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## HAXPES of Si(100) with Cr K $\alpha$ excitation

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Si (100) wafer was analyzed by high-energy photoelectron spectroscopy (HAXPES) using monochromatic Cr K $\alpha$  radiation (5414.7 eV). The HAXPES spectra reported here include a survey scan and high-resolution spectra of Si 1s, Si 2s, Si 2p core-levels.

**Keywords:** Si, HAXPES, Cr K $\alpha$

### INTRODUCTION

Silicon is still the most widely used material in the semiconductor industry. The recent arrival of laboratory HAXPES spectrometers on the market has given researchers the ability to probe deeper in multilayer materials. Here, we provide HAXPES data acquired with Cr K $\alpha$  radiation (5414.8 eV) on a bare silicon wafer which is useful for comparison with other Si compounds.

### SPECIMEN DESCRIPTION (ACCESSION # 01712)

**Host Material:** Si

**CAS Registry #:** 7440-21-3

**Host Material Characteristics:** Homogeneous; solid; single crystal; semiconductor; semiconductor; Other

**Chemical Name:** Silicon

**Host Composition:** Si

**Source:** Siltronix

**Form:** Silicon wafer

**Structure:** (100) face-centered cubic

**History & Significance:** Air exposed lightly p-doped ( $10^{16}$  at./cm<sup>3</sup>) Si wafer

**As Received Condition:** Piece of a 300 mm Si wafer

**Analyzed Region:** Same as host material

**Ex Situ Preparation/Mounting:** The sample was mounted on the sample holder using double sided conductive tape.

**In Situ Preparation:** The sample was sputter cleaned by Ar<sup>+</sup> ions (2 keV) for 8 minutes prior to measurements to remove the native oxide and the carbon contamination.

**Charge Control:** Low-energy electrons (1 eV, filament 1.1 A) and Ar<sup>+</sup> ions (500 eV)

**Temp. During Analysis:** 300 K

**Accession#:** 01712

**Technique:** XPS

**Host Material:** Si

**Instrument:** ULVAC-PHI Quantes

**Major Elements in Spectra:** Si

**Minor Elements in Spectra:** Ar

**Published Spectra:** 4

**Spectra in Electronic Record:** 4

**Spectral Category:** comparison

**Pressure During Analysis:** < 6.10<sup>-7</sup> Pa

**Pre-analysis Beam Exposure:** 0 s

### INSTRUMENT DESCRIPTION

**Manufacturer and Model:** ULVAC-PHI Quantes

**Analyzer Type:** spherical sector

**Detector:** multichannel resistive plate

**Number of Detector Elements:** 32

### INSTRUMENT PARAMETERS COMMON TO ALL SPECTRA

#### ■ Spectrometer

**Analyzer Mode:** constant pass energy

**Throughput (T=E<sup>N</sup>):** The energy dependence can be modeled using the following equation:  $\frac{A}{E_p} = \left(\frac{a^2}{a^2 + R^2}\right)^b$ , where a and b are constants, E<sub>p</sub> is the pass energy, A is the peak area and R is the retard ratio equal to E/E<sub>p</sub>, where E is the kinetic energy. Three spectral regions are recorded on a sputter cleaned sample at different pass energies. The values of a and b are then determined by a linear least square fit of the data applying the equation described above.

**Excitation Source Window:** Al

**Excitation Source:** Cr K $\alpha$  monochromatic

**Source Energy:** 5414.8 eV

**Source Strength:** 50 W

**Source Beam Size:** 100  $\mu$ m x 100  $\mu$ m

**Signal Mode:** multichannel direct

#### ■ Geometry

**Incident Angle:** 22 °

**Source-to-Analyzer Angle:** 46 °

**Emission Angle:** 45 °

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**Specimen Azimuthal Angle:** 0 °  
**Acceptance Angle from Analyzer Axis:** 0 °  
**Analyzer Angular Acceptance Width:** 20 ° × 20 °

#### ■ Ion Gun

**Manufacturer and Model:** ULVAC-PHI Quantes

**Energy:** 500 and 2000 eV

**Current:** 0.001 mA

**Current Measurement Method:** Faraday cup

**Sputtering Species:** Ar

**Spot Size (unrastered):** 100 μm

**Raster Size:** 3000 μm × 3000 μm

**Incident Angle:** 45 °

**Polar Angle:** 45 °

**Azimuthal Angle:** 45 °

**Comment:** Differentially pumped ion gun used for pre-sputtering of the sample and to prevent from reoxidation during analysis.

