GeSn nano-structures for HEP applications

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Advantages of GeSn for HEP detectors

- **Strain engineering**
  - **Absorption** in NIR to MWIR vs Sn content
  - Band gap with **indirect to direct transition for** Sn of around 7% @ 2 µm emission in bulk
  - **High mobility** due to smaller effective mass

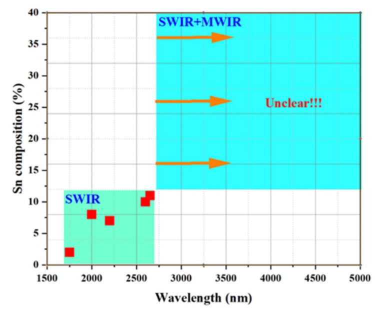
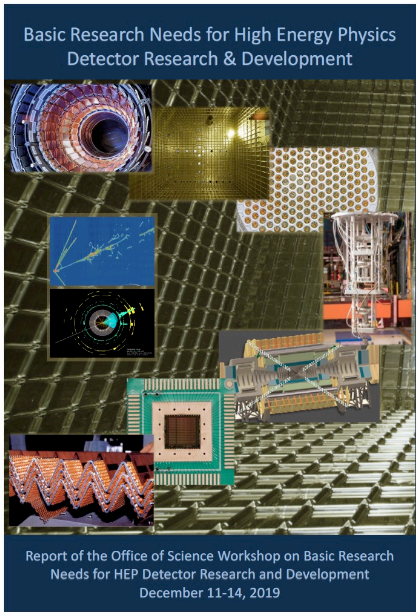


Figure 23. Sn content vs. cut-off wavelength of the GeSn PIN detector.



- **Applications to HEP Detectors**
  - Extend detectors response beyond 1.5 µm for Ge and 1 µm for Si
  - **Wavelength tuning** covering NIR to LWIR, i.e. 1 to 5 µm possible
  - **Multispectral devices demonstrated** i.e. working between 0.8 and 2 µm
  - **Reaching direct band gap** beyond Si/Ge or III-V devices that are difficult to integrate on Silicon
  - Monolithic integration with **metal-oxide-semiconductors (CMOS) technology**, i.e. lower manufacturing cost and easy adaptation

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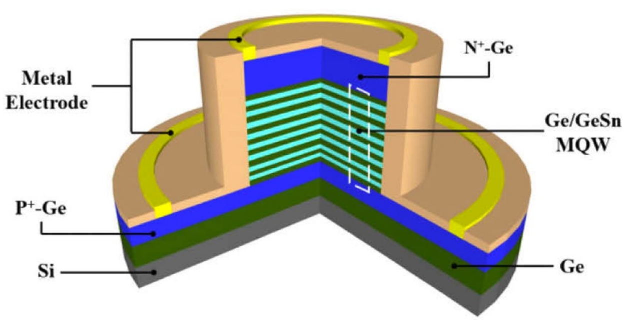
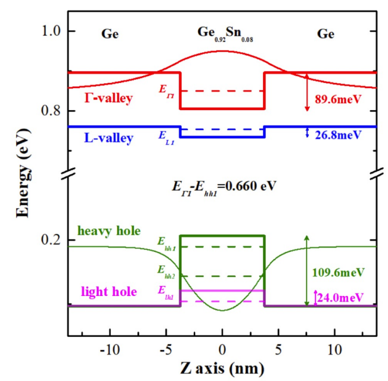
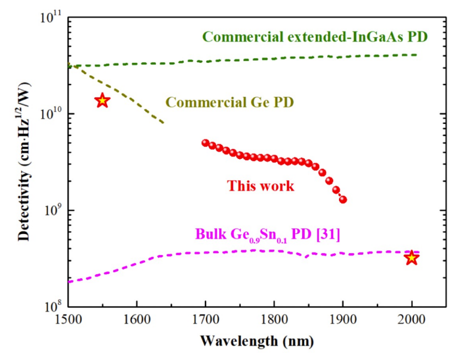
Recent progress

