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Characterizing Critical Buried Interfaces by Inelastic Background Analysis (IBA) using Lab-Scale Hard X-ray Spectroscopy

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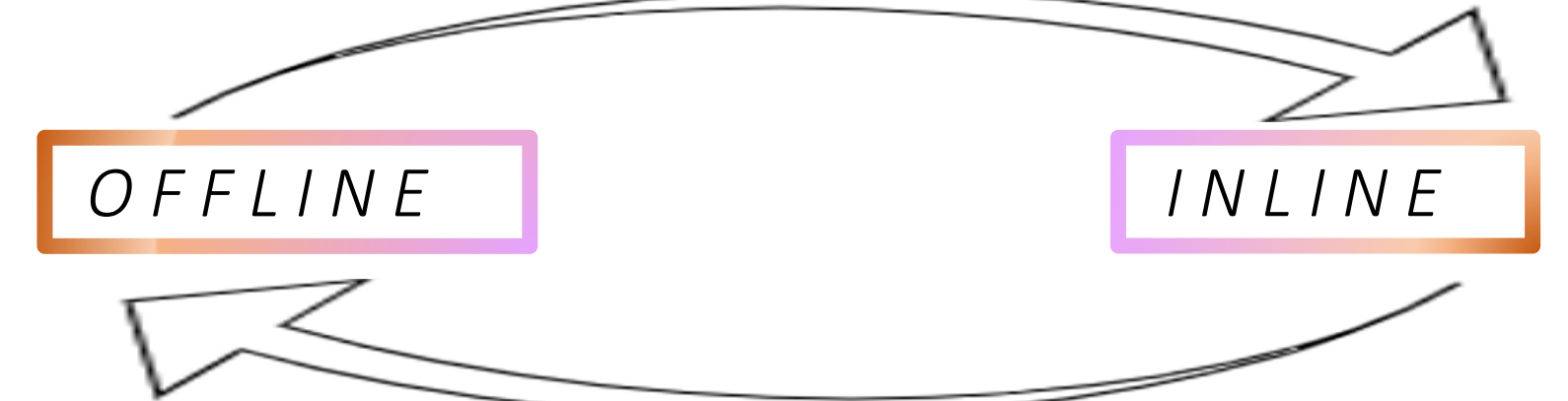
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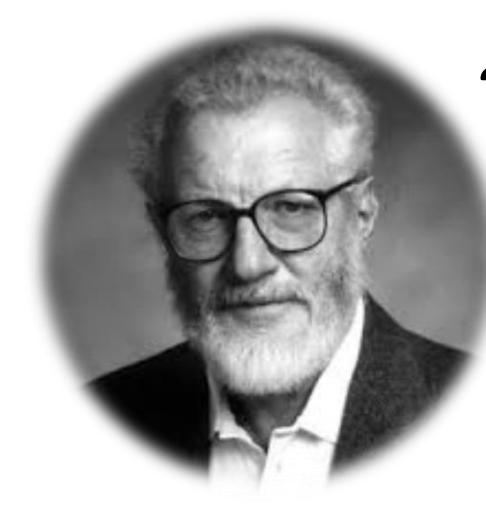
ABSTRACT: devices are shrinking while increasing in complexity. The buried interfaces in electronic materials are critical to their functionality but notoriously difficult to characterize. This work aims to expand an existing approach to non-destructive depth profiling of deeply buried interfaces by developing a generic and semi-automated method analyzing the inelastic background of XPS spectra

Objectives

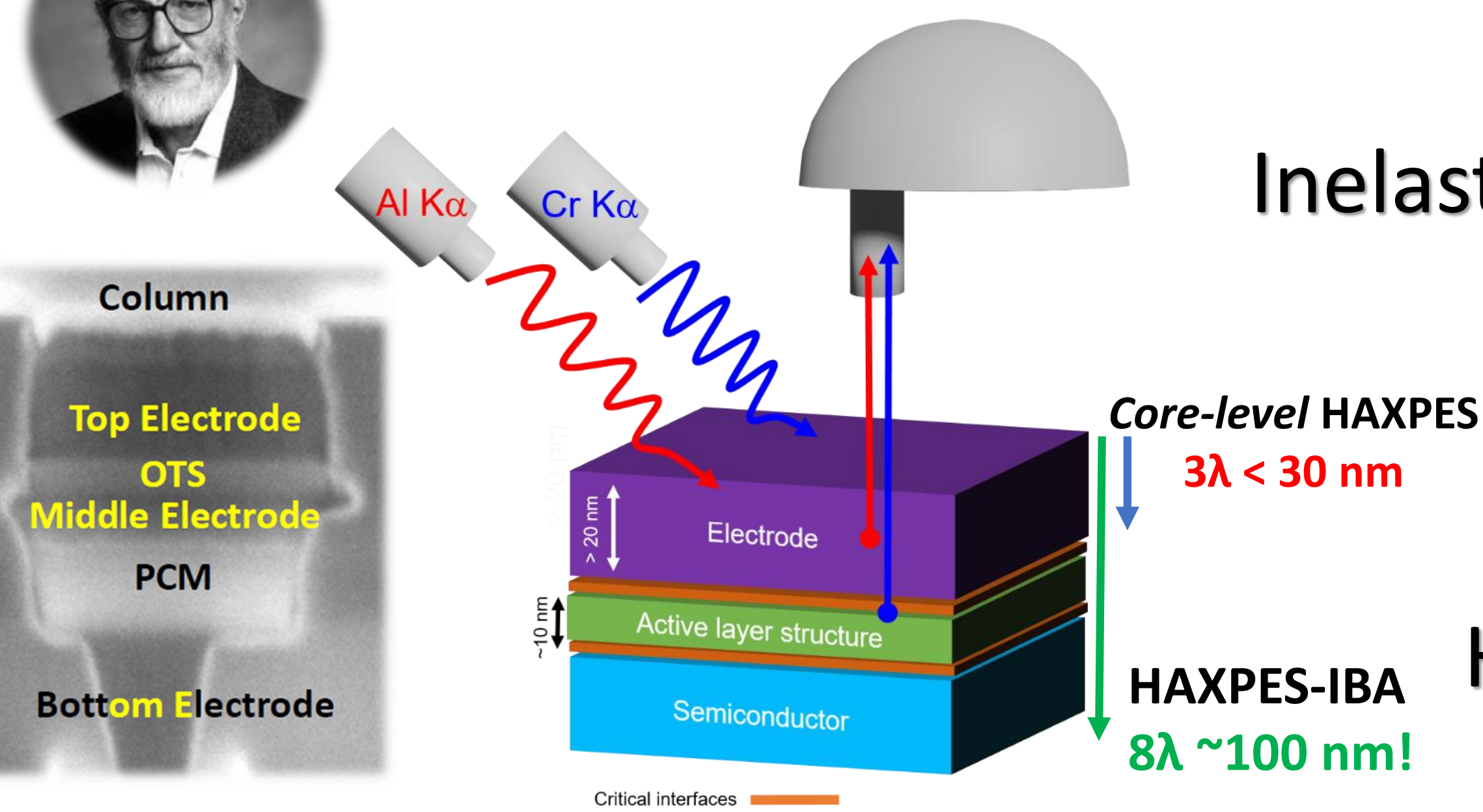
- 1: Apply IBA to lab-based HAXPES spectra for the characterization of interfaces and buried layers
- 2: Develop a generalized, semi-automatic method for evaluating results and fitting uncertainty in the IBA solution



