

Core Level XPS Spectra of Silicon Carbide Using Zirconium and Magnesium Radiations

A. R. Chourasia

Department of Physics, Texas A & M University—Commerce, Commerce, TX 75429

Core levels of silicon and carbon in the hexagonal form of silicon carbide have been studied by x-ray photoelectron spectroscopy. For this purpose, zirconium L_{α} (energy = 2042.4 eV) and magnesium K_{α} (energy = 1253.6 eV) radiations have been employed. The XPS data in the silicon $1s$, $2s$, $2p$, and Auger KLL , and carbon $1s$ and Auger KLL regions are presented. The data set will serve as a source of valuable information for analyzing spectra associated with silicon and carbon in the insulating sample of silicon carbide. © 2001 American Vacuum Society.
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Keywords: silicon carbide; core levels; x-ray photoelectron spectroscopy; zirconium; magnesium

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Accession # 00636

Technique: XPS

Host Material: SiC free-standing film (0001)

Instrument: Physical Electronics 5100 ESCA System

Major Elements in Spectrum: Si, C

Minor Elements in Spectrum: O

Printed Spectra: 13

Spectra in Electronic Record: 19

Spectral Category: comparison

Original Submission: 6/07/2001

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INTRODUCTION

The data presented in this article are related to the earlier reported work (Refs. 1 and 2). The calibration spectra are in accord with the standards (Ref. 3).

SPECIMEN DESCRIPTION

Host Material: SiC free-standing film (0001)

CAS Registry #: 409-21-2

Host Material Characteristics: homogeneous; solid; single crystal; semiconductor; ceramic

Chemical Name: silicon carbide

Host Composition: SiC

Form: self-standing film

Structure: 6H (0001) hexagonal

History & Significance: Many silicon compounds used in the semiconductor industry are insulating in nature. The Auger parameter is employed to study the chemical environment of atoms in such nonconducting materials. The present data set will form a basis for such an investigation.

As Received Condition: self-standing silicon carbide film

Analyzed Region: the surface is likely to be ion-damaged

Ex Situ Preparation/Mounting: The sample was ultrasonically cleaned with methanol. The sample was then screwed onto the PHI sample holder.

In Situ Preparation: The sample was lightly sputter etched using argon ions (current density = $4 \mu\text{A}/\text{cm}^2$). The sputtering time was 5 min. Approximately 4 nm of the surface was etched.

Charge Control: none

Temp. During Analysis: 300 K

Pressure During Analysis: $<6.6 \times 10^{-8}$ Pa

INSTRUMENT DESCRIPTION

Manufacturer and Model: Physical Electronics 5100 ESCA System

Analyzer Type: spherical sector

Detector: single channeltron detector

Number of Detector Elements: 1

INSTRUMENT PARAMETERS COMMON TO ALL SPECTRA

■ Spectrometer

Analyzer Mode: constant pass energy

Throughput ($T = E^N$): $N = -1$

Excitation Source Window: 2 μm beryllium window for Zr source; 2 μm aluminum window for Mg source

Source Strength: 300 W

Source Beam Size: 25 mm \times 25 mm

Analyzer Width: 3000 μm \times 10000 μm

Signal Mode: pulse single channel

■ Geometry

Incident Angle: 9°

Source to Analyzer Angle: 54°

Emission Angle: 45°

Specimen Azimuthal Angle: 0°

Acceptance Angle from Analyzer Axis: 0°

Analyzer Angular Acceptance Width: $4^\circ \times 4^\circ$

■ Ion Gun

Manufacturer and Model: Physical Electronics 04-300

Energy: 3000 eV

Current: 0.004 mA

Current Measurement Method: biased stage

Sputtering Species: Ar

Spot Size (unrastered): 800 μm

Raster Size: 15000 μm \times 15000 μm

Incident Angle: 40°

Polar Angle: 45°

Azimuthal Angle: 58°

Comment: Sputtering was performed using a differentially pumped ion gun.