#### DATA ANALYSIS METHOD

**Energy Scale Correction:** The decrease of photoionization cross-sections in HAXPES (Refs. 1 and 2) leads to a very low C 1s intensity. Therefore, the binding energy was referenced to the Si 2p binding energy position measured with Al K $\alpha$  radiation after shifting the C 1s peak to 284.8 eV. Doing so, the Si 2p binding energy was 99.4 eV. The spectra recorded with the Cr K $\alpha$  source were then rescaled by shifting the Si 2p to 99.4 eV. The procedure may yield uncertainties of 0.2 eV at most, because HAXPES and its larger probing depth may be sensitive to band bending of the nearly intrinsic Si surface, expected here to be small.

**Recommended Energy Scale Shift:** 1.6 eV for binding energy

**Peak Shape and Background Method:** Shirley background was employed to treat the data. No curve fitting was conducted on the spectra.

**Quantitation Method:** PHI Multipak software Version 9.9.0.8 was used to perform quantification. Empirically determined sensitivity factors (RSFs) were provided by the software. The RSFs were derived from the pure-element relative sensitivity factor as defined in ISO 18118:2015 (Ref 3) which were measured on pure element samples using a Cr K $\alpha$  source. They therefore account for the decrease of cross-section and different escape depth of photoelectrons using higher energy photons. RSFs are reported proportional to the RSF of F 1s equal to 1. The reported concentrations were calculated using these RSFs corrected to include the transmission function and asymmetry parameter.

#### ACKNOWLEDGMENTS

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#### DATA AVAILABILITY STATEMENT

*The data that supports the findings of this study are available within the article and its supplementary material.*

#### REFERENCES

1. M.B. Trzhaskovskaya and V.G. Yarzhemsky, *At. Data Nucl. Data Tables* **119**, 99 (2018).
2. M.B. Trzhaskovskaya and V.G. Yarzhemsky, *At. Data Nucl. Data Tables* **129-130**, 101280 (2019).
3. International Organization for Standardization 2015, *Surface chemical analysis - Auger electron spectroscopy and X-ray photoelectron spectroscopy - Guide to the use of experimentally determined relative sensitivity factors for the quantitative analysis of homogeneous materials*, ISO 18118:2015.

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SPECTRAL FEATURES TABLE							
Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV x cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
01712-02	Si 1s	1838.7	1.43	16156	4.653	100	Si
01712-03	Si 2s	150.3	1.69	665	0.436	...	Si
01712-04	Si 2p	99.0	1.44	459	0.110	...	Si