Final Objective: Bring offline HAXPES analysis to inline metrology for semiconductor technologies



2000: « The interface is the device »
Herbert Kroemer, Nobel Lecture



- XPS**
- Non-destructive core-level analysis
 - Minimal sample preparation
 - **Limited probing depth**

Inelastic Background Analysis (IBA)

- QUASES software package
- 10 nm probing depth with traditional XPS
- no additional instrumentation needed
- **Limitations : peak interference in background**

- HAXPES + IBA**
- Up to 150 nm probing depth when combined with background analysis
 - Expand collection of available peaks

Objective 1(a) Al₂O₃ / HfO₂

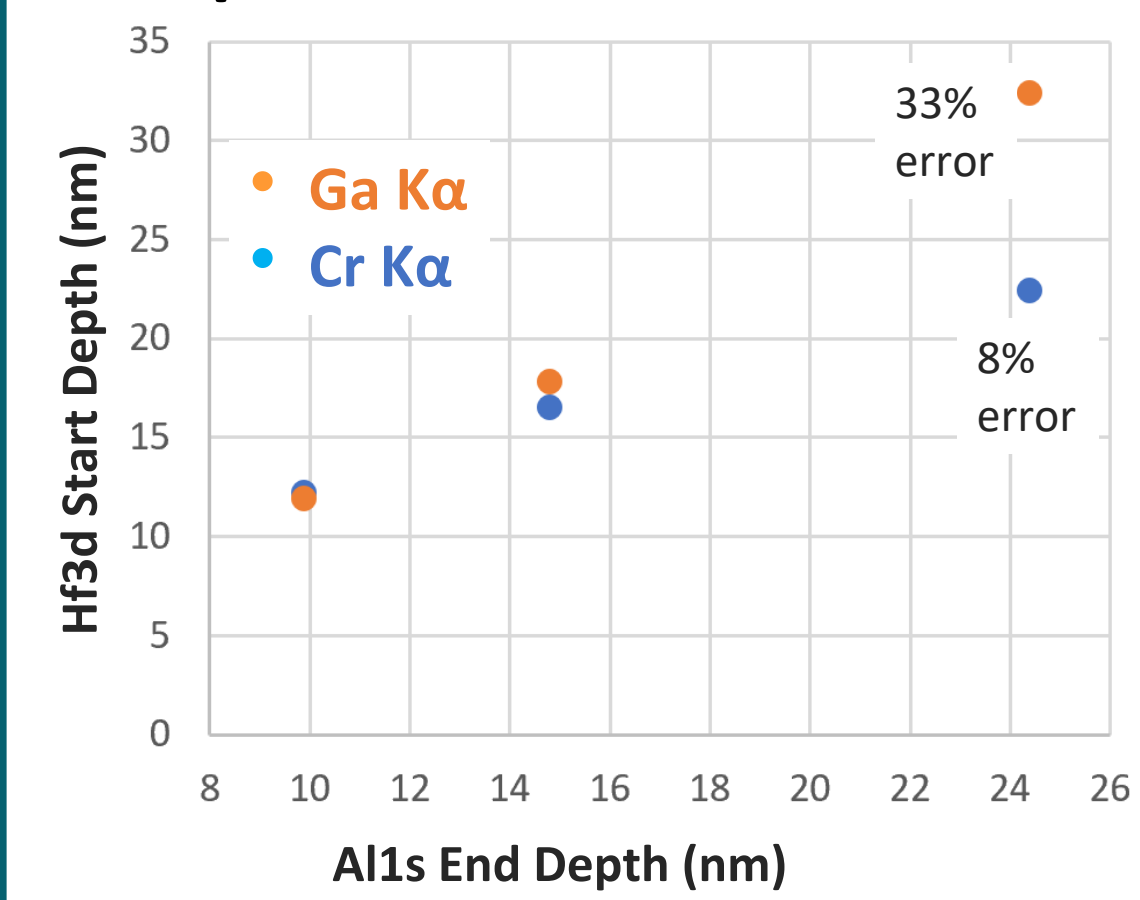
3 bilayer samples of High-k metal oxides with d(HfO₂)=2.5 nm