- Devices based on GeSn include **detectors, modulators and lasers**
- For higher Sn content, large lattice mismatch resulting in **misfit and threading dislocations** degrades device performance; i.e. leakage current, recombination centers etc.
- Using **nanostructures**
  - helps to **avoid strain relaxation**, similar to III-V alloys
  - Tune device parameters: absorption, mobility, energy band
- **Demonstrated example:** $Ge_{0.92}Sn_{0.08}$/Ge MQW *p-i-n* photo-detectors with high detectivity and low dark current based on the quantum confined Stark (QCSE) effect after *Zhou et al., Optics Express 28, 23 (2020)*





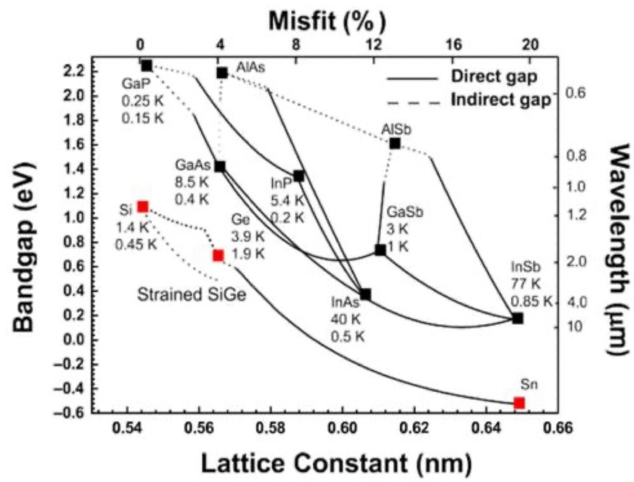


Growth considerations and challenges for GeSn

- **Lattice mismatch 16%**
- **Low Sn solubility** in $Ge_{1-x}Sn_x$ alloys
  - GeSn is eutectic alloy**,** thermal equilibrium solid solubility of Sn in the Ge matrix is as low as 1 at.% below 500℃ . Additionally, the eutectic temperature of Ge – Sn binary alloys is as low as 231.1℃.
- **Sn segregation** during the growth and post-processing is one of the problems associated with the formation of homogeneous $Ge_{1-x}Sn_x$ layers.

It strongly depends on substrate temperature

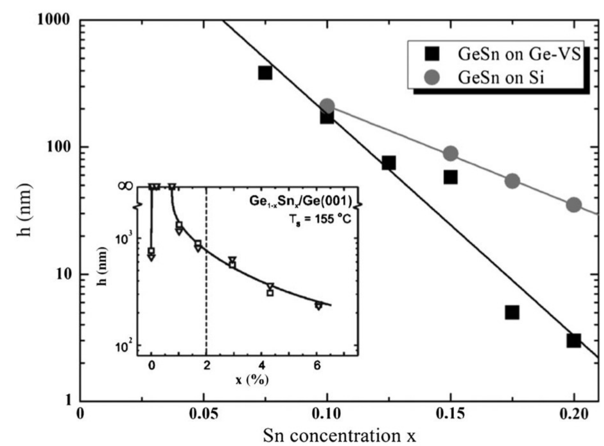
Lattice mismatch



Radamson et al., Nanomaterials (2022)