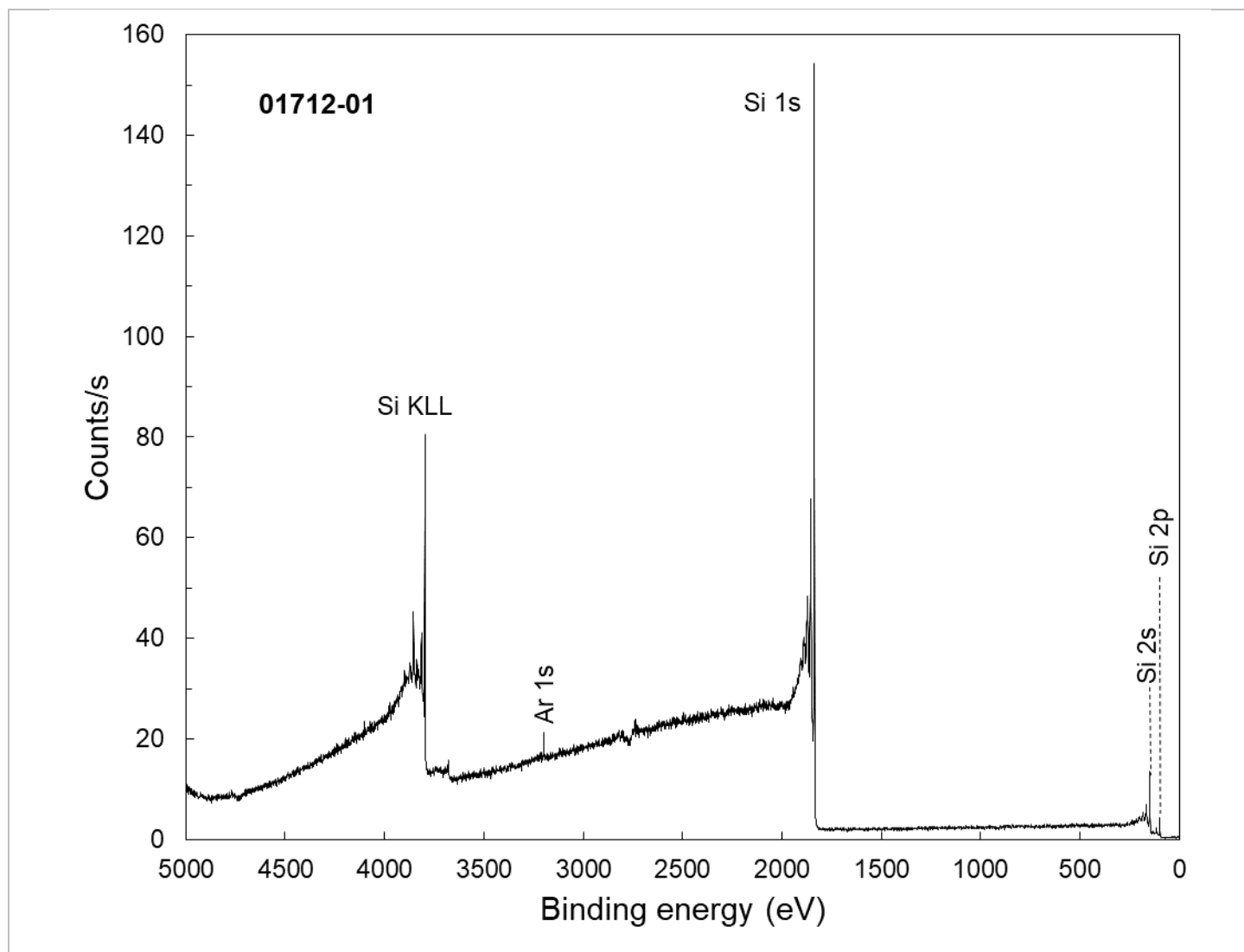
ANALYZER CALIBRATION TABLE							
Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV x cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
...	Ag3d <sub>5/2</sub>	368.12	0.63	114999	...	...	...
...	Cu2p <sub>3/2</sub>	932.61	0.96	40205	...	...	...
...	Au4f <sub>7/2</sub>	83.89	0.78	100500	...	...	...

The spectra in the analyzer calibration table were recorded using Al K $\alpha$  photons.

GUIDE TO FIGURES					
Spectrum (Accession) #	Spectral Region	Voltage Shift*	Multiplier	Baseline	Comment #
01712-01	Survey	0	1	0	...
01712-02	Si 1s	-1.6	1	0	...
01712-03	Si 2s	-1.6	1	0	...
01712-04	Si 2p	-1.6	1	0	...

