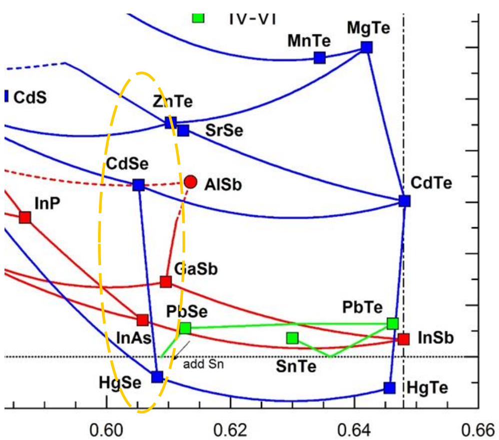
Wurtzite (WZ)
E_g = 1.72 eV
a = 4.299 Å
c = 7.015 Å



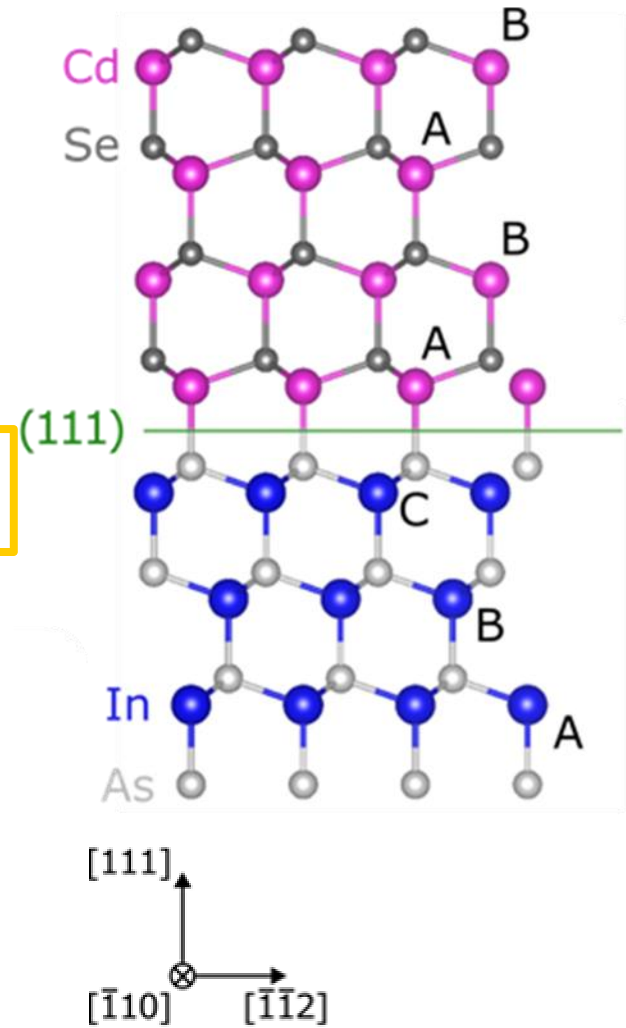
Zincblende (ZB)
E_g = 1.67 eV
a_0 = 6.050 Å

- CdSe mainly has two phases: zincblende, wurtzite.
- Wurtzite is the most stable phase at room temperature
- Our DFT calculations shows that formation energies for ZB and WZ phases differ by only **3.4 meV/atom**

Can we grow single-crystal wurtzite CdSe in ZB InAs substrates!



Our approach: Use InAs (111) substrates

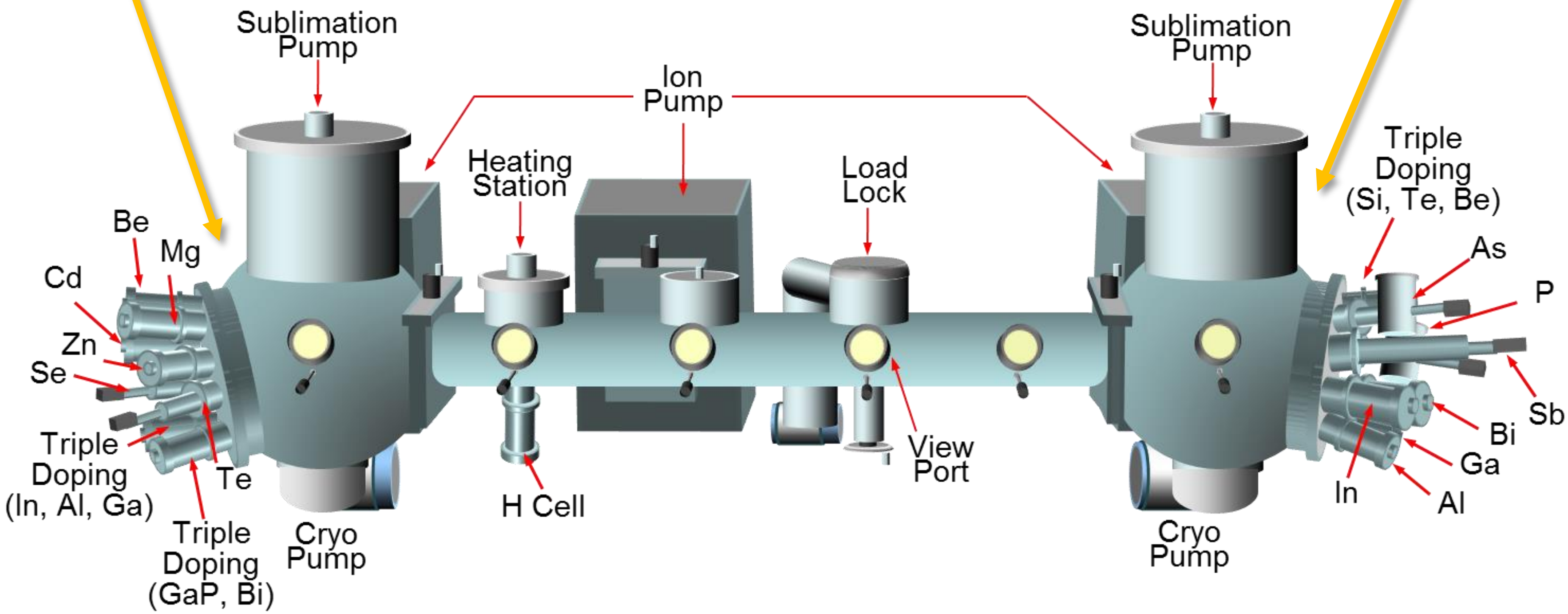


Dual-chamber MBE system for III-V/II-VI growth

Dual MBE chambers for growth of II-VI and III-V materials

II-VI thin film overgrowth

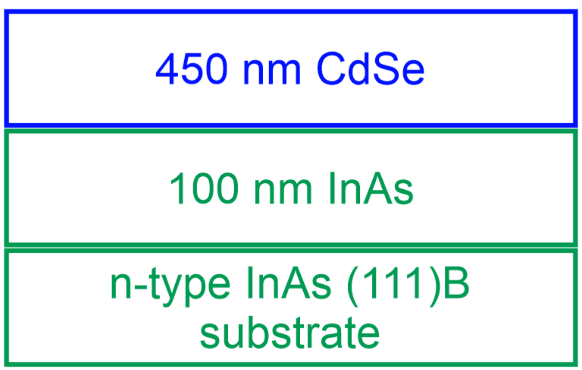
Substrate oxide removal and InAs buffer growth



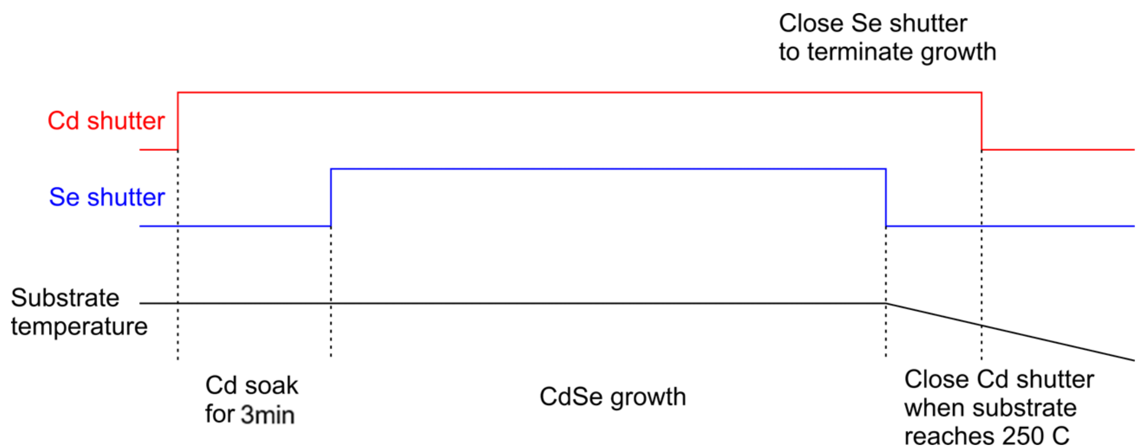
MBE growth of CdSe thin films

- CdSe thin films grown on InAs (100), (111)A, and (111)B substrates
- 100 nm InAs (111) buffer growth proceeds at 500 ^{o}C, ~0.5 ML/s, As/In = 40
- CdSe growth temperature 250 - 350 ^{o}C calibrated by optical pyrometer
- 3min Cd or Se soak employed to prepare heterointerface in either Cd- or Se-rich initial condition
- Cd/Se flux ratios range from 0.72(Se-rich) to 6.73(Cd-rich), typical CdSe growth rate ~0.8 ML/s