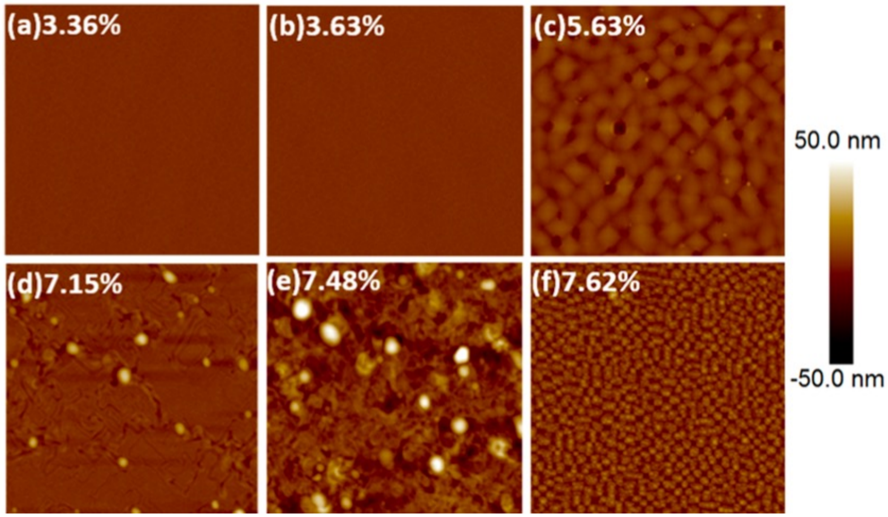
- For Sn content of 7% it is at 0.9%
  - Within moderate lattice mismatch with layer by layer growth for MBE
  - Critical thickness around 500 nm

- Lattice mismatch for Ge and Sn is 16%
  - Critical thickness below 1 ML



Arguirov et al., Photon Res 1,2 (2013)

Sn segregation

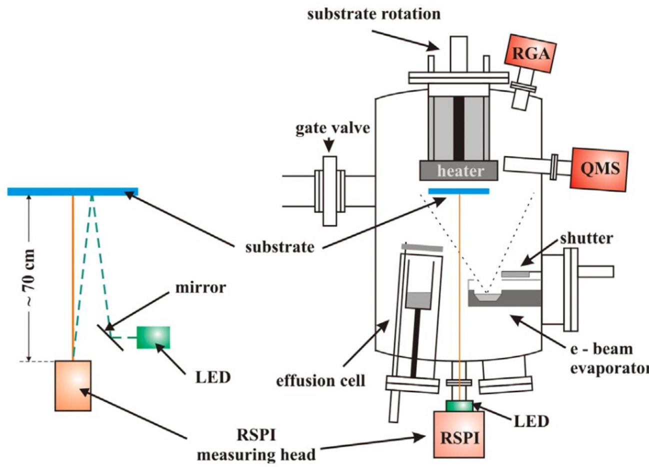


The Sn segregation can be clearly observed when the Sn concentration is above 7%. In FIG. 1. (d) and (e), Sn droplets are observed and become big with increasing Sn concentration. However, when the Sn concentration reaches 7.62%, the Sn droplets become much less, while the pyramids appear again

- Substrate temperature vs Sn-droplets formation
- In this study, GeSn thin films on Ge (001) with various Sn concentrations from 3.36 to 7.62% were grown by MBE.
- It is estimated that 7.62% Sn concentration could be the limitation at the growth temperature of 200 ℃

Solutions to MBE growth of GeSn

- To address segregation and low solubility use **Ultra-low temperature molecular beam epitaxy (MBE)**
  - Reported growth temperatures giving best results are at 160℃
  - At 200℃, surface segregation observed
- Growth on Si wafer with **Ge-VS** (virtual substrate)
- Reported **pseudo-morphic growth** for layer thicknesses between 260 to 30 nm
- No PL reported from these films