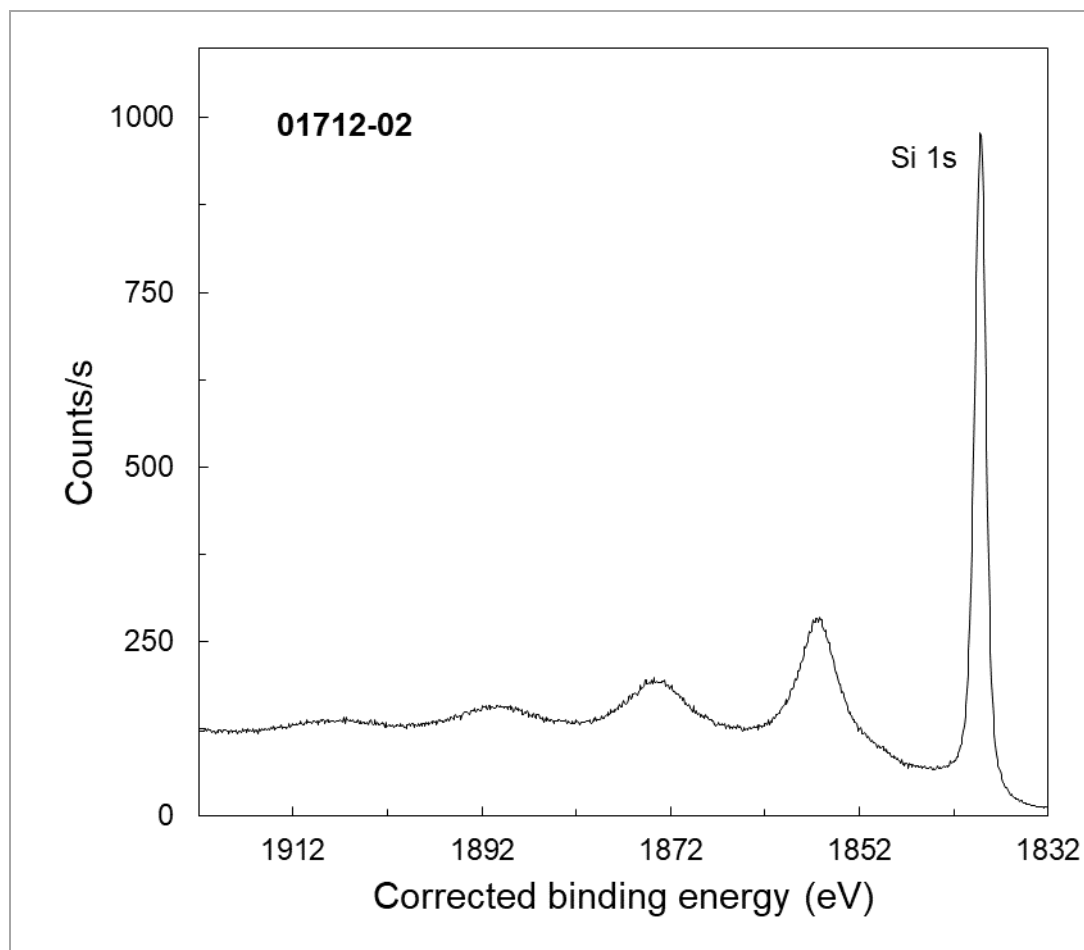
\*Voltage shift of the archived (as-measured) spectrum relative to the printed figure. The figure reflects the recommended energy scale correction due to a calibration correction, sample charging, flood gun, or other phenomenon.

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Accession #	01712-01
Host Material	Si
Technique	XPS
Spectral Region	survey
Instrument	ULVAC-PHI Quantes
Excitation Source	Cr K $\alpha$ monochromatic
Source Energy	5414.8 eV
Source Strength	50 W
Source Size	0.1 mm x 0.1 mm
Analyzer Type	spherical sector analyzer
Incident Angle	22°
Emission Angle	45°
Analyzer Pass Energy	280 eV
Analyzer Resolution	2.33 eV
Total Signal Accumulation Time	5240 s
Total Elapsed Time	5760 s
Number of Scans	10
Effective Detector Width	31 eV

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■ Accession #: 01712-02

■ Host Material: Si

■ Technique: XPS

■ Spectral Region: Si 1s

Instrument: ULVAC-PHI

Quantes

Excitation Source:

Cr K $\alpha$  monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1 mm

Analyzer Type: spherical sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

Analyzer Resolution: 1.17 eV

Total Signal Accumulation

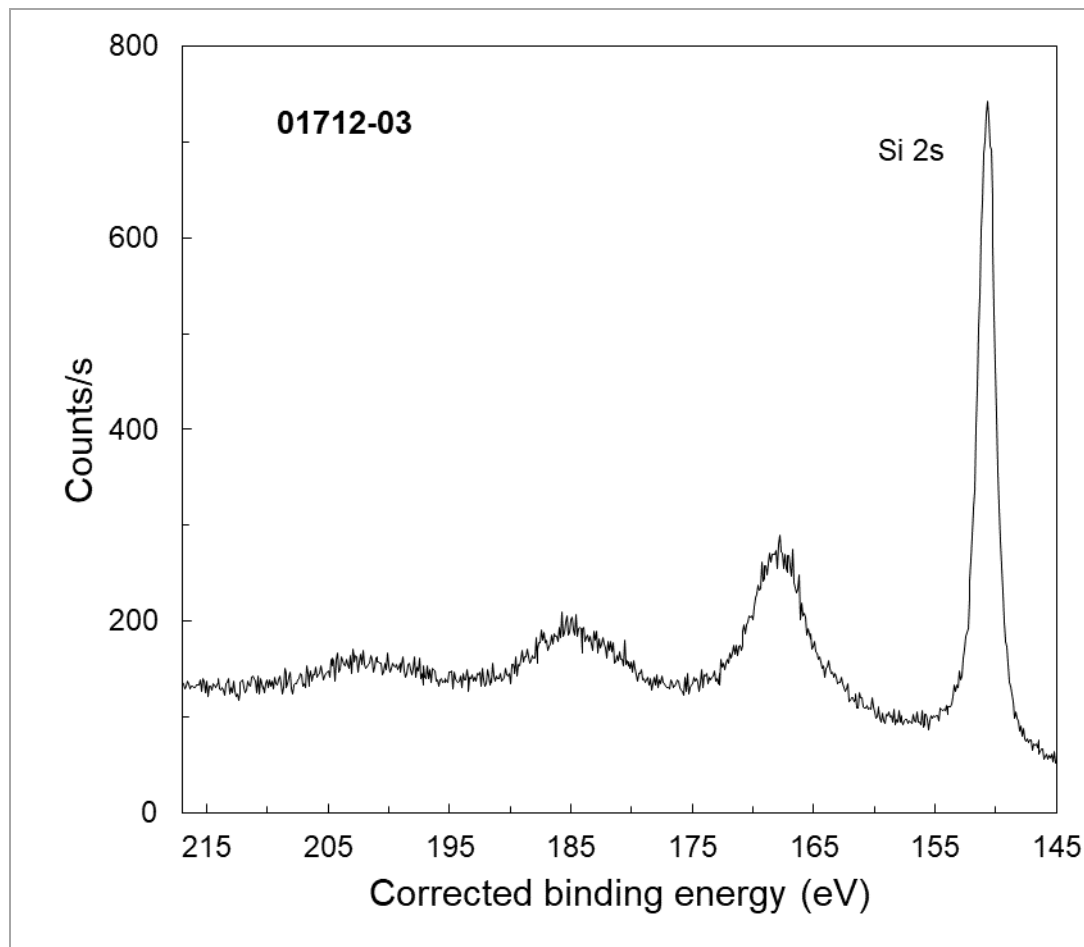
Time: 4098 s

Total Elapsed Time: 4506 s

Number of Scans: 10

Effective Detector Width: 12.4 eV

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■ **Accession #:** 01712-03

■ **Host Material:** Si

■ **Technique:** XPS

■ **Spectral Region:** Si 2s

Instrument: ULVAC-PHI

Quantes

Excitation Source:

Cr K $\alpha$  monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1 mm

Analyzer Type: spherical sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

Analyzer Resolution: 1.17 eV

Total Signal Accumulation

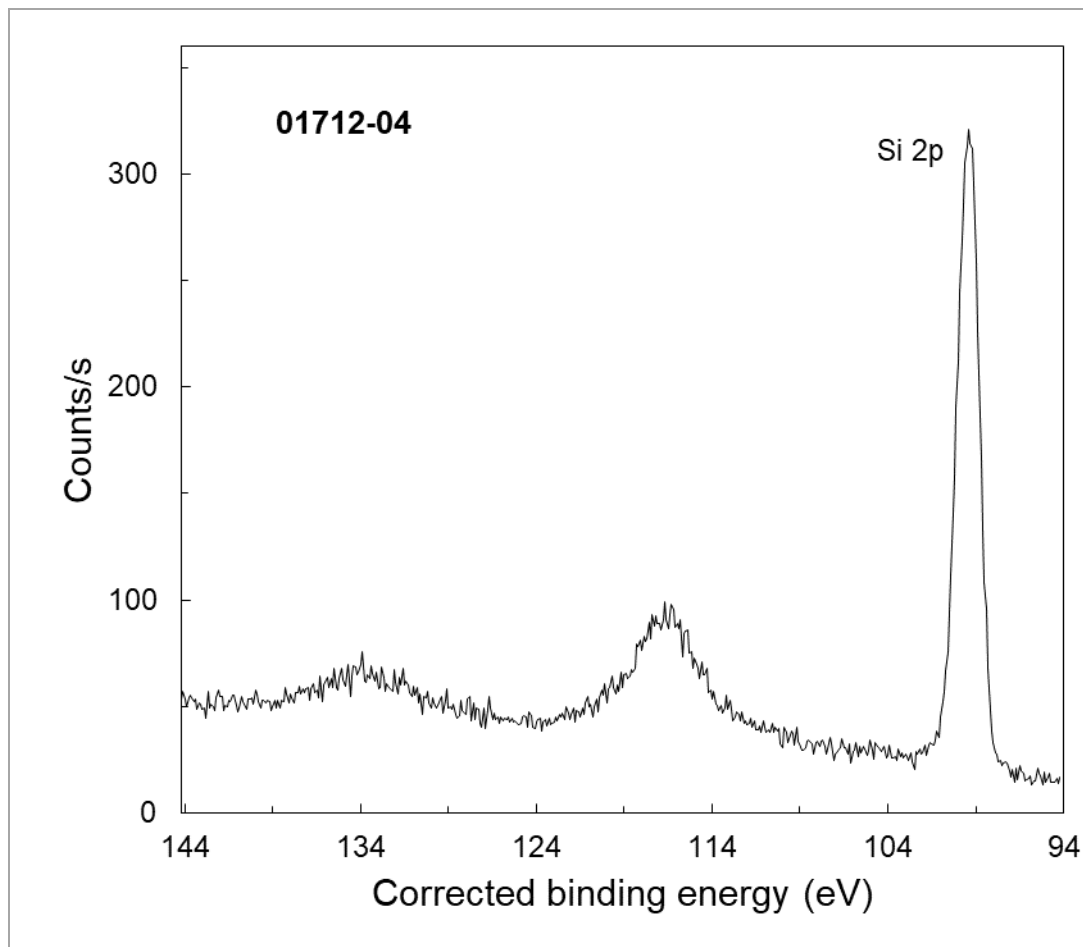
Time: 4050 s

Total Elapsed Time: 4458 s

Number of Scans: 12

Effective Detector Width: 12.4 eV

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- Accession #: 01712-04
- Host Material: Si
- Technique: XPS
- Spectral Region: Si 2p