Typical sample structure

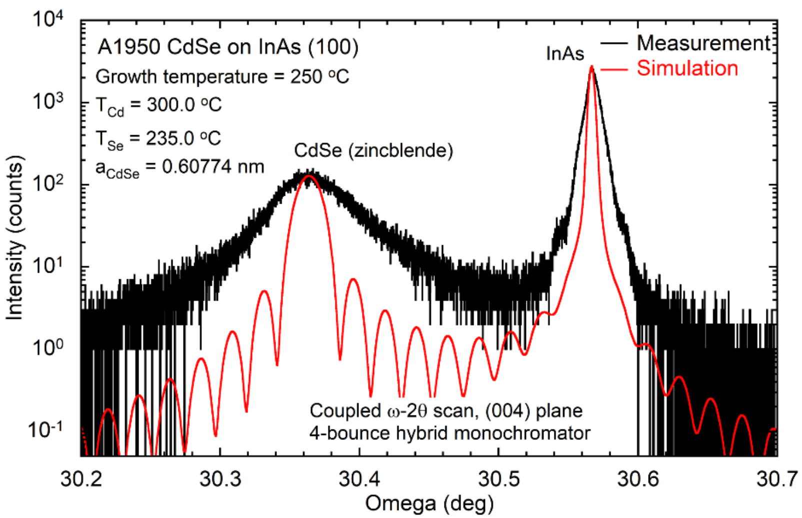


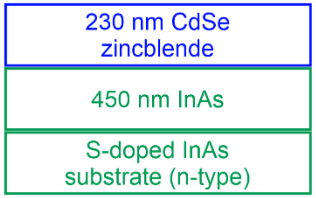
Shutter operation sequence for Cd soak

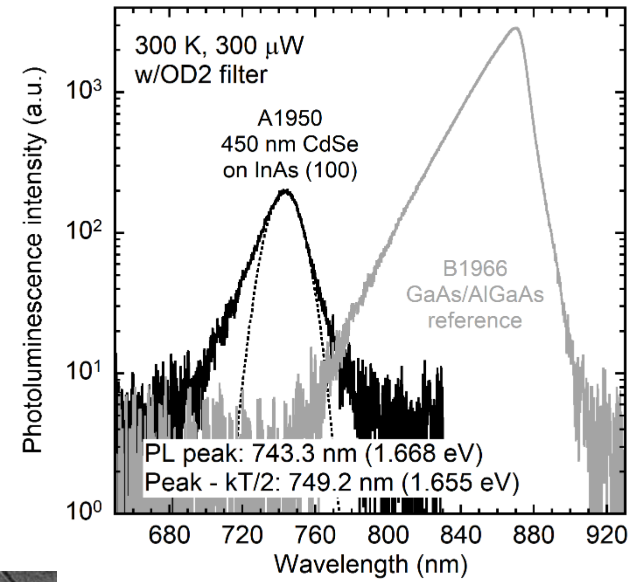


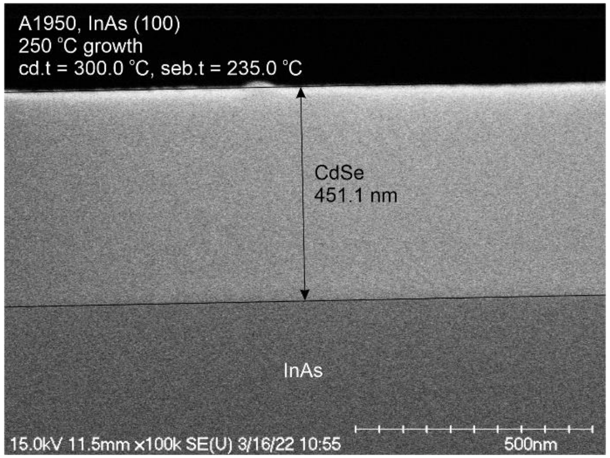
Zincblende CdSe on InAs(100)

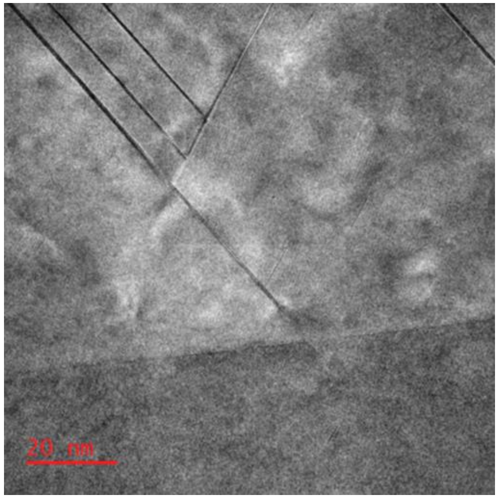
450 nm thick single-crystal zincblende (cubic) CdSe film grown on InAs (100) at 250 ºC, 0.82 ML/s, Cd/Se flux ratio of 1.35