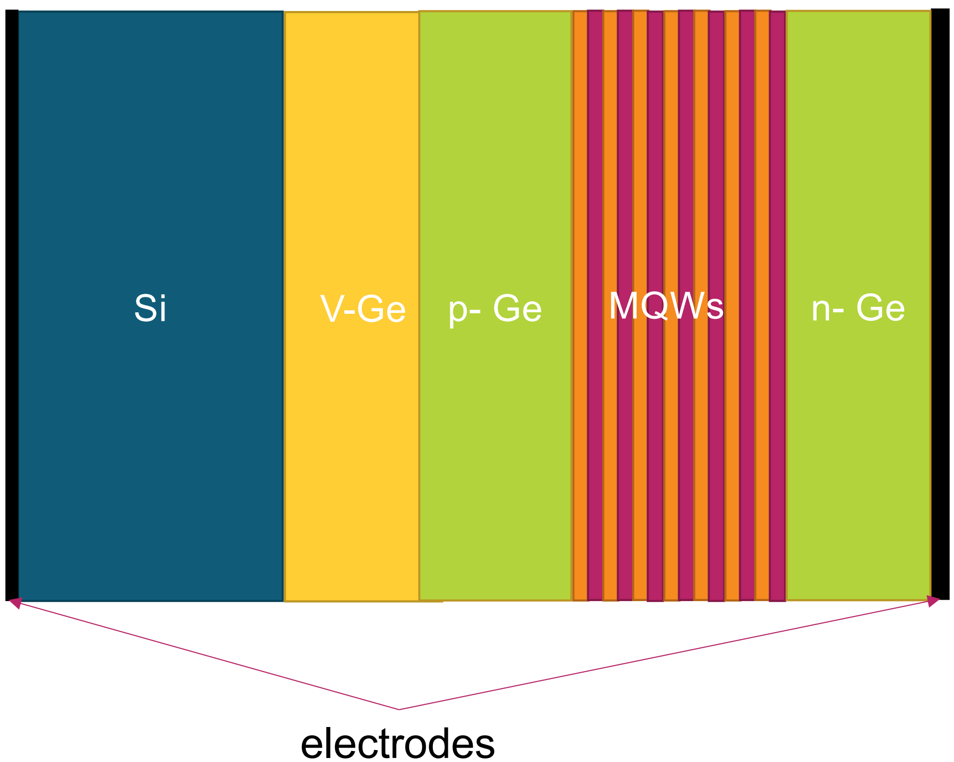
Growth chamber design

Table 2
Values of angular displacement for GeSn layers with different Sn contents and the corresponding tetragonal strain.

Sample	Sn content RBS	a_o [nm] (Vegard's law)	f [%] lattice mismatch with Ge	$\Delta\Theta_{theo}$ [deg] pseudomorph	$\Delta\Theta_{exp}$ [deg]	Tetragonal strain [%]
C	0.047	0.56966	0.69	−0.34	−0.30	1.0
D	0.06	0.57074	0.88	−0.44	−0.39	1.4
E	0.08	0.5724	1.18	−0.58	−0.53	1.9
F	0.11	0.5749	1.62	−0.80	−0.77	2.7
G	0.125	0.57614	1.84	−0.91	−0.93	3.2

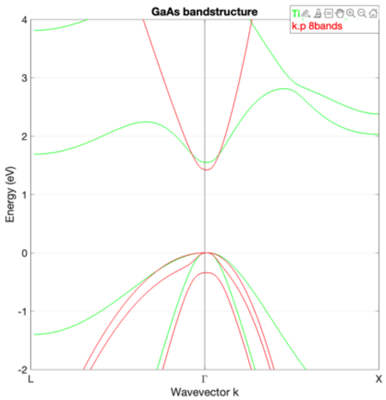
Buca et al., Journal of Crystal Growth 384, 71–76 (2013)

