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HAXPES of Si(100) with Cr Kα excitation

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Si (100) wafer was analyzed by high-energy photoelectron spectroscopy (HAXPES) using monochromatic Cr Kα 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 Kα

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

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 Kα 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^3) 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^+ 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^+ ions (500 eV)

Temp. During Analysis: 300 K

Pressure During Analysis: < 6.10^{-7} 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^N): The energy dependence can be modeled using the following equation: $\frac{A}{E_p} = (\frac{a^2}{a^2+R^2})^b$, where a and b are constants, E_p is the pass energy, A is the peak area and R is the retard ratio equal to E/E_p, 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_α monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Beam Size: 100 μm x 100 μm

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 x 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 photoionzation 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 Kα 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 Kα 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 Kα 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.

Surface Science Spectra

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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

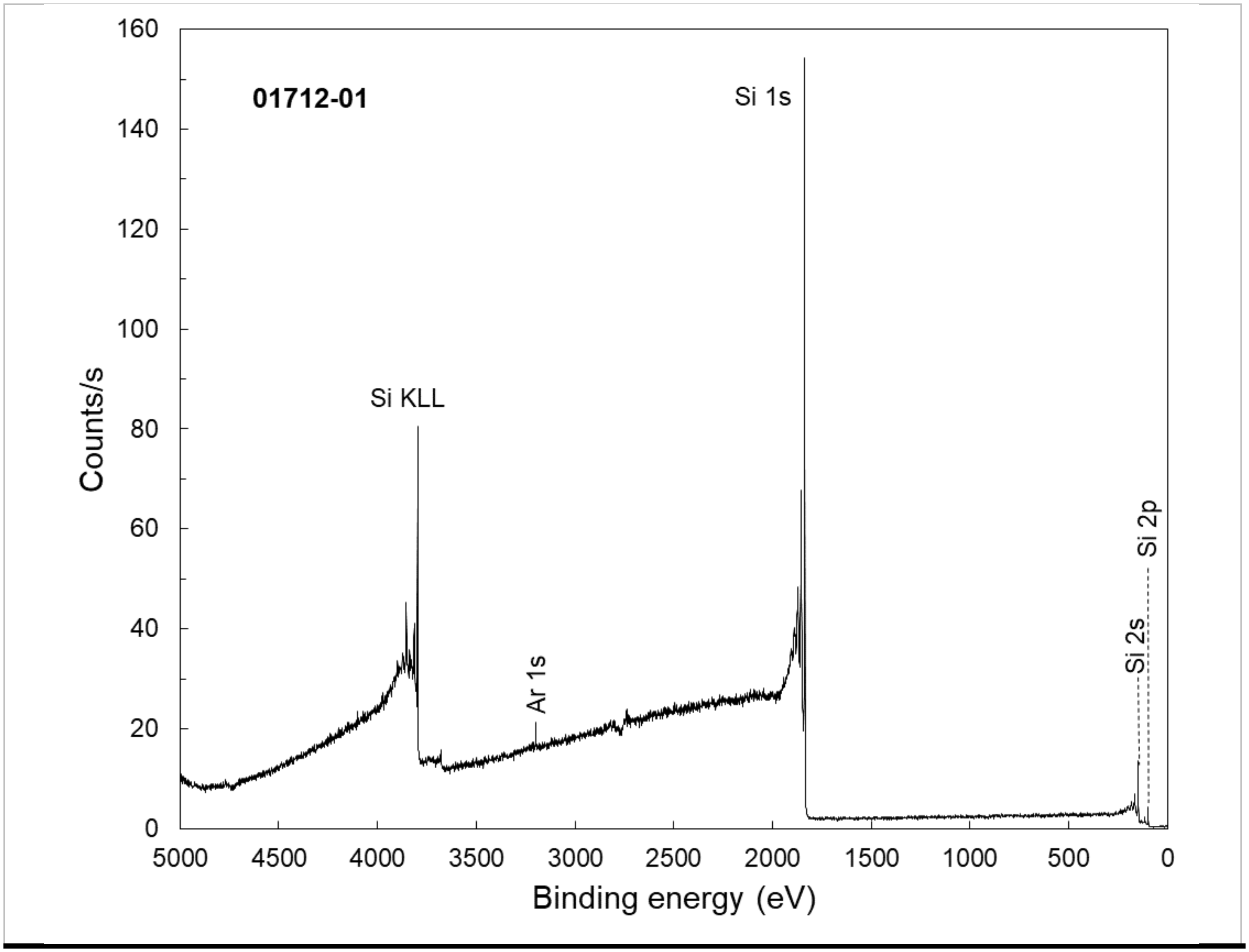
Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV x cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
...	Ag3d$_{5/2}$	368.12	0.63	114999	...	...	...
...	Cu2p$_{3/2}$	932.61	0.96	40205	...	...	...
...	Au4f$_{7/2}$	83.89	0.78	100500	...	...	...