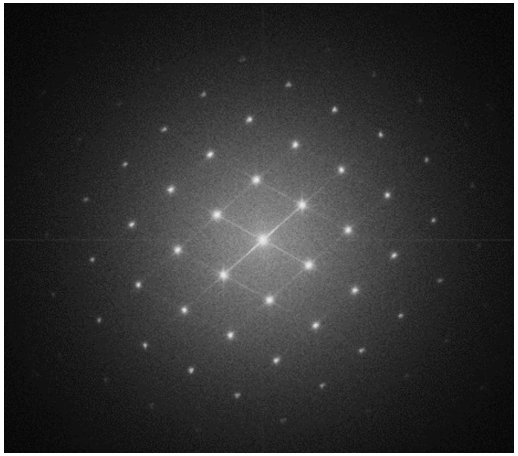




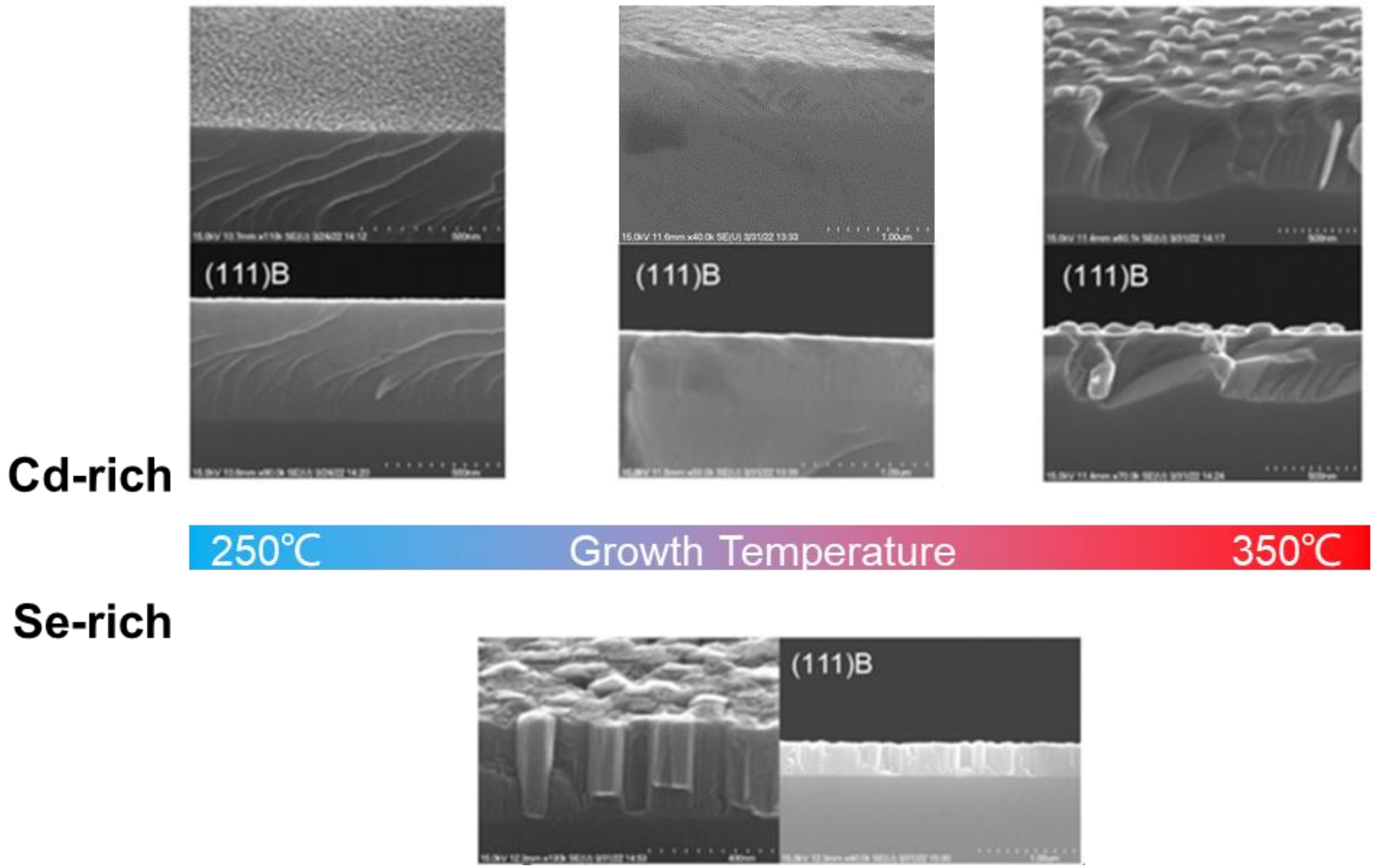






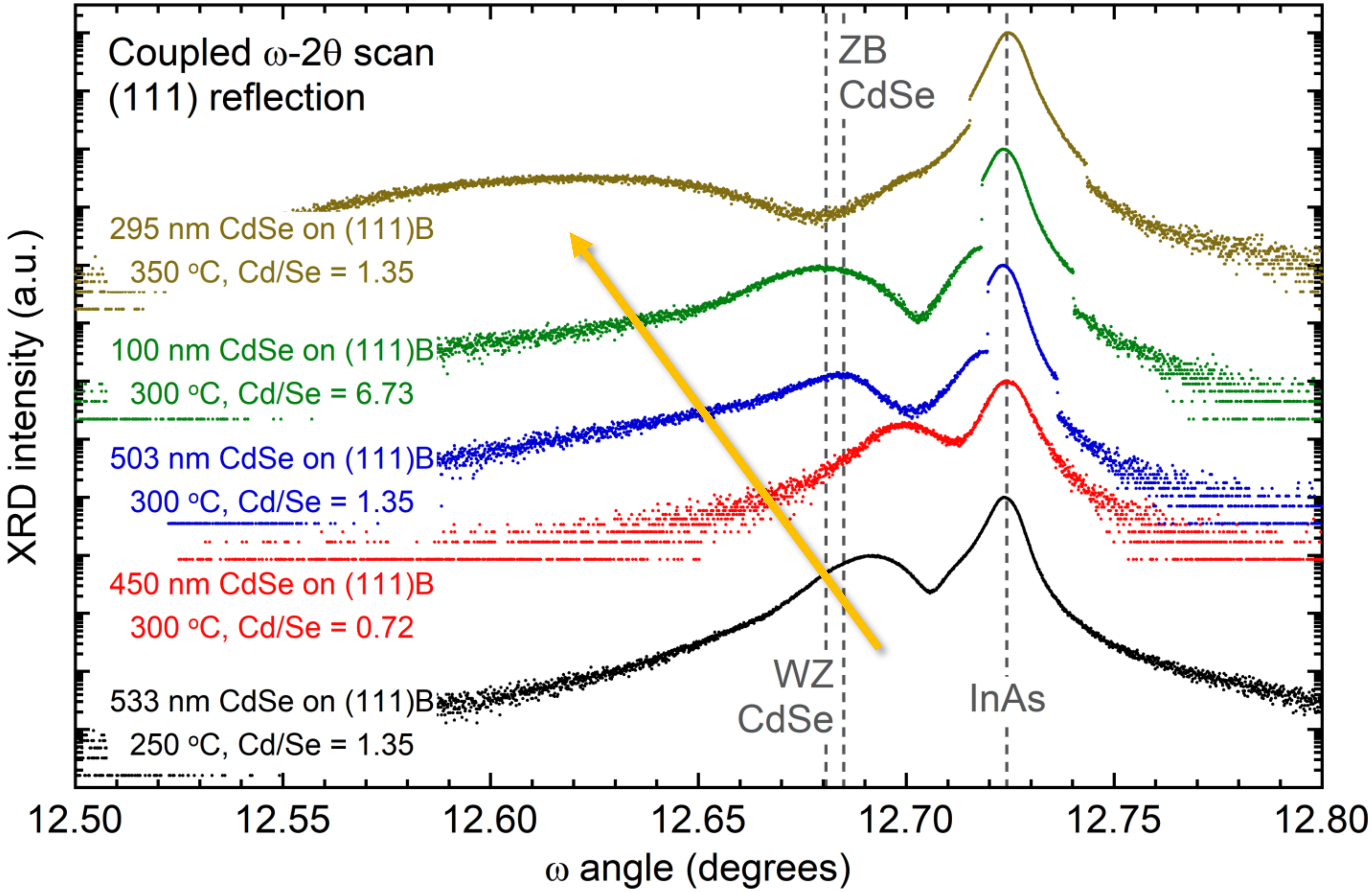


SEM cross-sectional images of the MBE layers



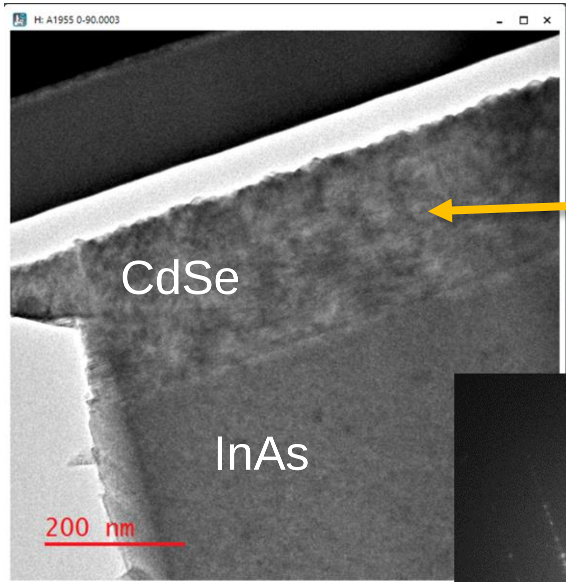
- Cd-rich growth yields highly oriented crystalline films and Se-rich growth yields polycrystalline films with nano columns ~10-100 nm
- Surface roughness increases with growth temperature and nano crystals appear on surface of 350 ℃ grown sample

X-ray diffraction

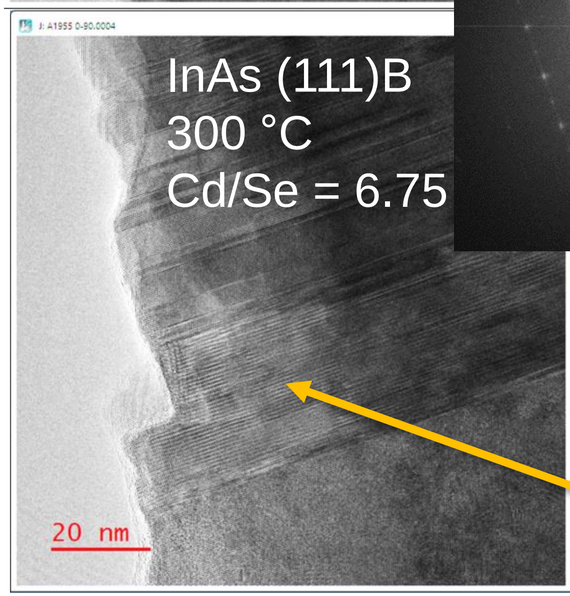


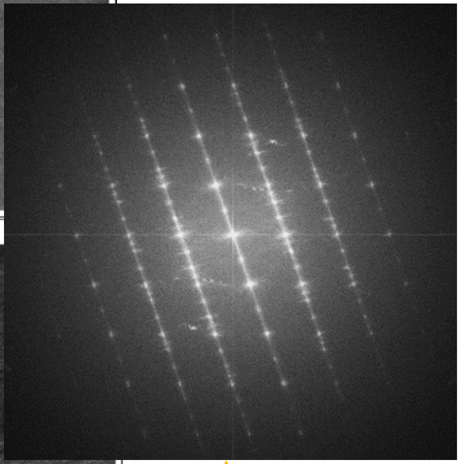
- Single crystal layer peaks have been observed.
- The ZB strained CdSe (111) peak nearly **overlaps** with WZ CdSe (0002) XRD peak
- Increased XRD FWHM correlates with film roughness/polycrystallinity in SEM images