Device concept

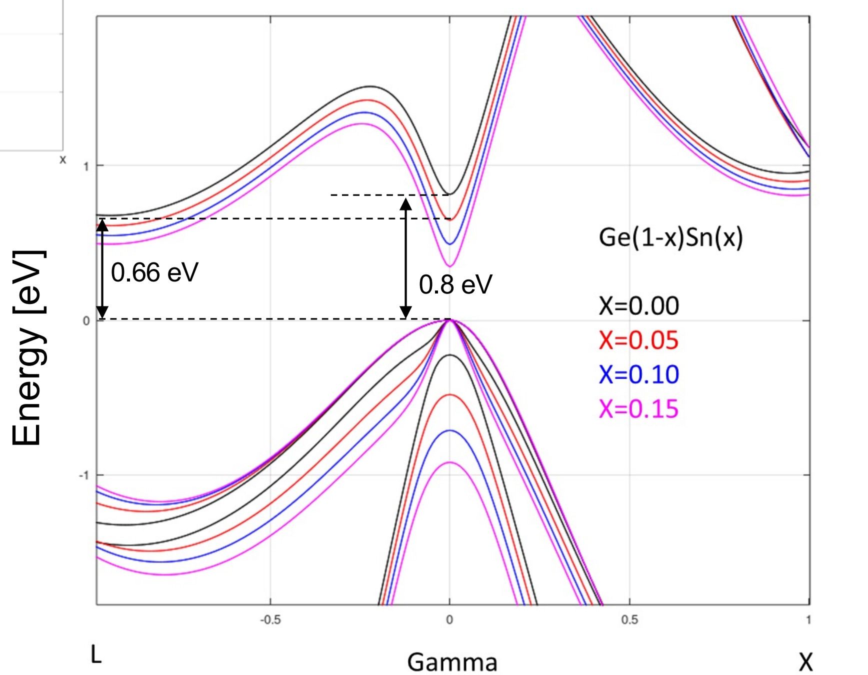


Band structure modelling results

Tight binding vs 8 k.p



GeSn 30 k.p model vs strain



- Band modelling using k.p perturbation method
- 8 k.p vs 30 k.p
  - 8 k.p model sufficient around Gamma point
  - 30 k.p reproduces bands better for higher wave-vectors
  - Consistent with Tight binding model
    - Some of the parameters are based on 'educated guesses' as data still lacking
    - Opportunity to fill these gap within this research