The spectra in the analyzer calibration table were recorded using Al Kα photons.

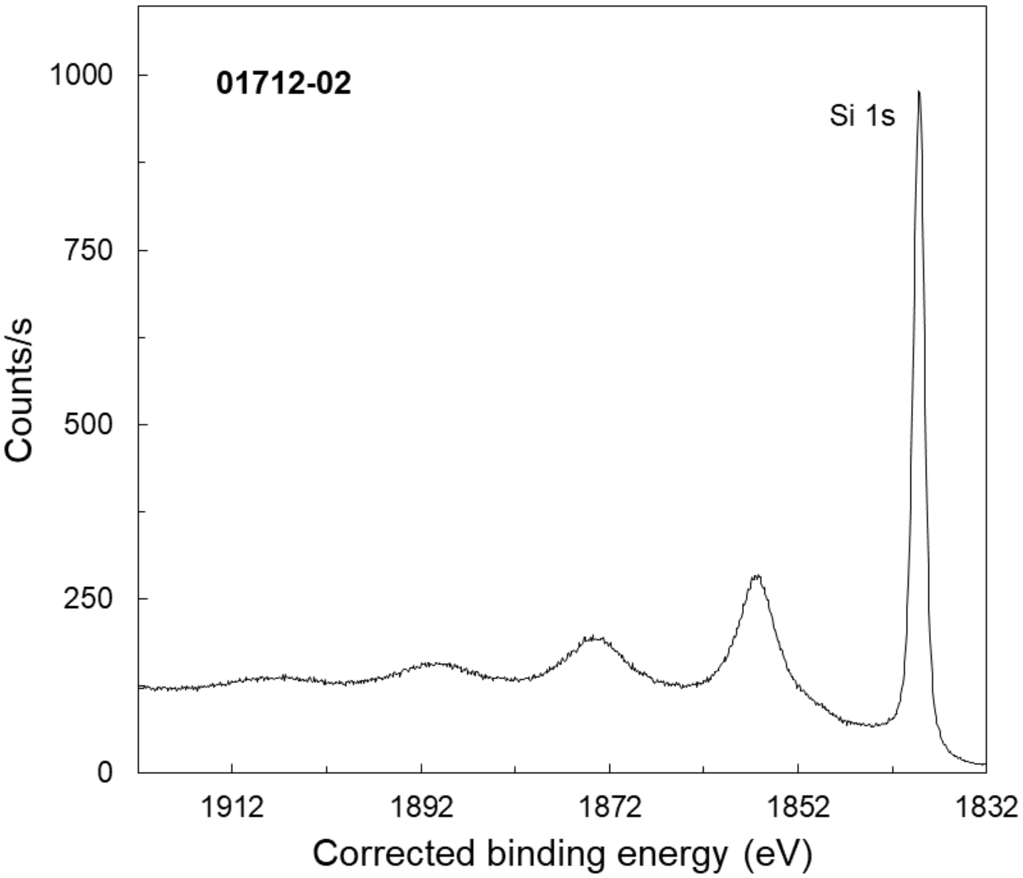
GUIDE TO FIGURES

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.