TEM images

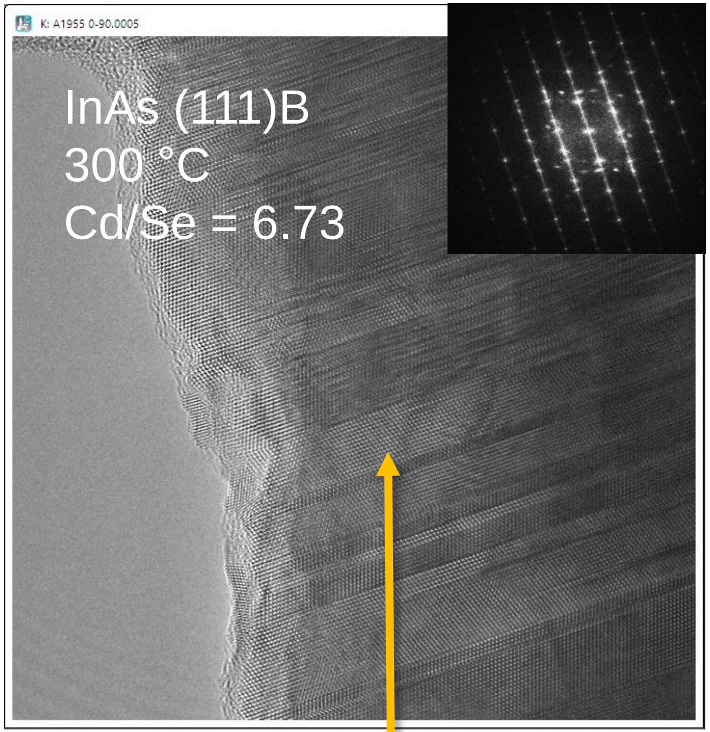


Numerous basal plane stacking faults observed and the CdSe layer is defective





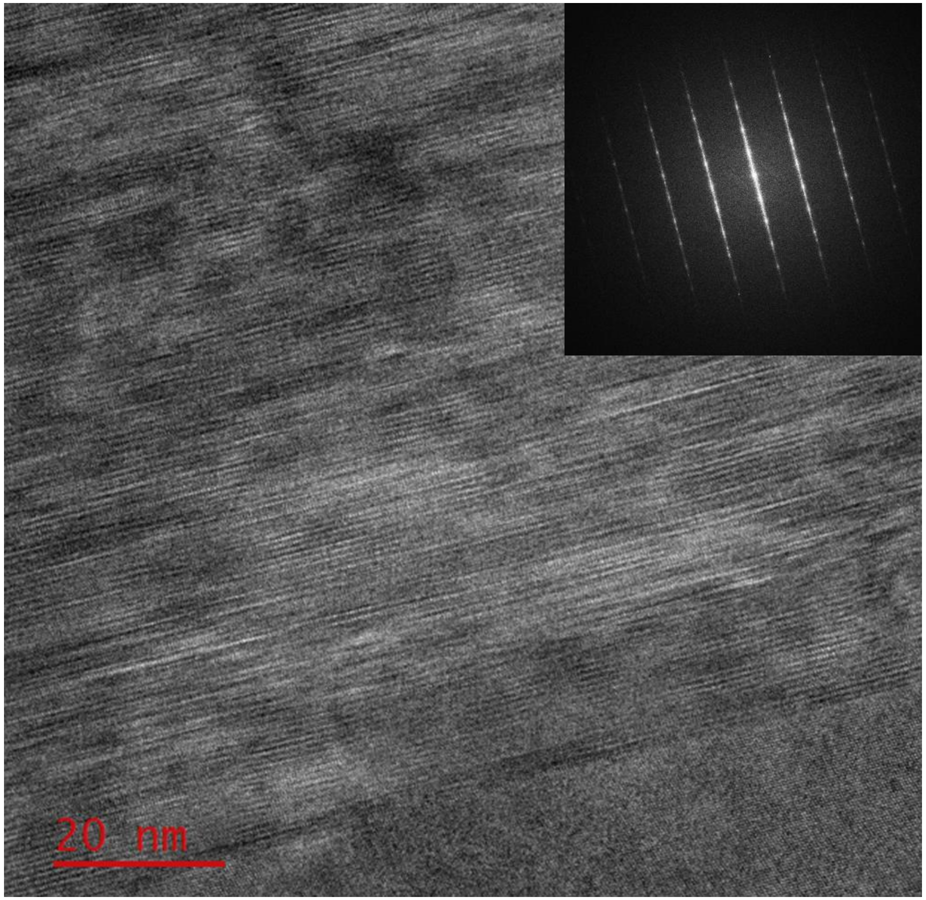
Mostly WZ but patches of ZB and considerable stacking disorder. Mixed-phase growth is confirmed

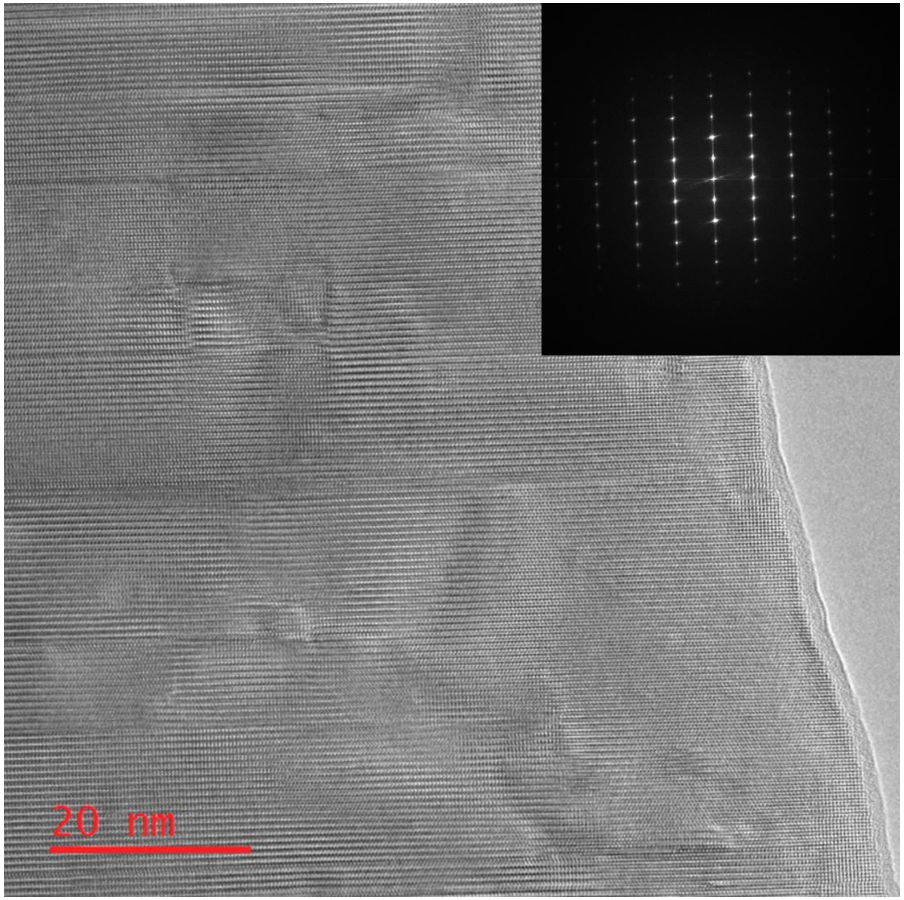


[110] projection – Lots of twins in FFT and stacking faults. ZB and WZ layers are distinguished.