☐ Compare Cr Kα and Ga Kα HAXPES results

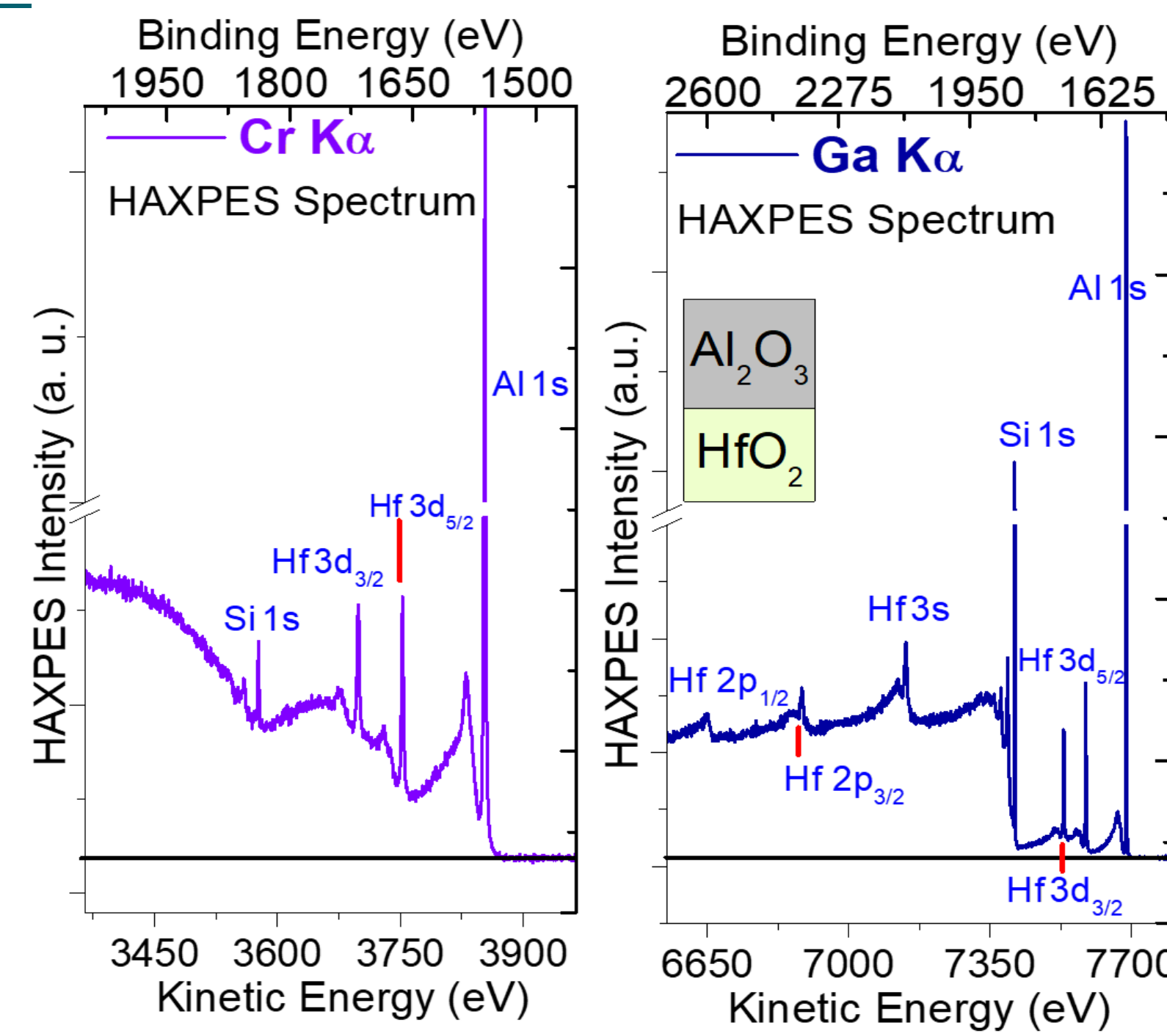
Surface layers	Name	Surface Layer Thickness (nm)
Al ₂ O ₃	A1	9.9
Al ₂ O ₃	A2	14.8
Al ₂ O ₃	A3	24.4

- Cr Kα hv = 5414.72 eV
IMFP Hf3d = 6.6 - 6.7 nm
- Ga Kα hv = 9251.74 eV
IMFP Hf3d = 11.8 - 12.2 nm

Comparison of Interface Positions



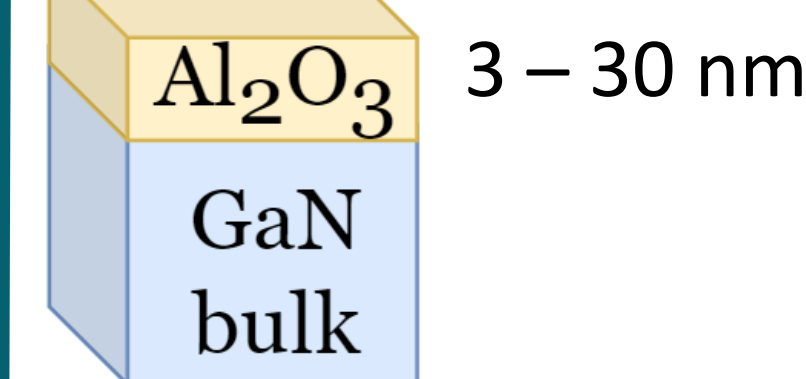
- Hf3d is not in accordance with Al1s interface position and Ga Kα HAXPES energy did not improve IBA model
- Increasing source energy increases inelastic losses in the kinetic energy range further from the peak (Hf3d), which is interrupted by other peaks (Si1s) in these spectra
- Must carefully choose source energies for individual sample (peak overlap and buried layer thickness)