Accession #	01712-01
Host Material	Si
Technique	XPS
Spectral Region	survey
Instrument	ULVAC-PHI Quantes
Excitation Source	Cr K_{α} 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



- **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 °

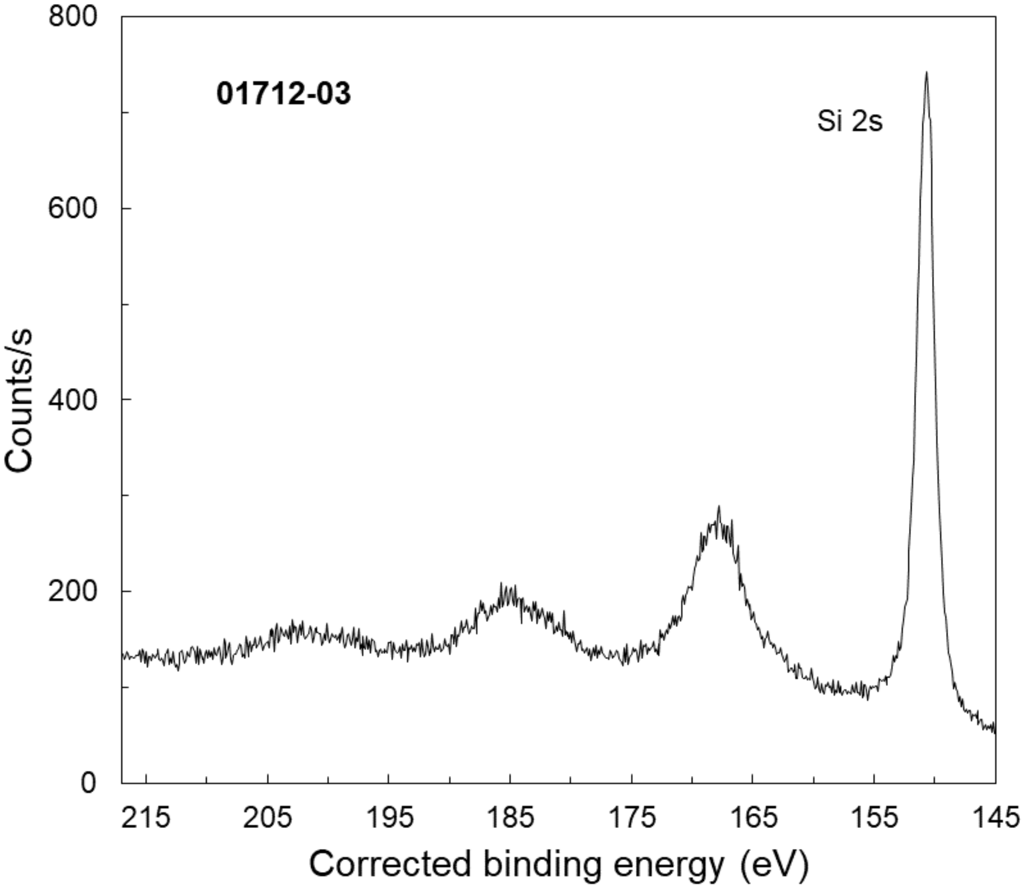
Analyzer Pass Energy 112 eV