Improved crystalline quality with annealing

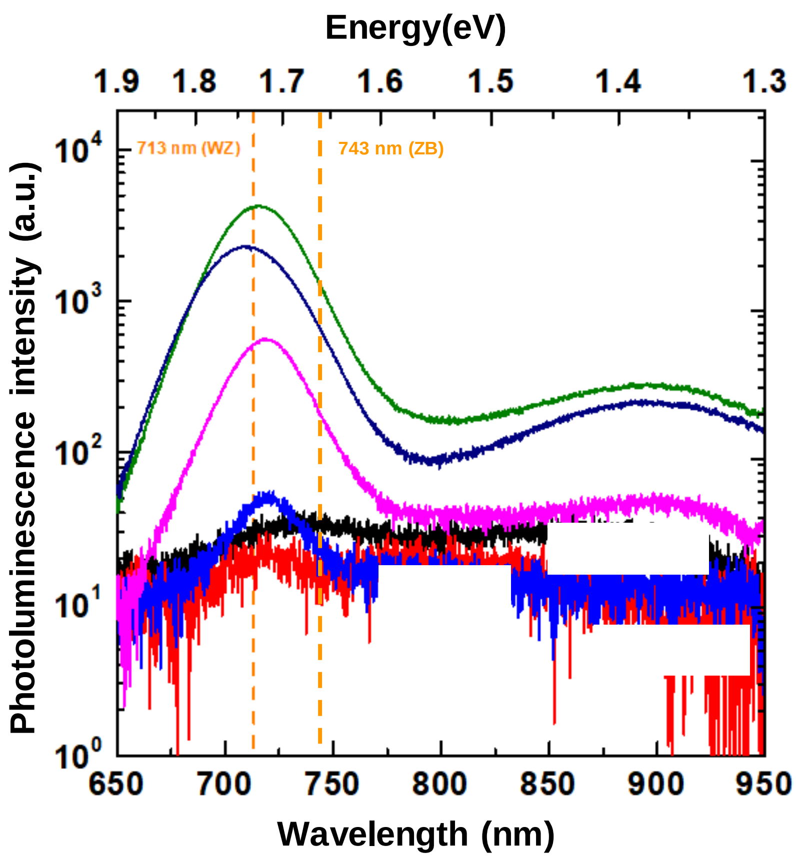
MBE as-grown CdSe → Annealed CdSe

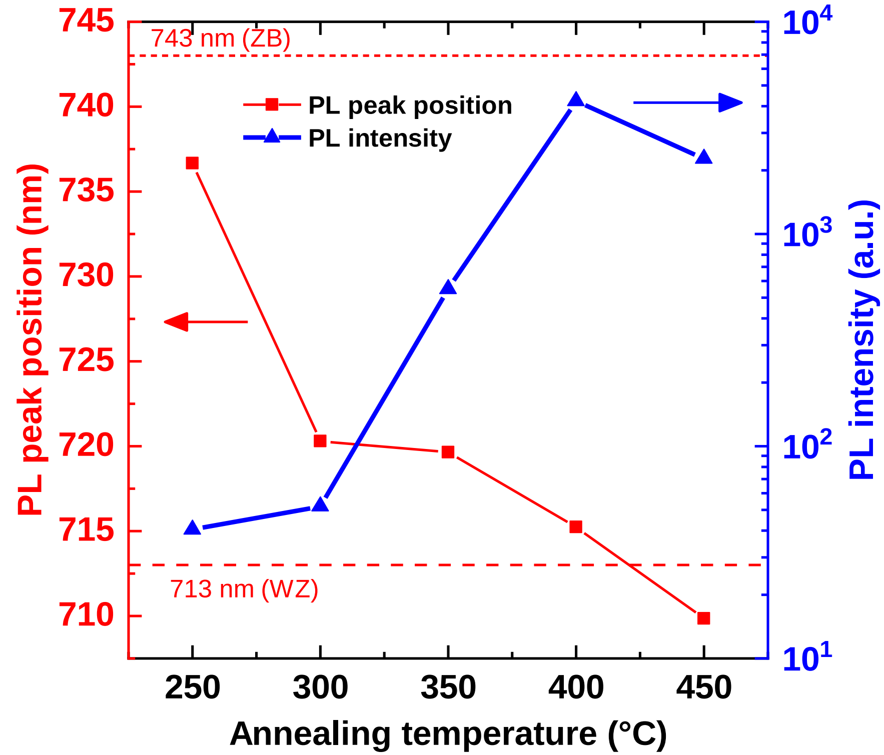




- 300 – 450 °C annealing on samples with a SiN_x cap at for 5 minutes under ambient N_2
- High-resolution TEM and corresponding FFT confirm WZ structure for post-annealing sample

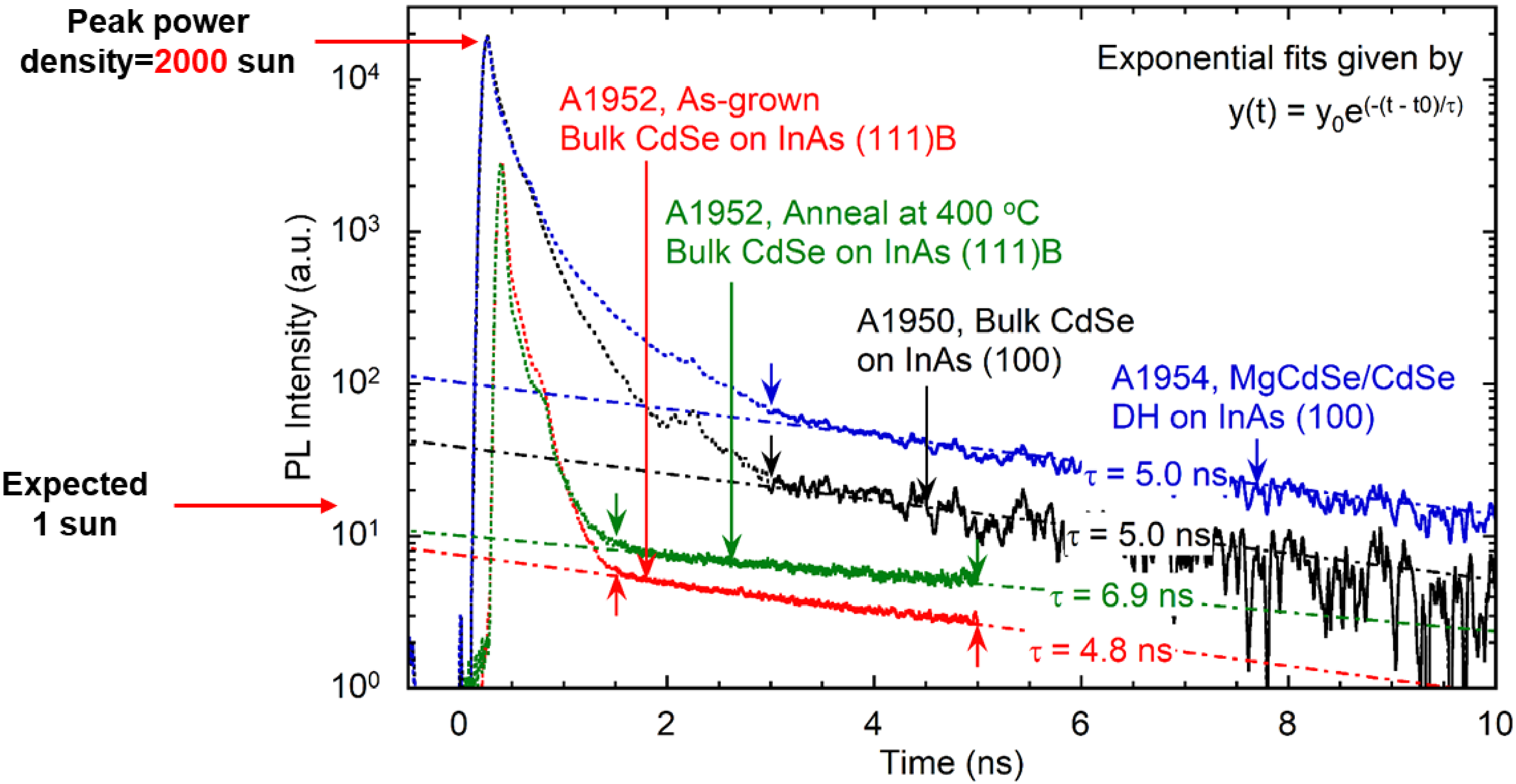
Steady-state photoluminescence





- ~530 nm CdSe on InAs (111)B, grown at 250 °C, Cd/Se flux ratio = 1.35
- **PL intensity maximized with 400 °C anneal**

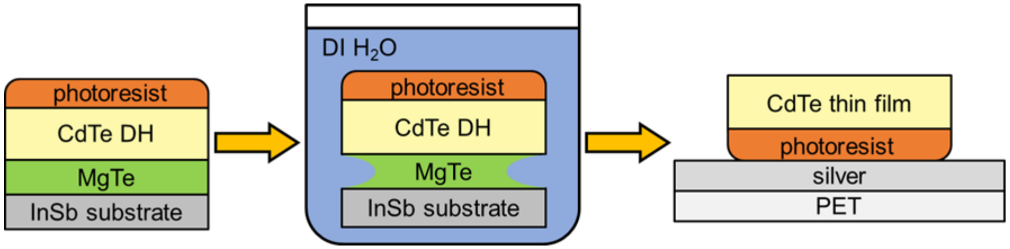
Time-resolved photoluminescence

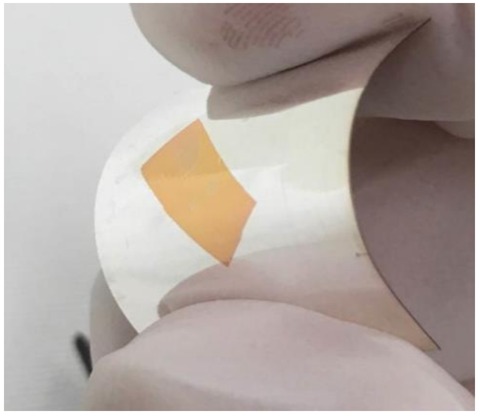


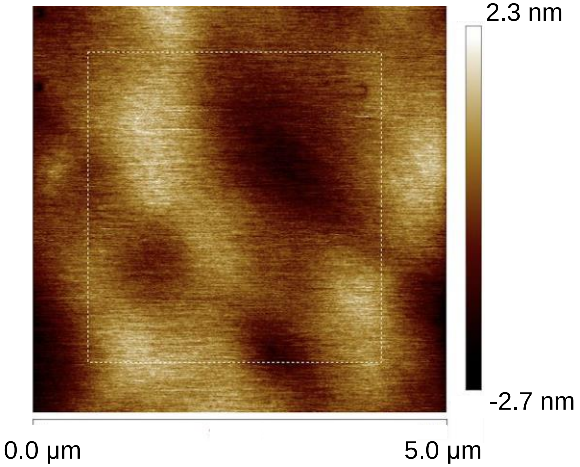
TRPL measurements have demonstrated single exponential decay under 1 sun condition