Objective 1(b) Al₂O₃ / GaN

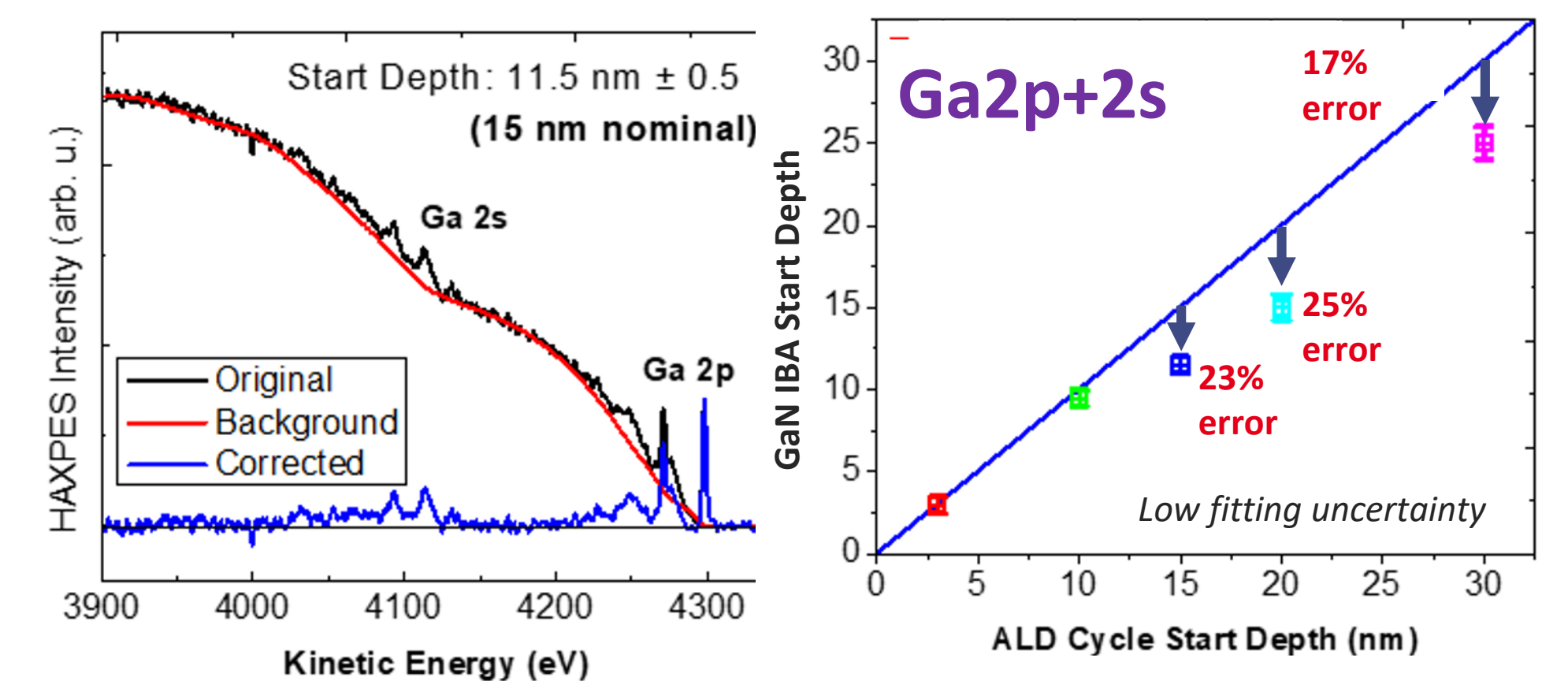
5 bilayer samples representative of HEMT device