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



- **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

Surface Science Spectra ACCEPTED MANUSCRIPT

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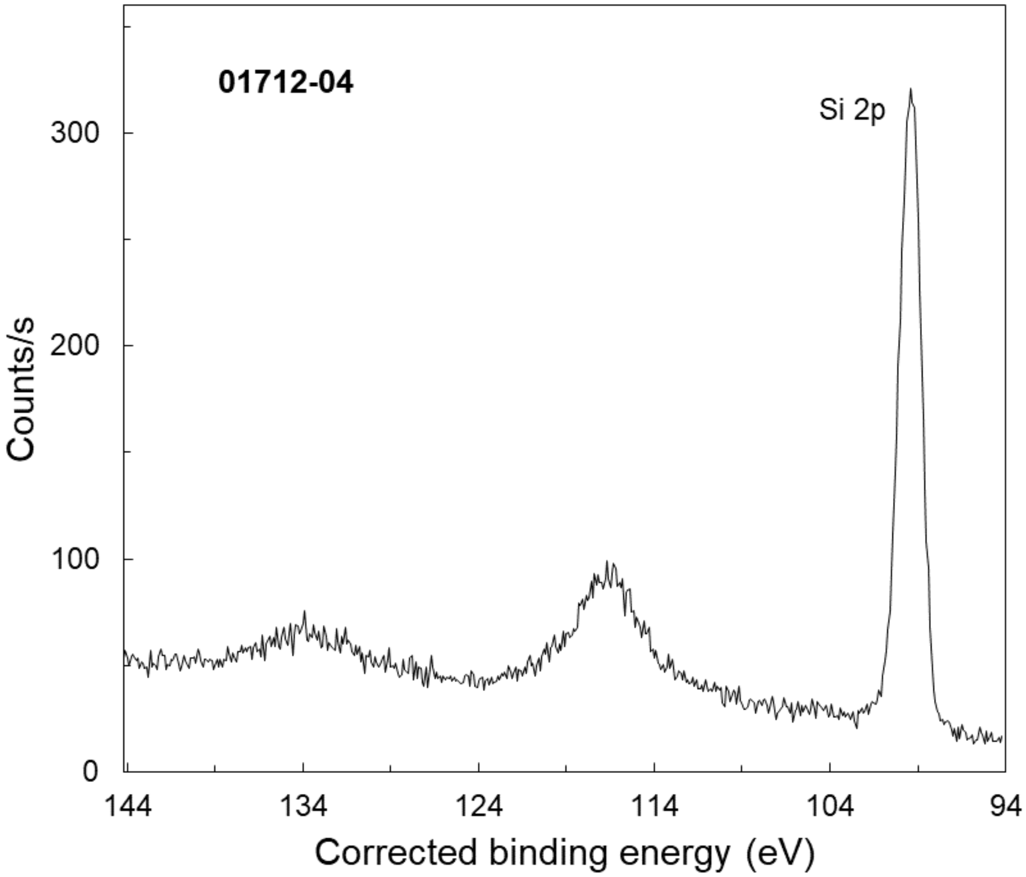

- **Accession #:** 01712-04
- **Host Material:** Si
- **Technique:** XPS
- **Spectral Region:** Si 2p