DATA ANALYSIS METHOD

Peak Shape and Background Method: The area under the curve is calculated in the following steps:

(1) The raw data defining the curve is used to calculate the absolute area under the curve. The area is evaluated by parabolic interpolation.

(2) The area of the background is calculated using the formula for calculating the area of a trapezoid, $1/2 \times [(b + c) \times (n - 1)]$, where b = the number of counts for the beginning end point, c = the number of counts for the ending end point, and n = total number of data points. The area of the background is then subtracted from the absolute area under the curve.

(3) The area is normalized for time by dividing the area by the time/step used to acquire the data.

(4) The area is normalized for the size of the unit step by multiplying the area by the step size.

Software is provided by Physical Electronics.

Quantitation Method: The atomic concentration for element X =

$[I_X/(S_X T_X)]/[\sum I_X/(S_X T_X)]$, where I = area under the peak, S = sensitivity factor, and T = total acquisition time per data point. The \sum represents the sum over all the elements present. The software is provided by Physical Electronics.

ACKNOWLEDGMENTS

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REFERENCES

1. A. R. Chourasia, S. J. Hood, and D. R. Chopra, *J. Vac. Sci. Technol. A* **14**, 699 (1996).
2. A. R. Chourasia, *Surf. Sci. Spectra* **5**, 115 (1998).
3. J. F. Moulder, W. F. Stickle, P. E. Sobol, and K. D. Bomben, *Handbook of X-ray Photoelectron Spectroscopy* (Physical Electronics, Eden Prairie, MN, 1992).

SPECTRAL FEATURES TABLE

Spectrum ID #	Element/Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV-cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
00636-02	Si 1s	1840.5	3.38	27790
00636-03	Si 2s	151.7	3.02	2513
00636-04	Si 2p	100.45	2.49	1565	0.270	25.1	...
00636-05	Si KLL	427.4	2.70	56681
00636-06	C 1s	283.3	3.10	2345	0.250	40.5	...
00636-07	O 1s	530.8	4.68	5249	0.660	34.4	...
00636-09	Si 2s	151.65	2.13	18598
00636-10	Si 2p	100.45	1.75	20409	0.270	43.9	...
00636-11	C 1s	283.35	1.89	21889	0.250	49.6	...
00636-13	O 1s	532.30	2.27	7527	0.660	6.5	...

ANALYZER CALIBRATION TABLE

Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV-cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
14	Ag 3d _{5/2}	368.25	1.87	21803
15	Au 4f _{7/2}	83.95	2.11	8516
16	Cu 2p _{3/2}	932.60	2.15	46290
17	Ag 3d _{5/2}	368.25	0.88	246128
18	Au 4f _{7/2}	84.05	1.00	191946
19	Cu 2p _{3/2}	932.65	1.19	452023