☐ Apply QUASES-Generate reference spectra

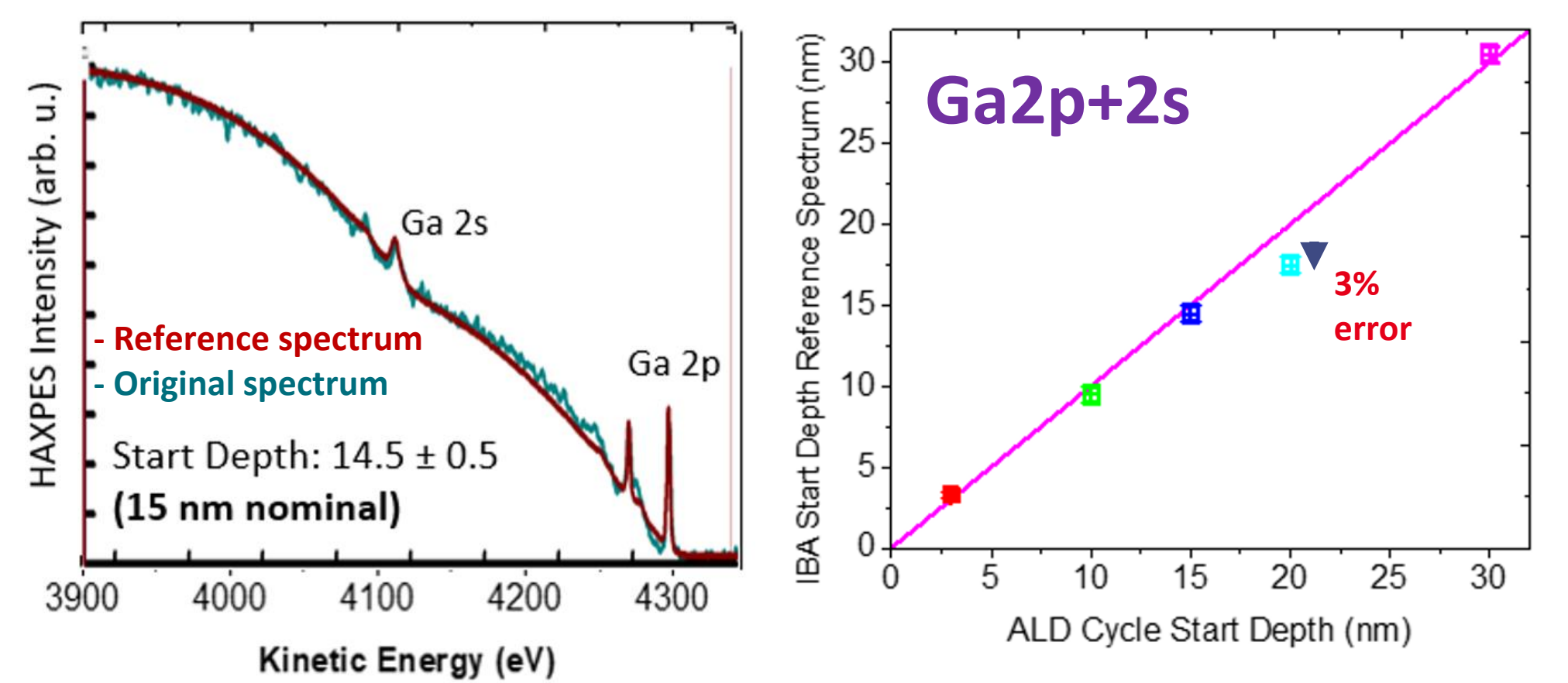


- Start Depth of buried Ga2p too close to surface
- Creates broad interface with Al₂O₃
- Start Depth of buried Ga2p is in accordance with anticipated interface with Al₂O₃ obtained by IBA of Al1s and O1s
- Al1s and O1s were best modeled with QUASES-Analyze and the Universal cross-section

QUASES-Analyze – no reference



QUASES-Generate – GaN bulk reference spectrum



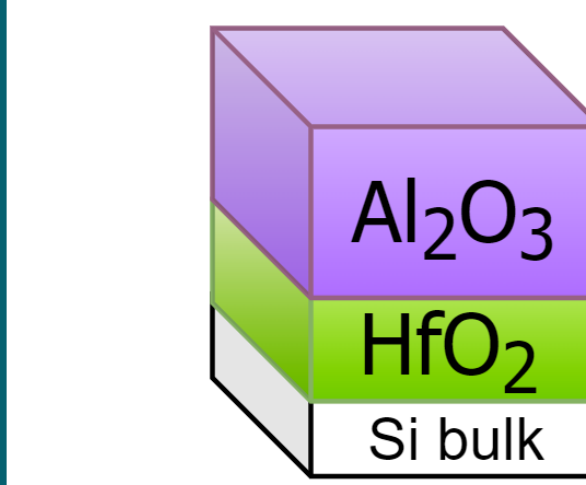
Objective 2. Error Calculation for Evaluation of IBA Solution

Calculate the error between a range of points on the x-axis, and look for the lowest error in possible solutions

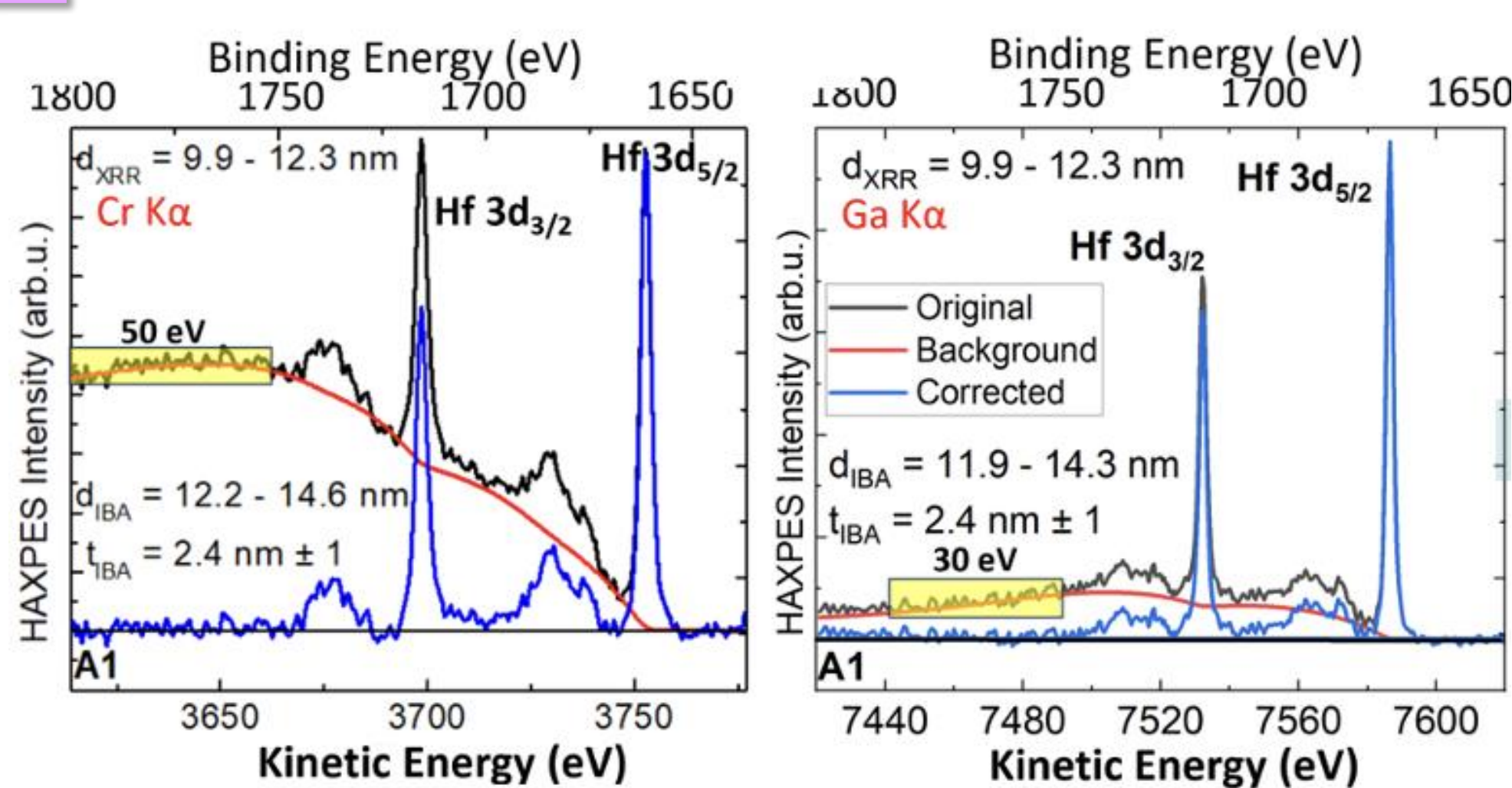
Problem: The size and location of the background region for comparison changes with:

$$MSE = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

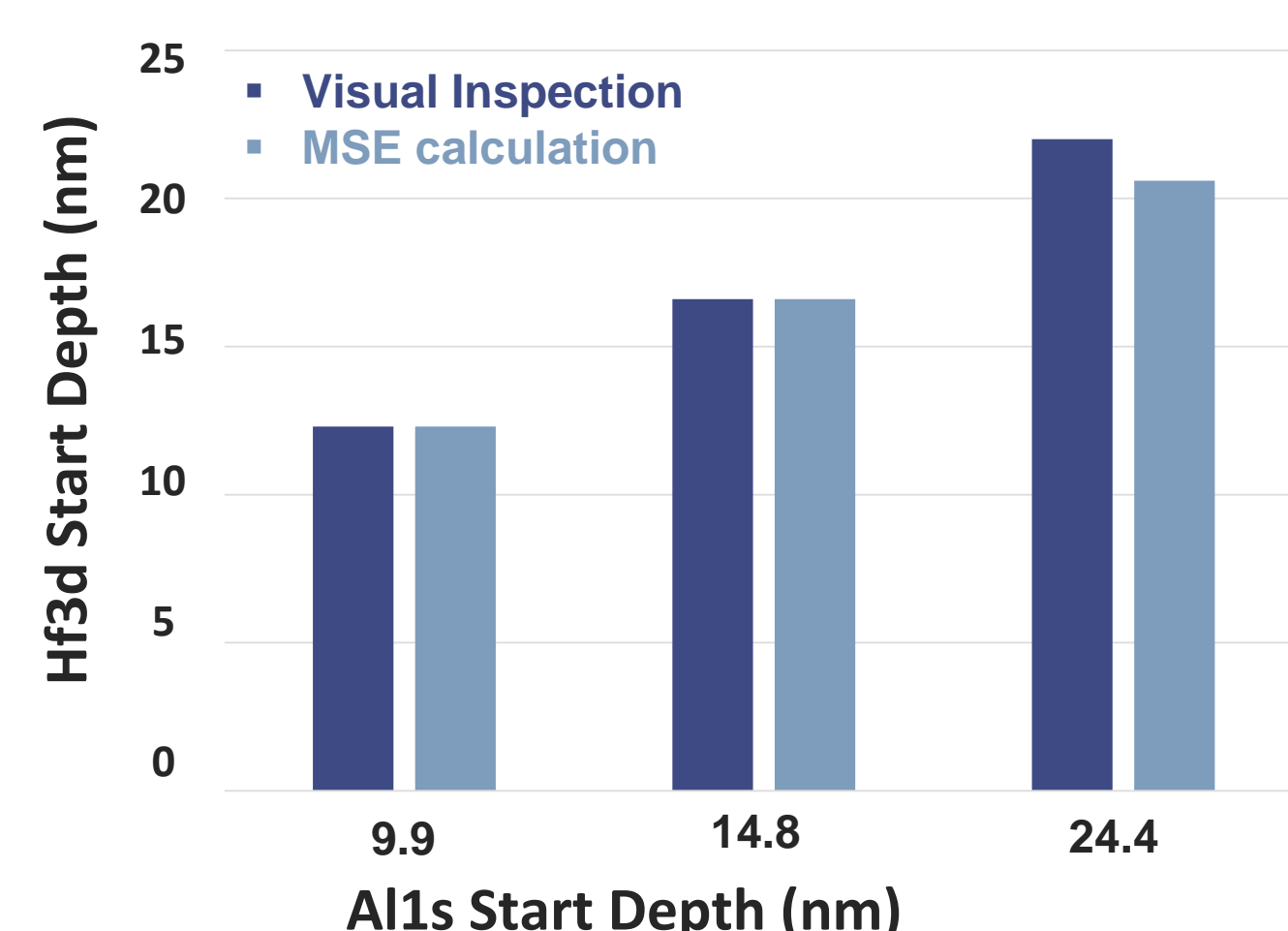
Y_i = Recorded Spectrum
 \hat{Y}_i = Modeled inelastic background