Instrument: ULVAC-PHI Quantes
Excitation Source: Cr K_α 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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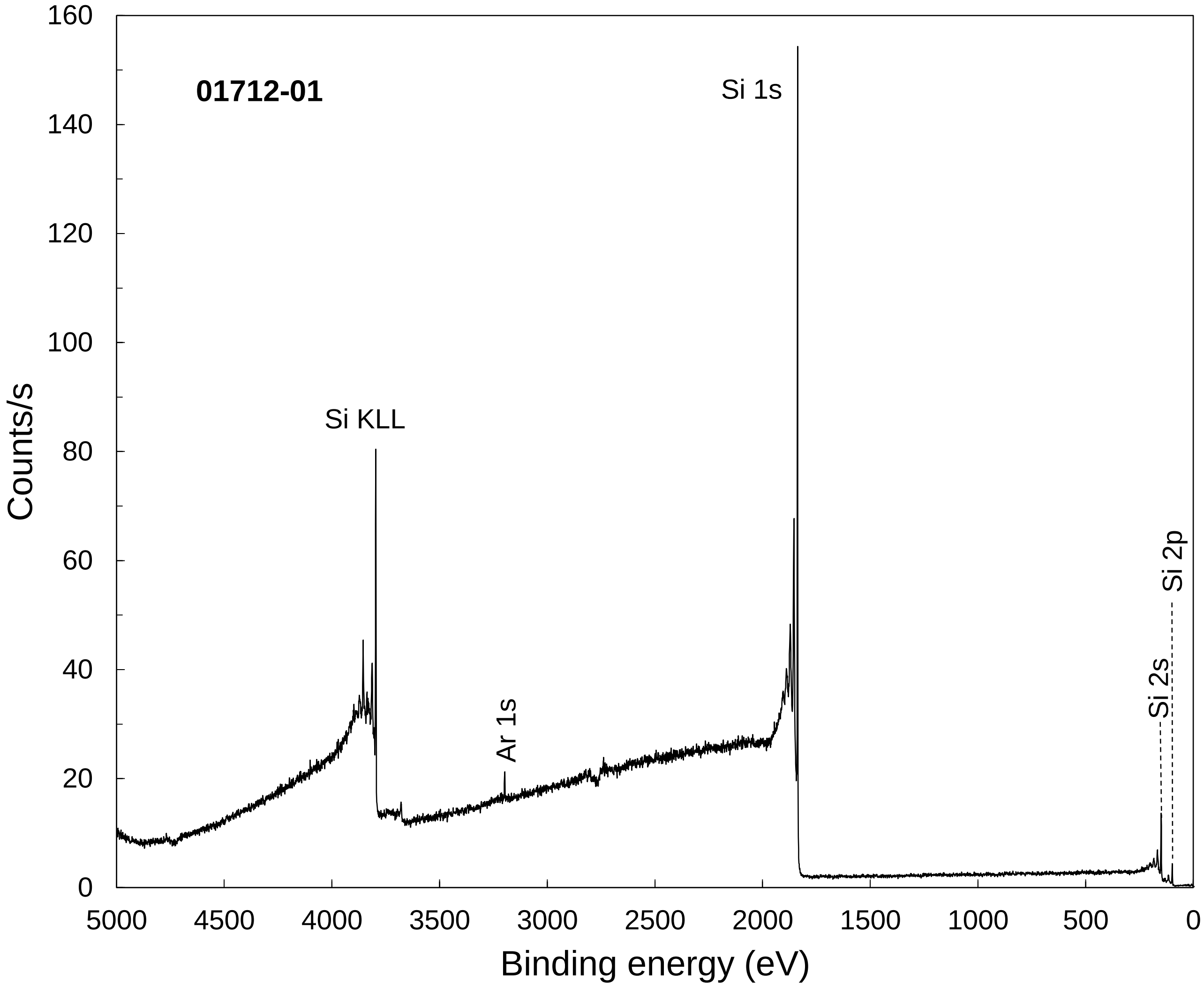