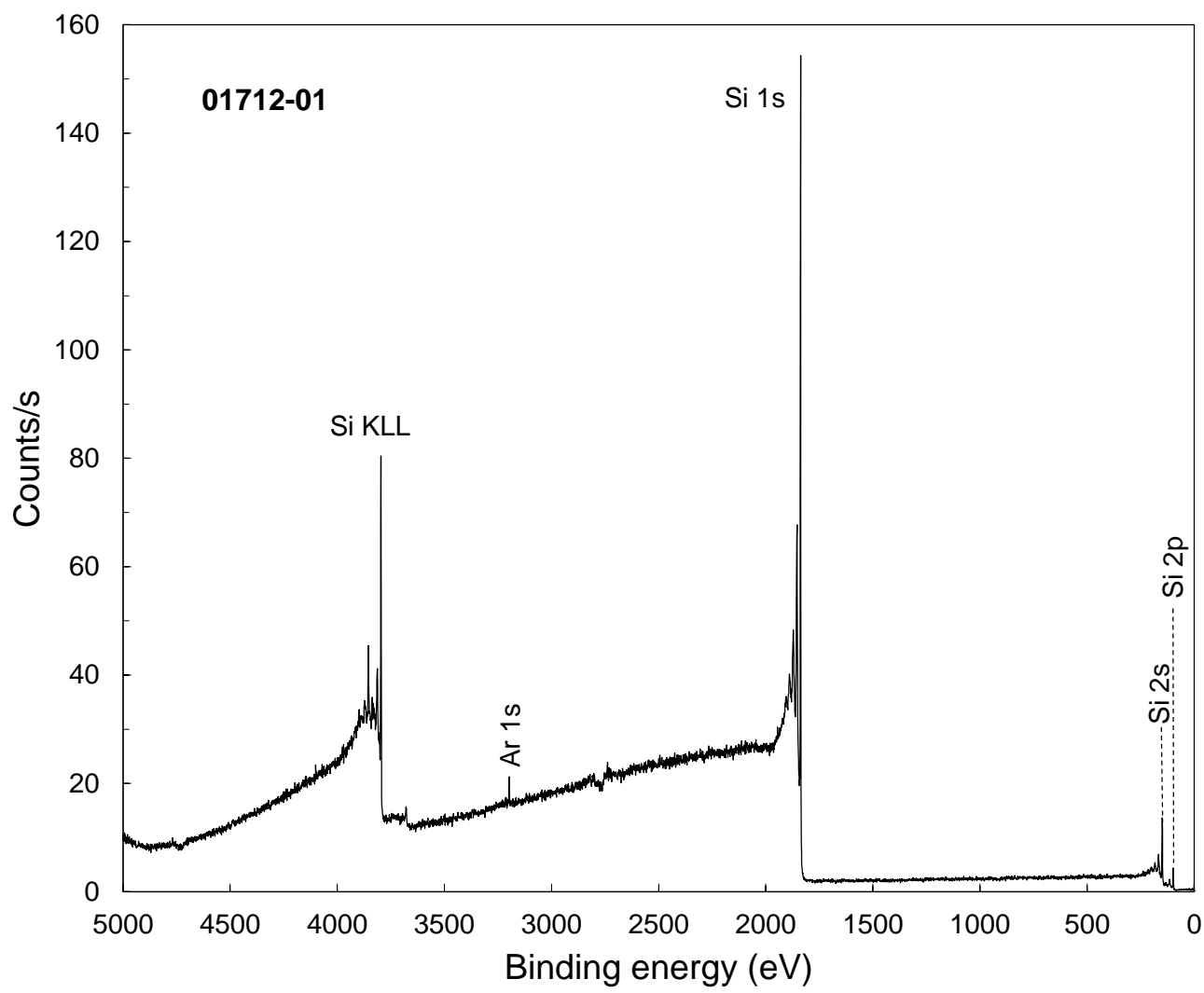
Instrument: ULVAC-PHI  
 Quantes  
 Excitation Source:  
 Cr K $\alpha$  monochromatic  
 Source Energy: 5414.8 eV  
 Source Strength: 50 W  
 Source Size: 0.1 mm x 0.1 mm  
 Analyzer Type: spherical sector  
 Incident Angle: 22 °  
 Emission Angle: 45 °  
 Analyzer Pass Energy 112 eV  
 Analyzer Resolution: 1.17 eV  
 Total Signal Accumulation  
 Time: 3972 s  
 Total Elapsed Time: 4374 s