Photon Energy

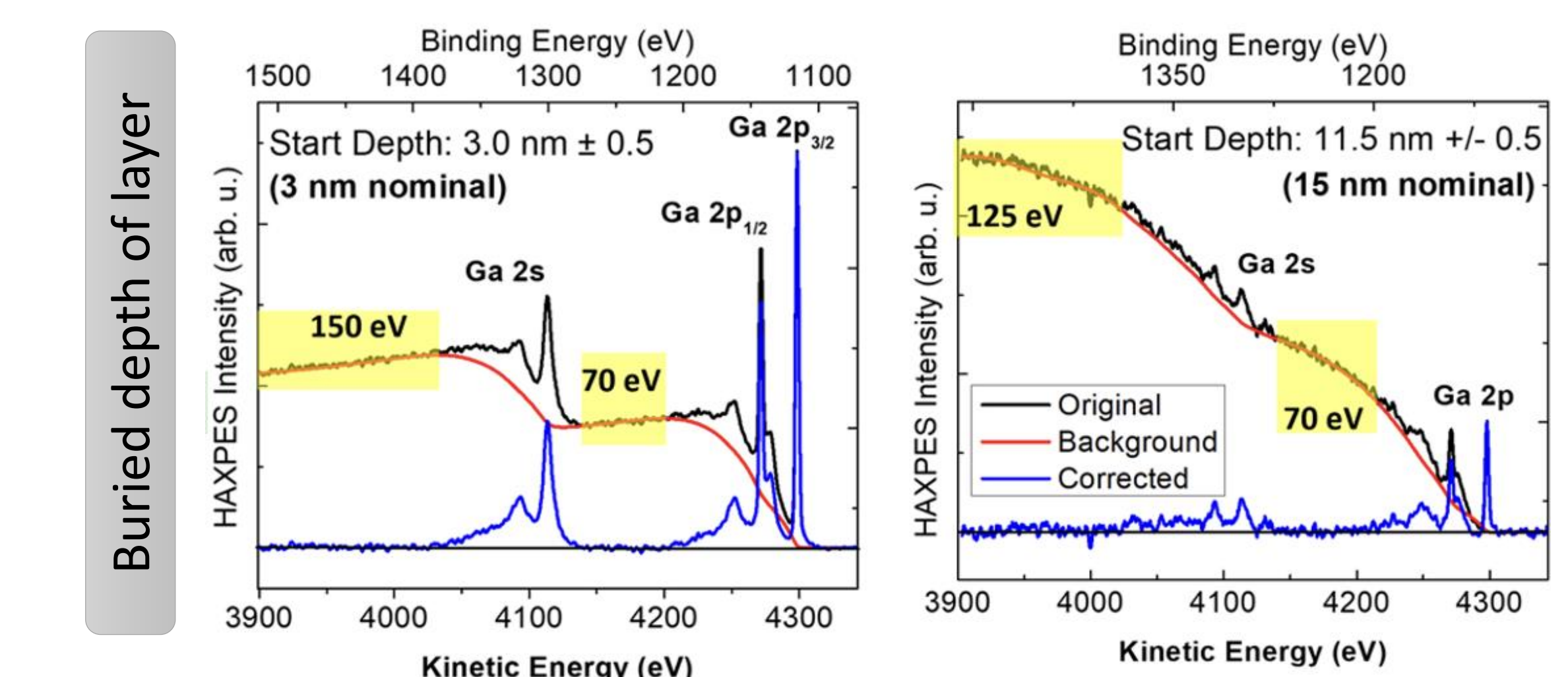


☐ Restrict energy range

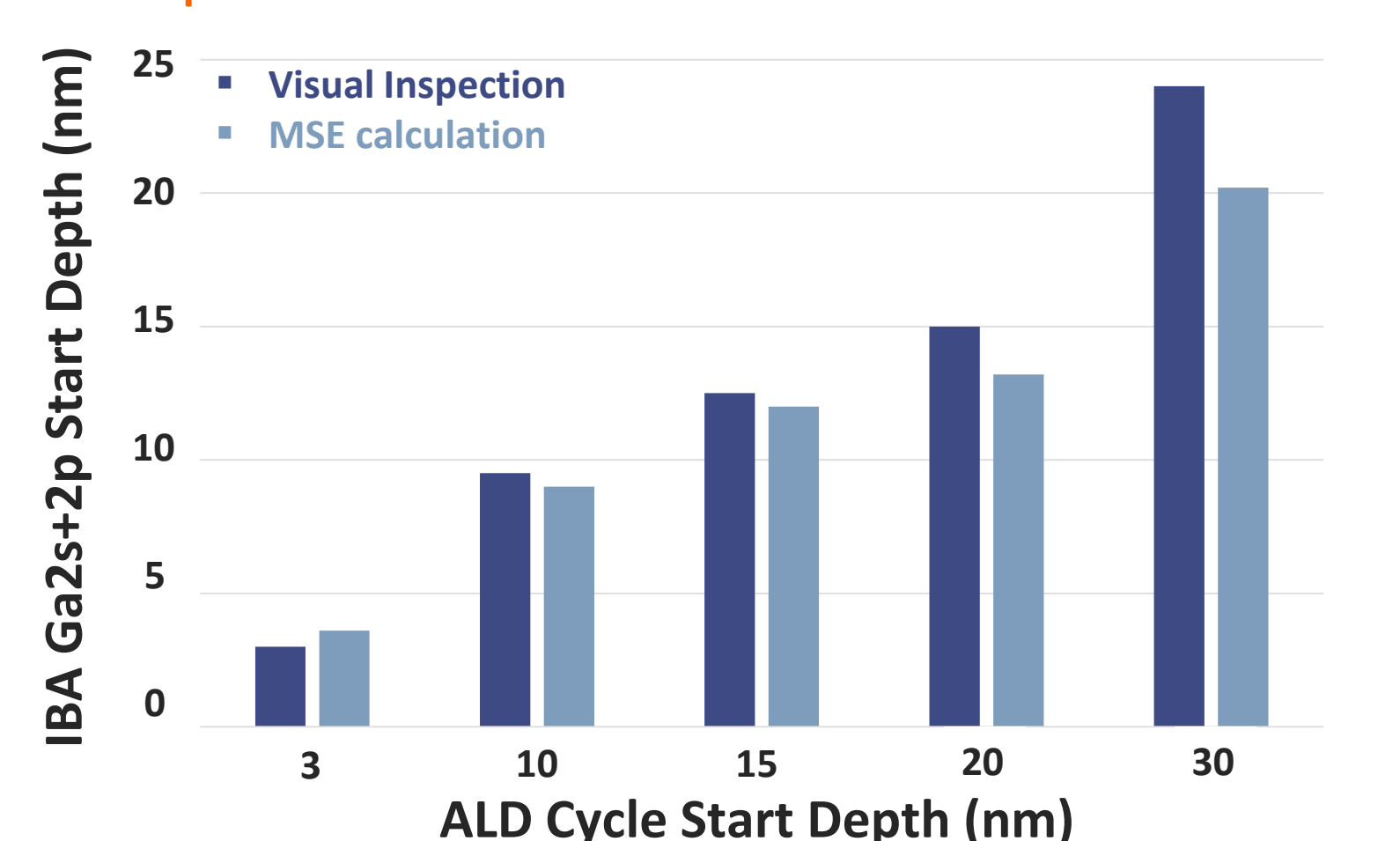
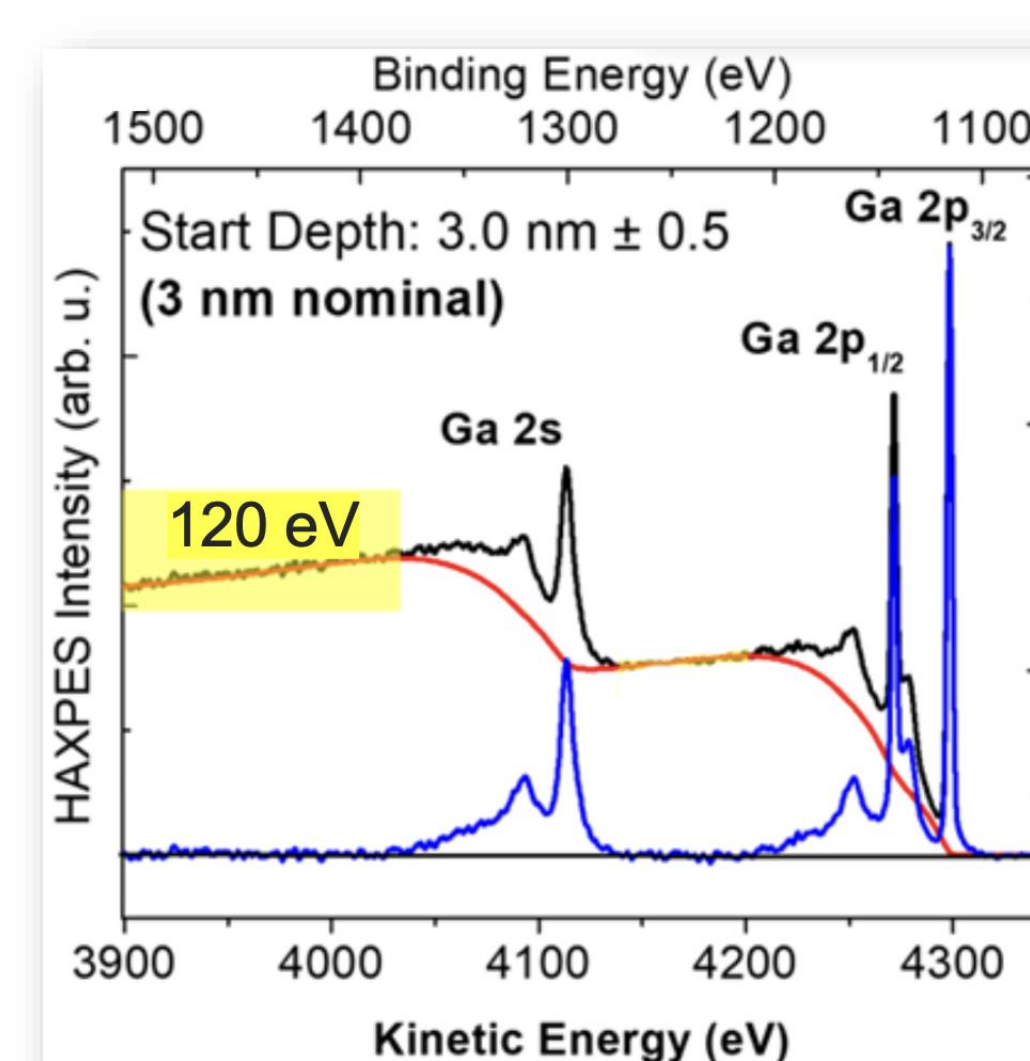


- Hf3d is not in agreement with Al1s interface position and Ga Kα HAXPES energy did not improve IBA model
- HAXPES-IBA solutions from visual inspection and error calculation agree

Buried depth of layer



☐ Restrict possible solution



- HAXPES-IBA solutions from visual inspection and error calculation agree
- Visual inspection overestimates start depth

More elegant algorithms are needed for a general error calculation but it could be a useful tool for avoiding user bias in IBA

[1] S. Tougaard, Practical guide to the use of backgrounds in quantitative XPS, J. Vac. Sci. Technol. A, 39 (2021) 011201.

[2] T. R. Bure, O. Renault, E. Nolot, T. Lardin, C. Robert-Goumet, N. Pauly, Assessing advanced methods in XPS and HAXPES for determining the thicknesses of high-k oxide materials: from ultra-thin layers to deeply buried interfaces. Appl. Surf. Sci. 609 (2023) 155317.

[3] O. Renault, P. Deleuze, J. Courtin, R. T. Bure, N. Gauthier, E. Nolot, C. Robert-Goumet, N. Pauly, E. Martinez, K. Artyushkova, New directions in the analysis of buried interfaces for device technology by hard X-ray photoemission. Faraday Discuss., 236 (2022) 288.