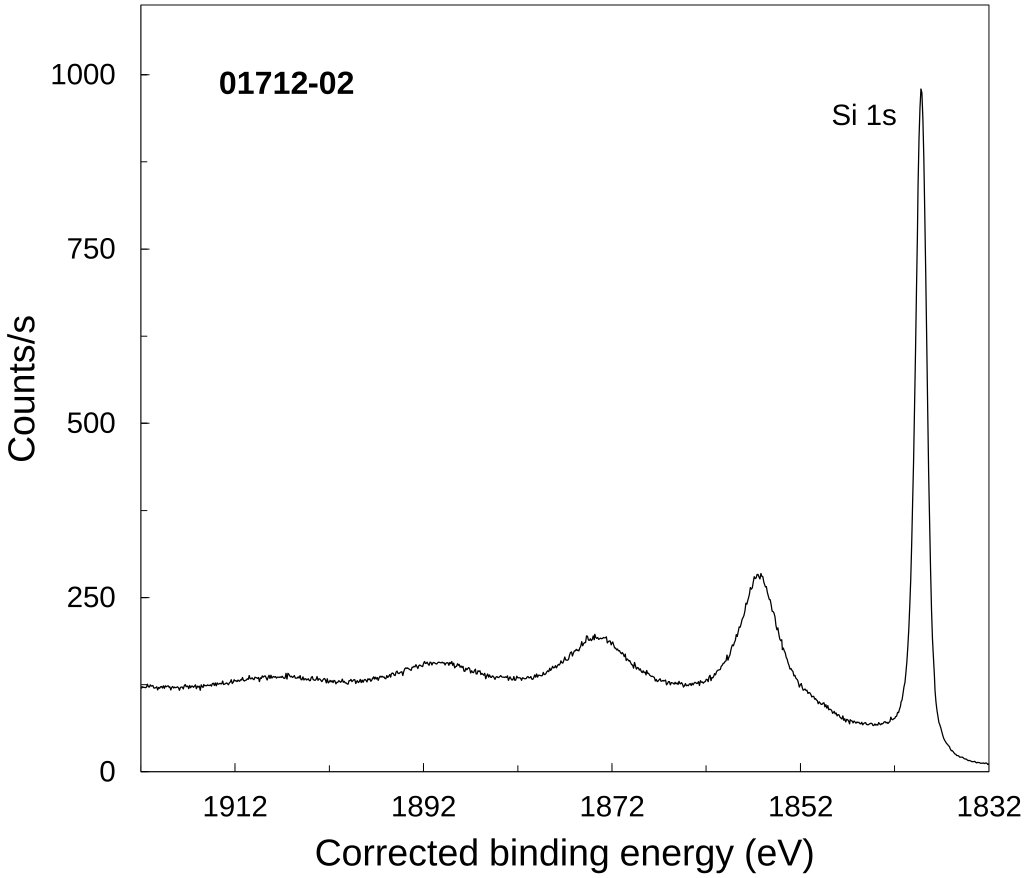
01712-02
Si 1s
Counts/s
0
250
500
750
1000
1912
1892
1872
1852
1832
Corrected binding energy (eV)

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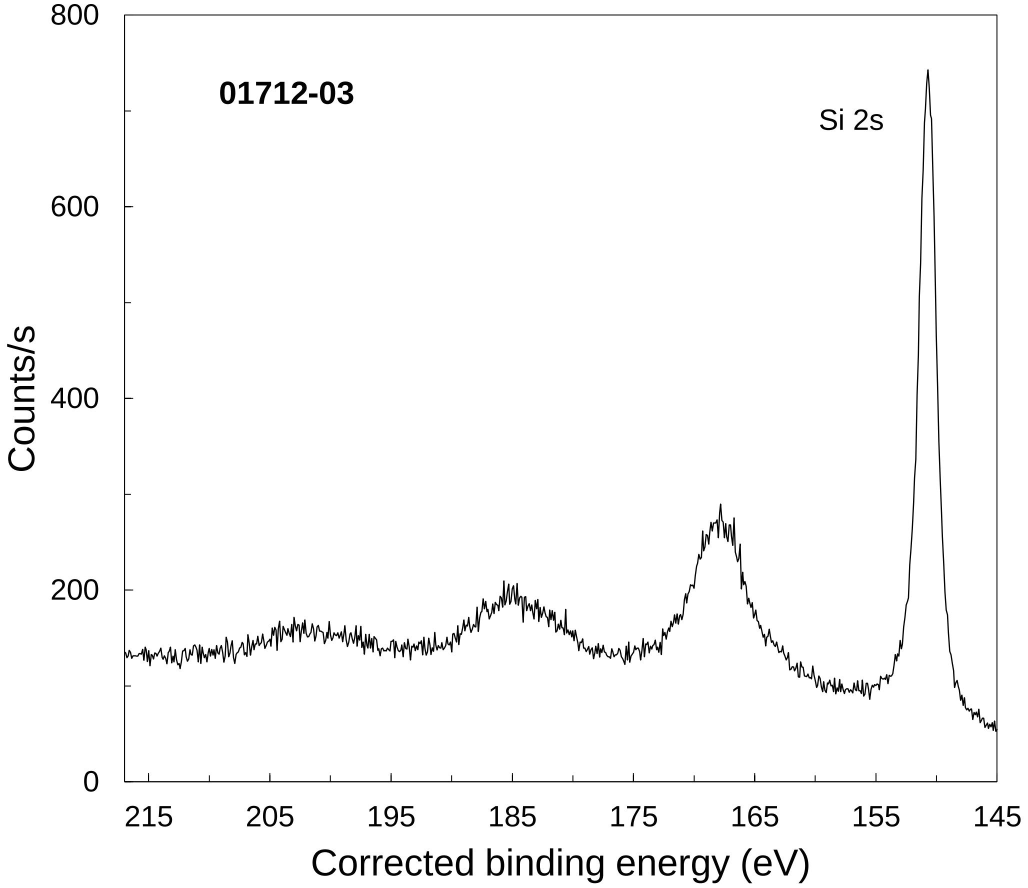