Epitaxial Lift-off of CdTe/MgCdTe DH Thin Films

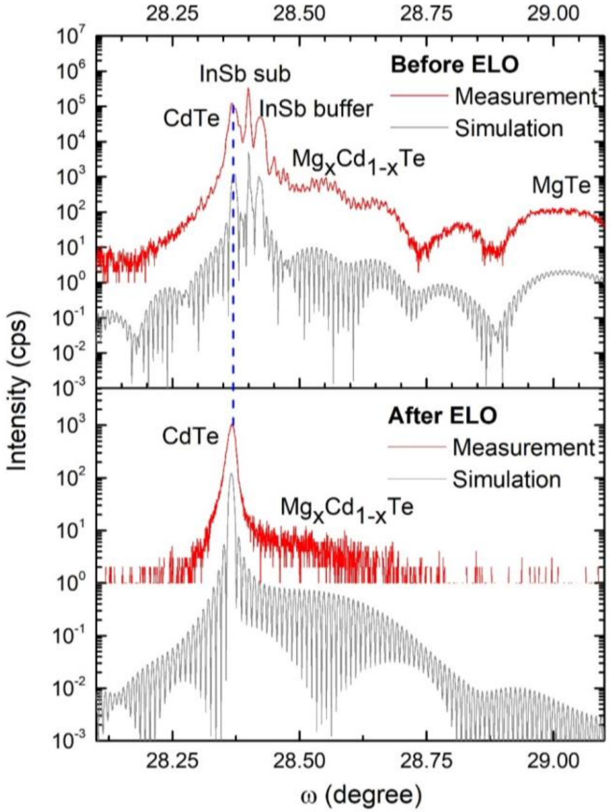
Thin film: better performance, light weight, low cost, II-VI/silicon tandem configuration







RMS roughness: 0.67 nm



J. Ding, C.-Y. Tsai, Z. Ju, and Y.-H. Zhang. *Appl. Phys. Lett.* **118**, 181101 (2021) (Editor's pick and a features article).

Water-soluble lift-off technology for CdTe solar cells

Contributors: Xin Qi[1], Jia Ding[1], Zheng Ju[2], Stephen Schaefer[1], and Yong-Hang Zhang[1]

[1]School of Electrical, Computer, and Energy Engineering,

[2]Department of Physics,

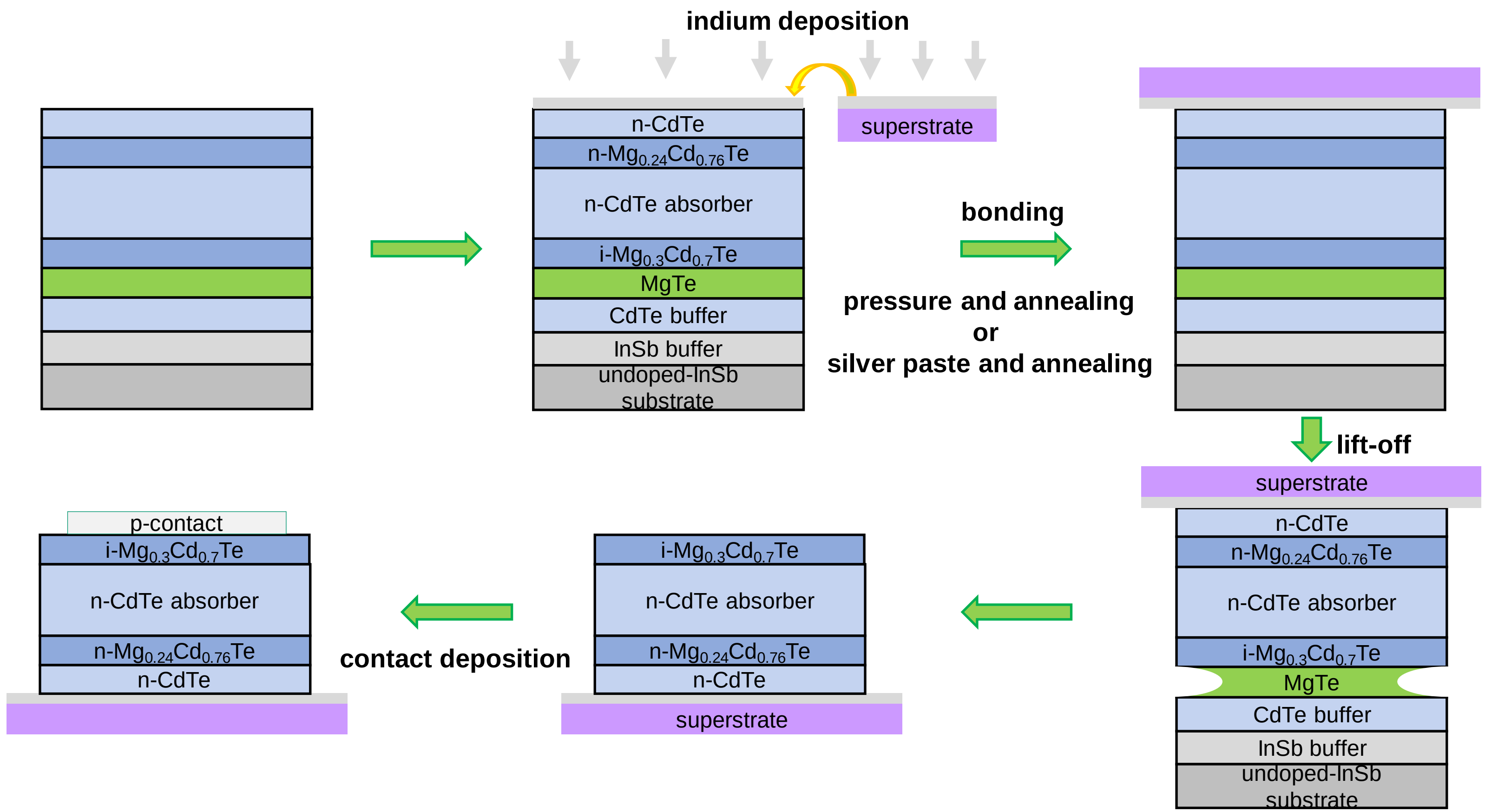
Arizona State University, Tempe, AZ 85281, USA

[4]California Technology Center, First Solar Inc., Santa Clara, CA, 95050, USA

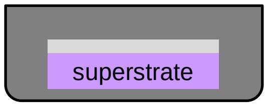
This work was partially supported by AFRL and ASU.

The goal is to demonstrate ultra-thin Cd(Se)Te, and possibly CdSe, solar cells with record performance.

ELO Process for Device Fabrication

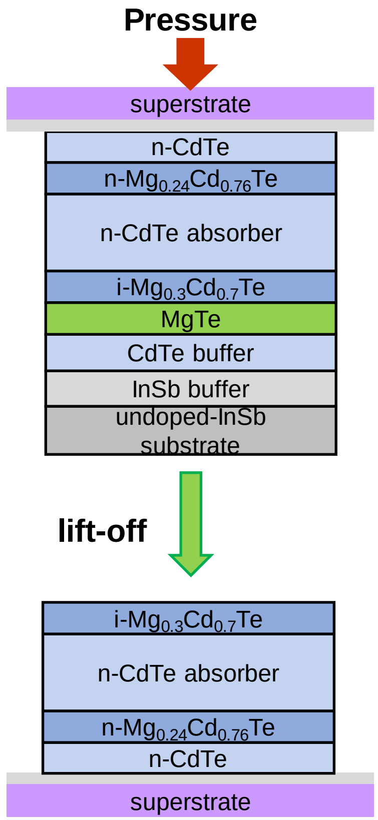


Thin films after ELO

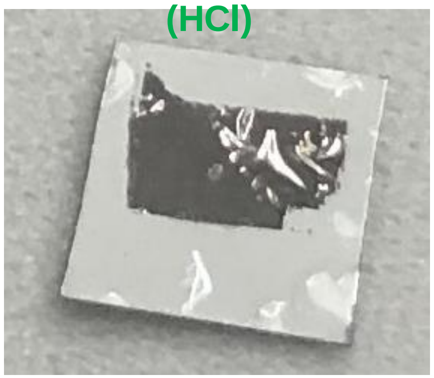


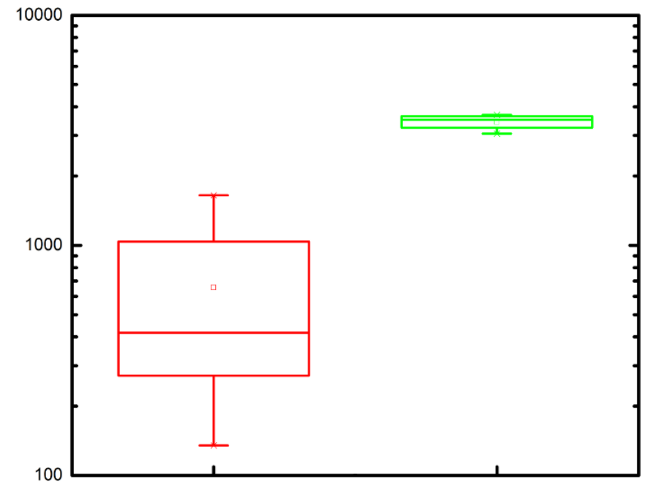
bonding

Dip in HCl



polyimide / indium (HCl)