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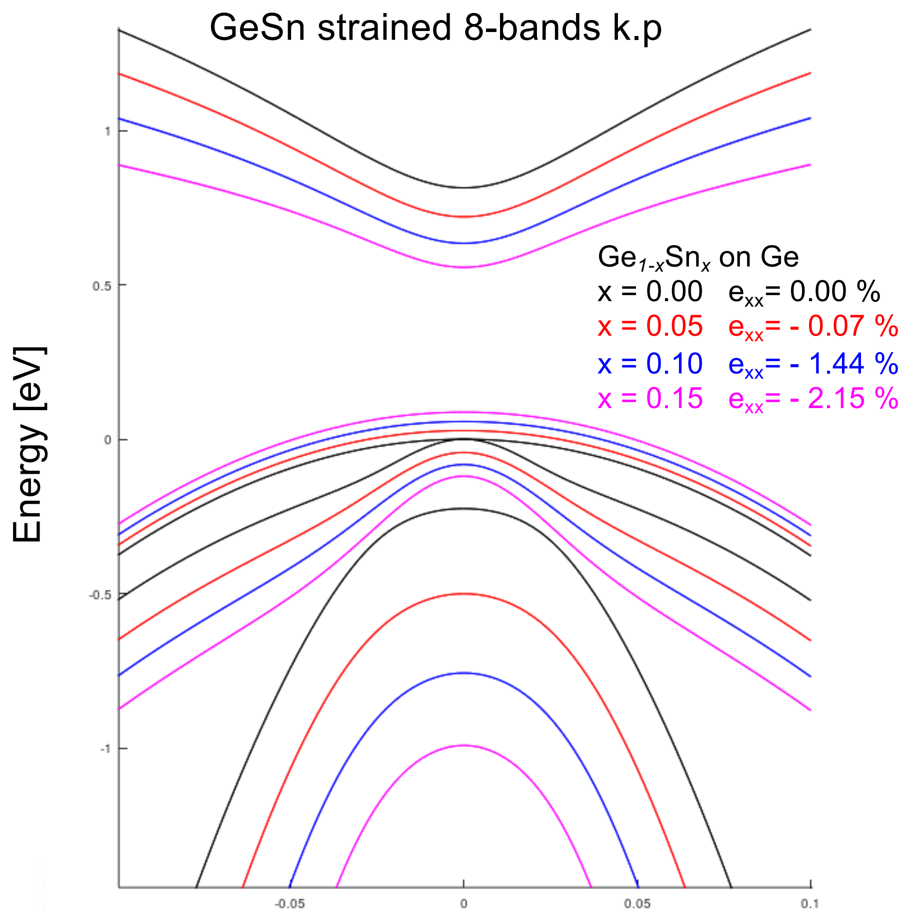
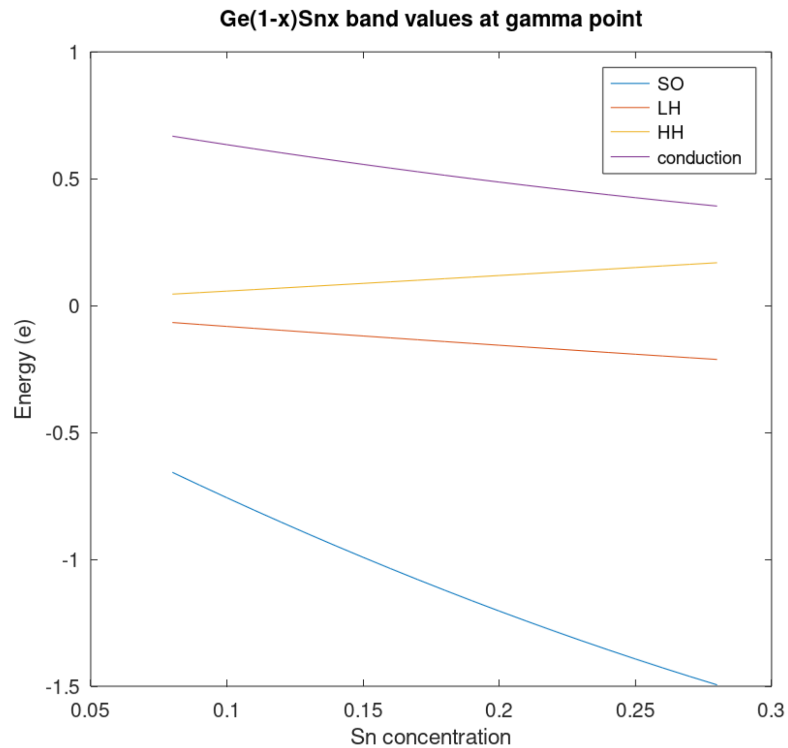
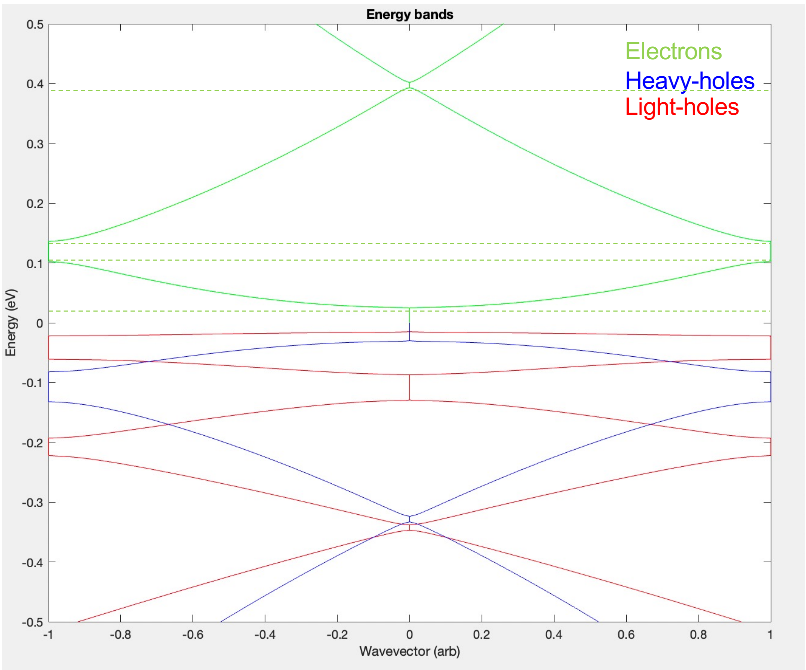
Band structure modelling GeSn including strain