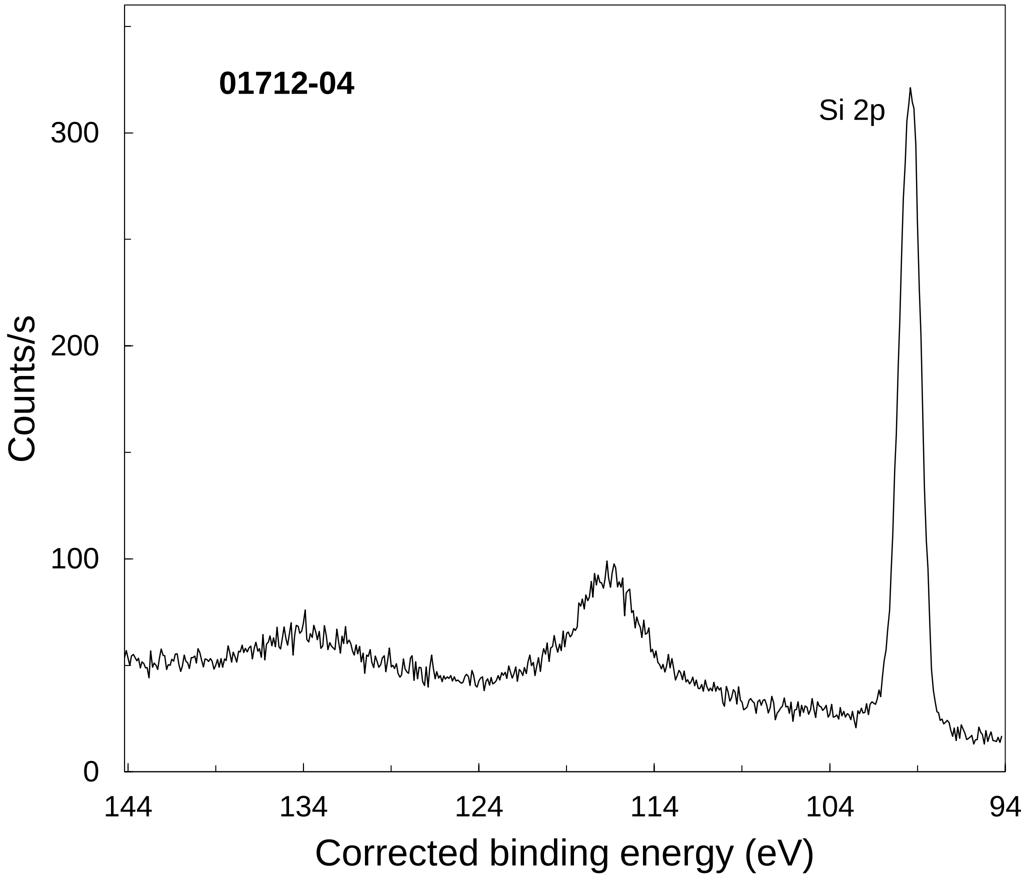
01712-04
Si 2p
Counts/s
0
100
200
300
144
134
124
114
104
94
Corrected binding energy (eV)