Number of Scans: 17

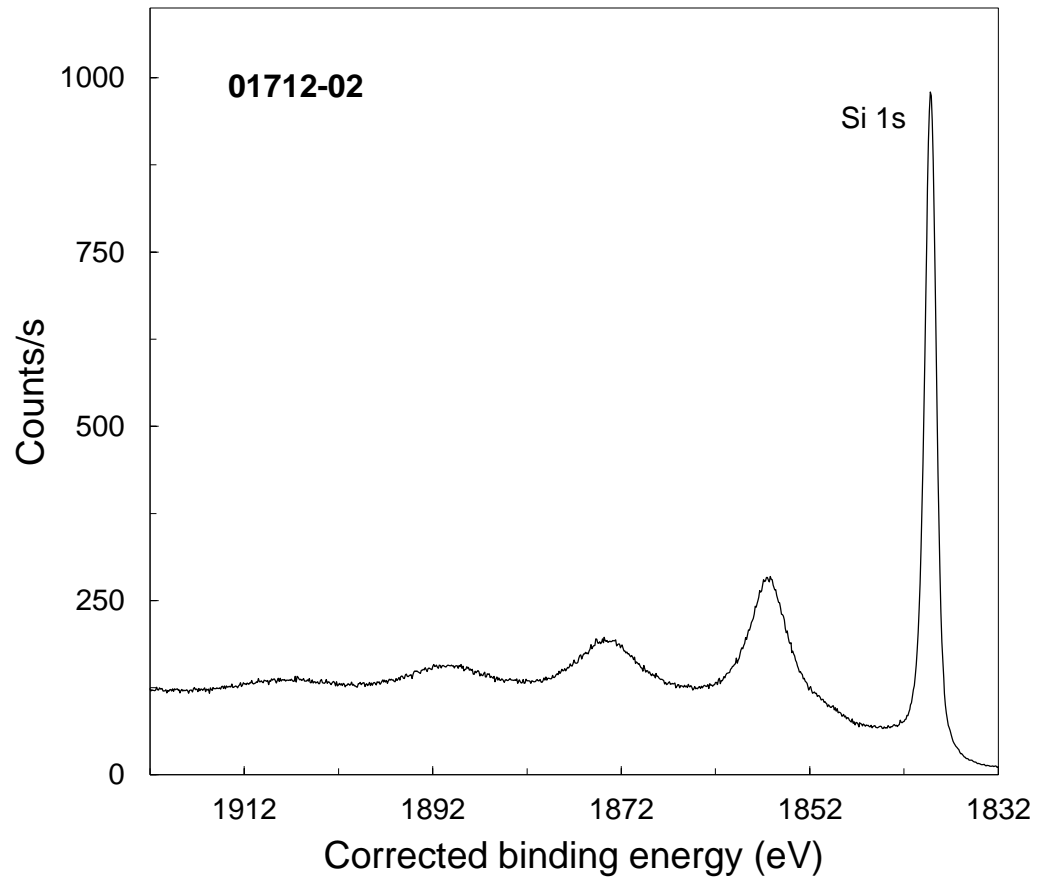
Effective Detector Width: 12.4 eV



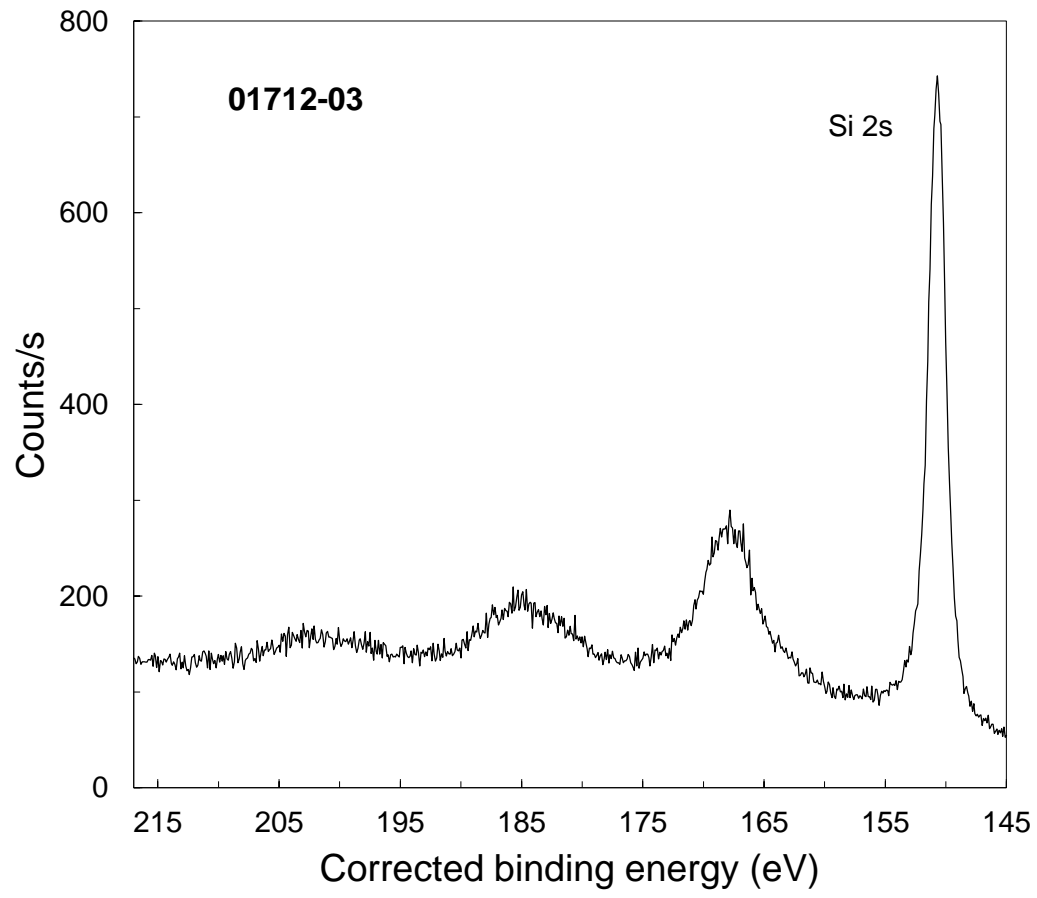
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