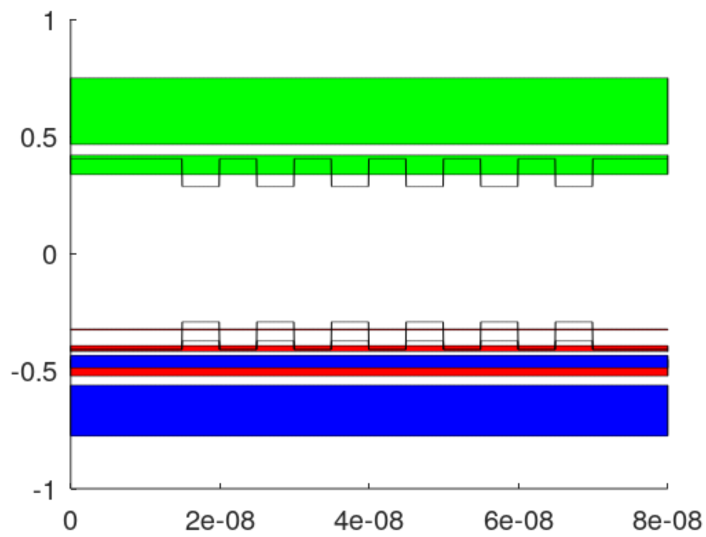
Heterostructures modelling



Bands dispersion in MQWs

- Using modified Kronig-Penney model
- assuming QWs made of Ge and $Ge_{0.9}Sn_{0.1}$

with superlattice period of a+b = (7.5 + 2.5) nm



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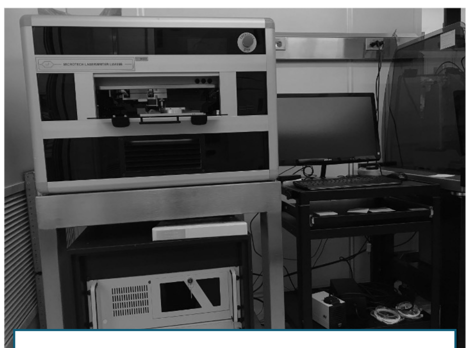
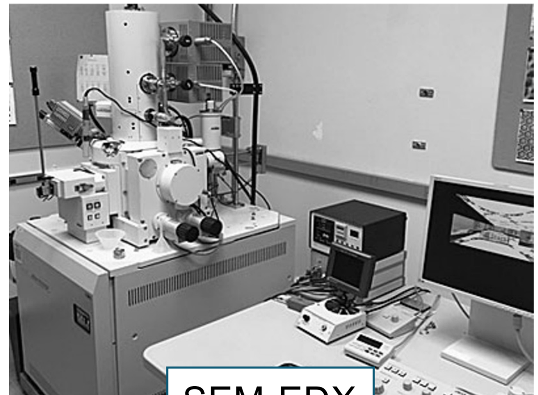
Brookhaven National Laboratory-IO fabrication capabilities