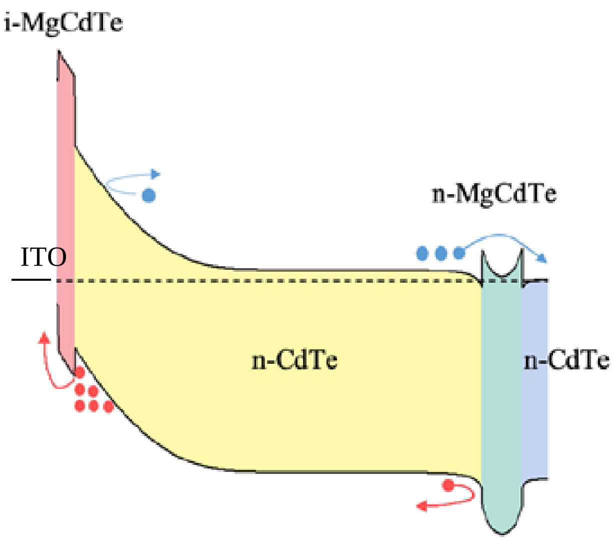


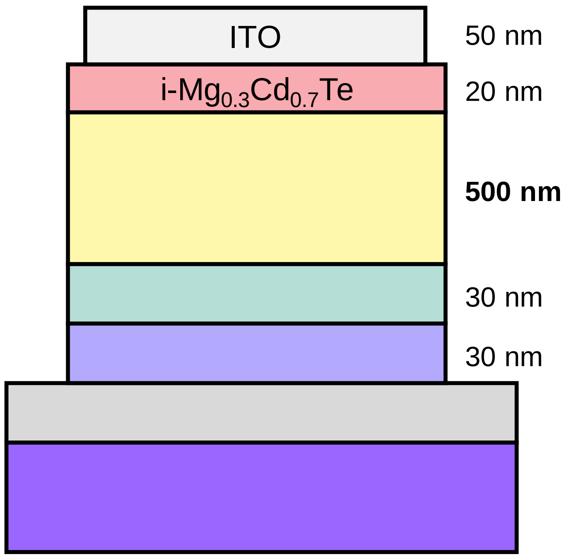
polyimide / indium

polyimide / indium (HCl)

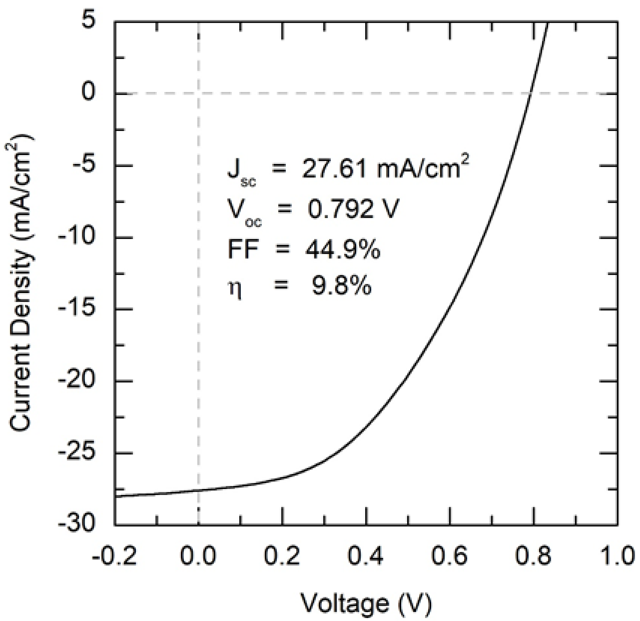
Xin Qi, Jia Ding, Zheng Ju, Stephen Schaefer, Yong-Hang Zhang, IEEE PVSC, 2022.

ELO CdTe/MgCdTe DH Solar Cell





polyimide / indium



Flexible Monocrystalline CdTe/MgCdTe DH thin-film solar cell.

Xin Qi, Jia Ding, Zheng Ju, Stephen Schaefer, Yong-Hang Zhang, IEEE PVSC, 2022.

Summary

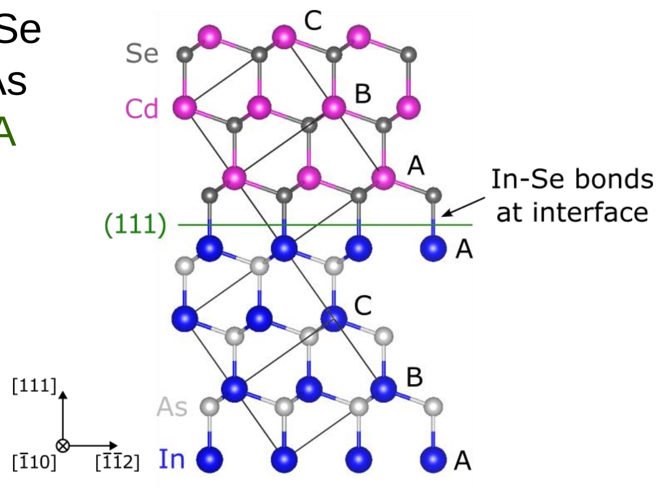
- MBE growths of CdSe at 250 – 350 ^{o}C with Cd/Se flux ratios from 0.72 – 6.73 are demonstrated
- Zincblende CdSe on InAs(100) is achieved with excellent crystallinity
- CdSe grown on InAs (111) has mixed wurtzite and zincblende phases
- PL spectra confirm that ZB layer emits at 743 nm and WZ at 713 nm.
- Structural defects limit the PL quantum efficiency and carrier lifetime.
- Annealing coverts most ZB phase into WZ phase at elevated temperatures

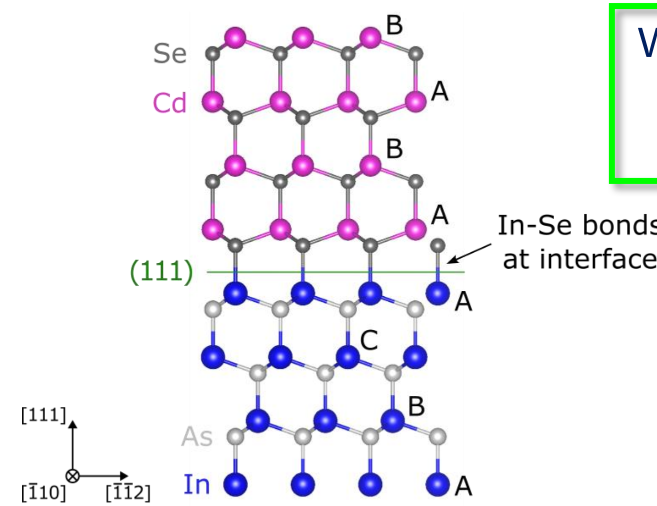
Acknowledgement

This work is supported by the NSF I/UCRC SPF2050 and First Solar Inc.