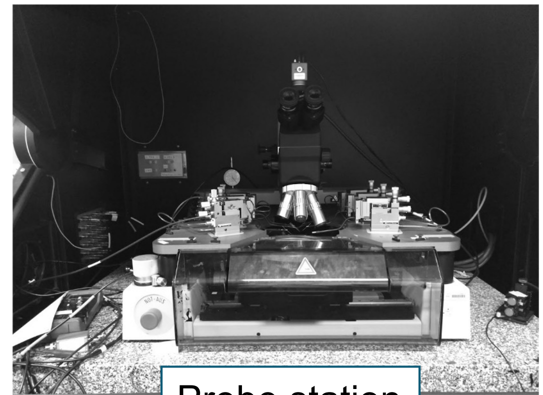
Sputtering, e-beam, thermal


Direct laser writing tool

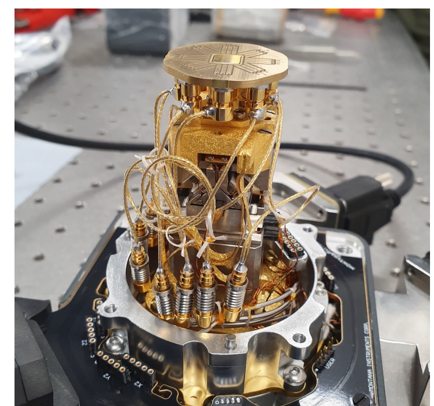
Thermal evaporation

Augmented by access to CFN shared facilities


SEM-EDX


Probe station


Clean room


Cryogenic probe station

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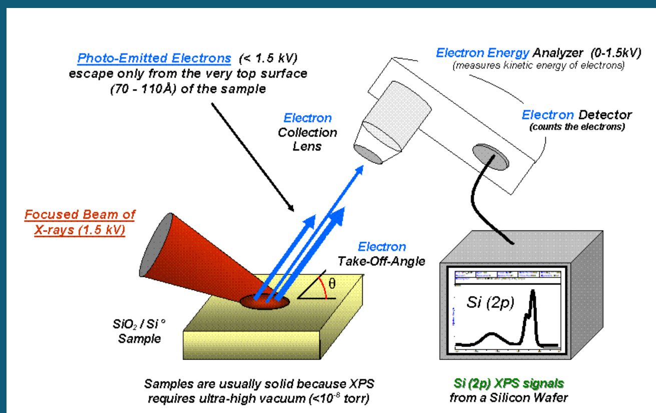
Brookhaven National Laboratory NSLS-II characterization

Hard X-ray PhotoElectron Spectroscopy



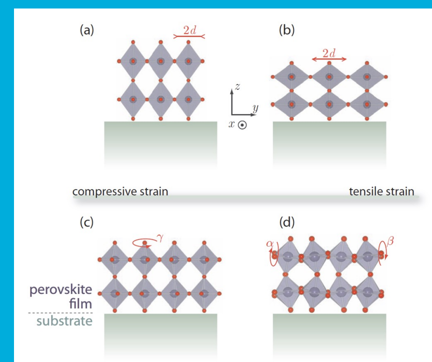
Variable Kinetic Energy HAXPES

•Tune the HAXPES depth sensitivity (photoelectron kinetic energy) by tuning the X-ray excitation energy using a synchrotron X-ray beamline

•The X24A endstations form a unique measurement suite for surface to near bulk HAXPES by spanning X-ray excitation energy from 0.2 to 5 keV

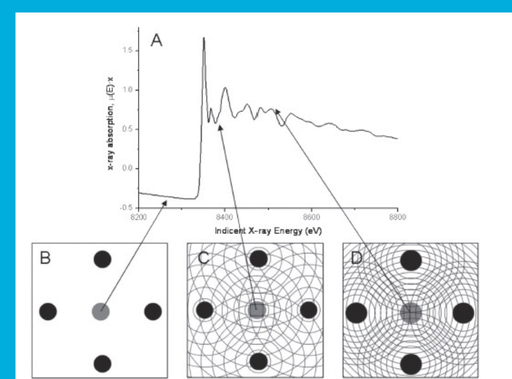
Example: Si electron binding energy 2p ~99 eV and 1s ~1840 eV, surface to bulk sensitivity (Lab source has fixed energy Al Kα)

Extended X-ray Absorption Fine Structure



Strain can result in changes in bond lengths or bond angles. This can be measured using EXAFS

J. M. Rondinelli and N. A. Spaldin, Adv. Mater. **23**, 3363 (2011)



Future work outlook

- Modelling of device performance using band-structure mapping and derived parameters i.e. gain, absorption (short term)
- Device growth and development (short term)
- Device integration (long term)

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