Our approach: CdSe on polar InAs (111) plane

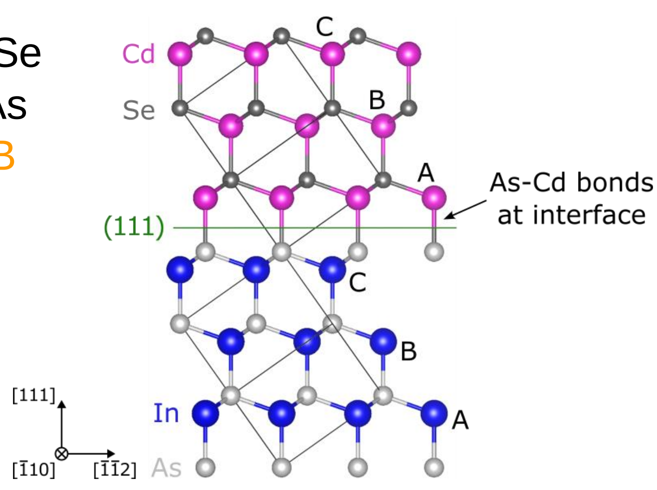
ZB CdSe on InAs (111)A

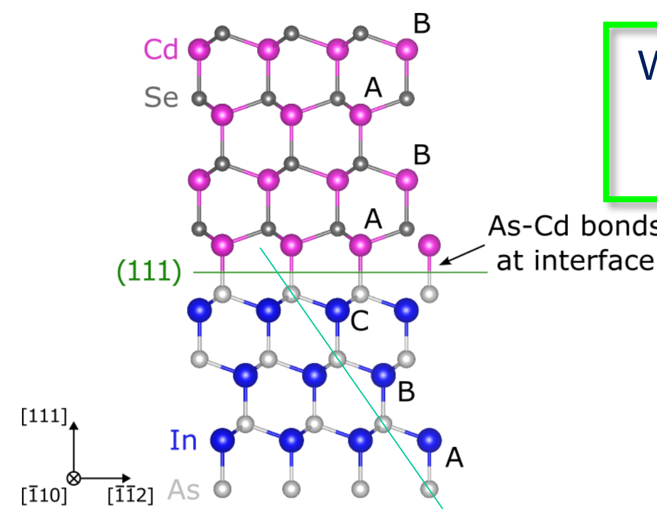




WZ CdSe on InAs (111)A

ZB CdSe on InAs (111)B





WZ CdSe on InAs (111)B

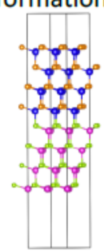
DFT simulation of CdSe/InAs interface

SLAB Calculations (PAW-LDA):

Ref SLABS	kpts	E (eV)	ΔE (eV)	AVG Cd-Se (Å)	AVG In-As (Å)	AVG Cd-As (Å)	AVG In-Se (Å)	AVG Se-As (Å)	AVG Cd-In (Å)
CdSe-111	2x2x1	-208.37108		--	--	--	--	--	--
ENCUT = 450 eV	4x4x2	**-208.19186**		**2.603±0.038**	--	--	--	--	--
InAs-111	2x2x1	-279.46809		--	--	--	--	--	--
ENCUT = 450 eV	4x4x2	**-278.94932**		--	**2.610±0.017**	--	--	--	--
Ref AVGS	**4x4x2**	**-243.57059**		**2.607**					
CdSe-InAs	2x2x1	-243.40899	+0.511	2.604±0.031	2.609±0.035	--	2.666	--	--
ENCUT = 450 eV	**4x4x2**	**-243.03879**	**+0.532**	**2.602±0.032**	**2.613±0.029**	--	**2.664**	--	--
CdSe-AsIn	2x2x1	-239.41214	+4.507	2.604±0.034	2.617±0.020	--	--	2.676	--
ENCUT = 450 eV	**4x4x2**	**-239.12875**	**+4.442**	**2.602±0.041**	**2.615±0.017**	--	--	**2.642**	--
SeCd-InAs	2x2x1	-240.99548	+2.924	2.608±0.025	2.606±0.026				2.770
ENCUT = 450 eV	**4x4x2**	**-240.67545**	**+2.895**	**2.608±0.025**	**2.611±0.016**				**2.767**
SeCd-AsIn	2x2x1	-243.42352	+0.496	2.609±0.016	2.611±0.032	2.605			
ENCUT = 450 eV	**4x4x2**	**-243.04843**	**+0.522**	**2.608±0.015**	**2.609±0.031**	**2.607**			

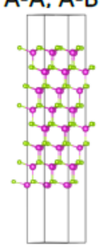
In this table the formation energy ΔE of A-A, A-B and B-B type interfaces is obtained by

ΔE =



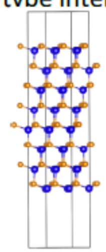
Interface CdSe-InAs is CdSe-B (bottom) InSe-A (top)

- ½



Pure CdSe

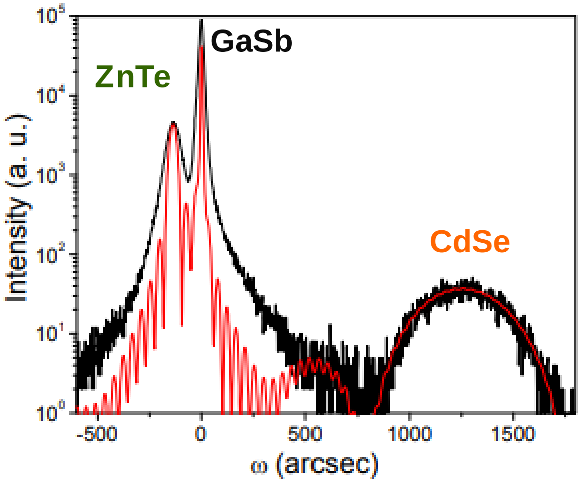
- ½

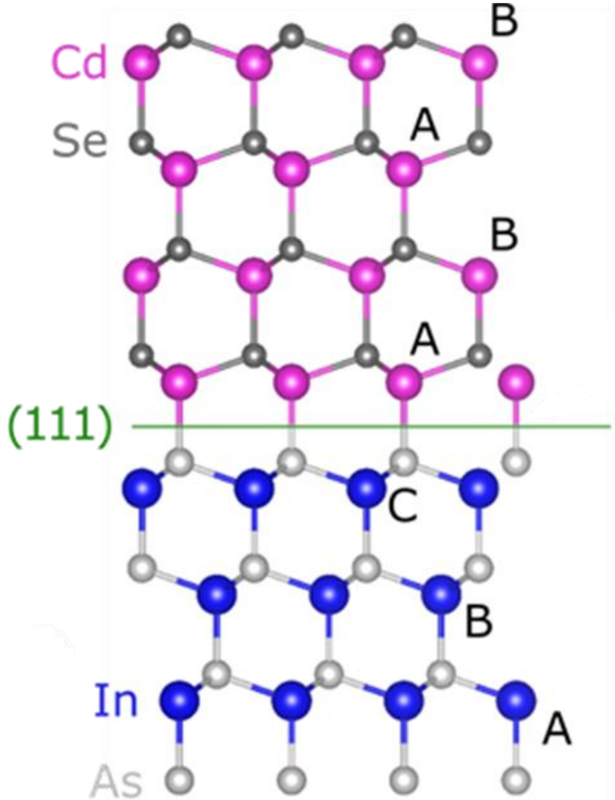


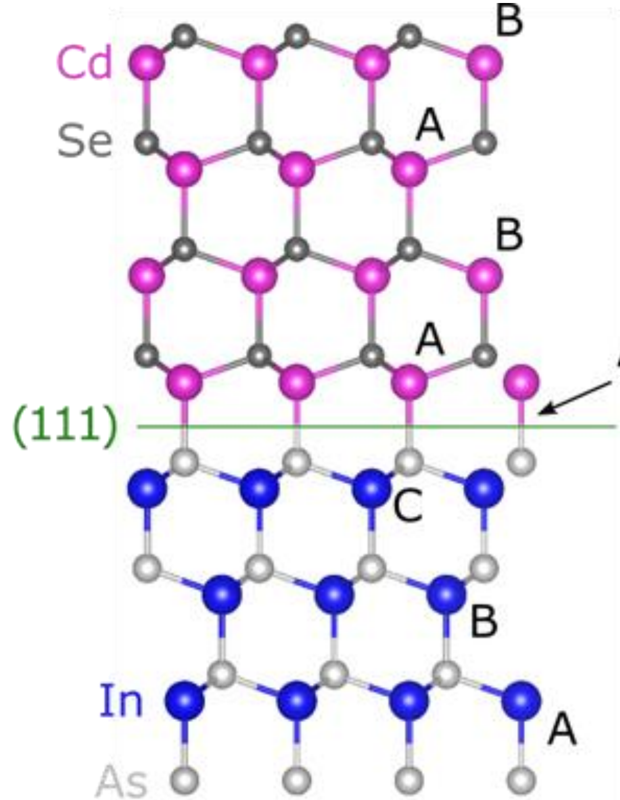
Pure InAs

Note: the formation energies obtained in this way contain the interface energy, and the energy associated with removing one free CdSe-B surface and one free InAs-A surface (see below for a description of a new method for obtaining these individual contributions

Based on the above the interfaces CdSe-A / InAs-B and CdSe-B / InAs-A <u>much more favorable</u> than CdSe-A/InAs-A or CdSe-B/InAs-B


GaSb
ZnTe
CdSe
Intensity (a. u.)
ω (arcsec)
-500
0
500
1000
1500


Cd
Se
B
A
B
A
(111)
C
B
In
As
A


Cd
Se
B
A
B
A
(111)
C
B
In
As
A