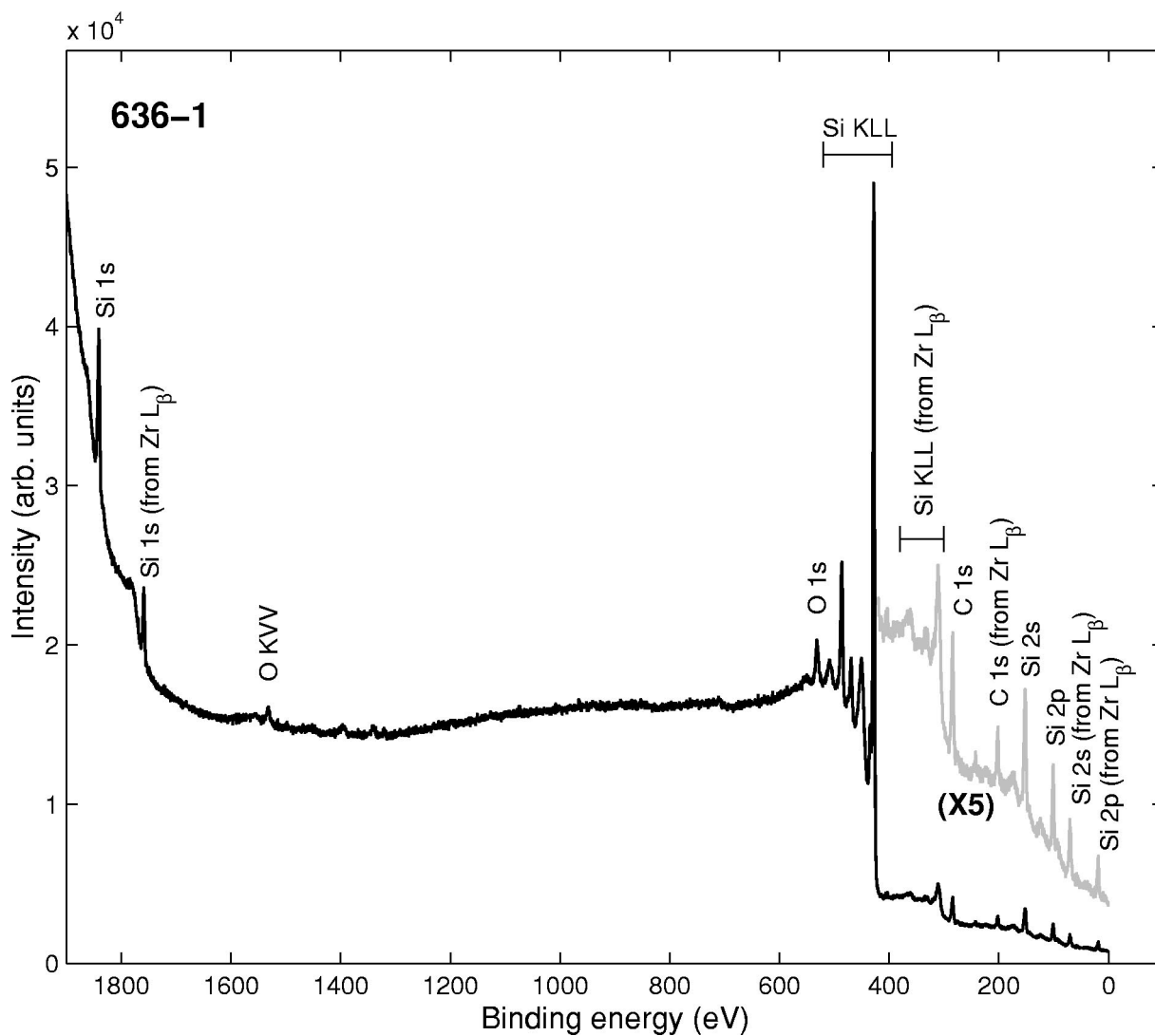
GUIDE TO FIGURES

Spectrum (Accession) #	Spectral Region	Sample Voltage*	Multiplier	Baseline	Comment #
636-1	Survey	0	1	0	1
636-2	Si 1s	0	1	0	1
636-3	Si 2s	0	1	0	1
636-4	Si 2p	0	1	0	1
636-5	Si KLL	0	1	0	1
636-6	C 1s	0	1	0	1
636-7	O 1s	0	1	0	1
636-8	Survey	0	1	0	2
636-9	Si 2s	0	1	0	2
636-10	Si 2p	0	1	0	2
636-11	C 1s	0	1	0	2
636-12	C KLL	0	1	0	2
636-13	O 1s	0	1	0	2
636-14 [NP]**	Ag 3d	0	1	0	1, 3
636-15 [NP]	Au 4f	0	1	0	1, 3
636-16 [NP]	Cu 2p	0	1	0	1, 3
636-17 [NP]	Ag 3d	0	1	0	2, 3
636-18 [NP]	Au 4f	0	1	0	2, 3
636-19 [NP]	Cu 2p	0	1	0	2, 3

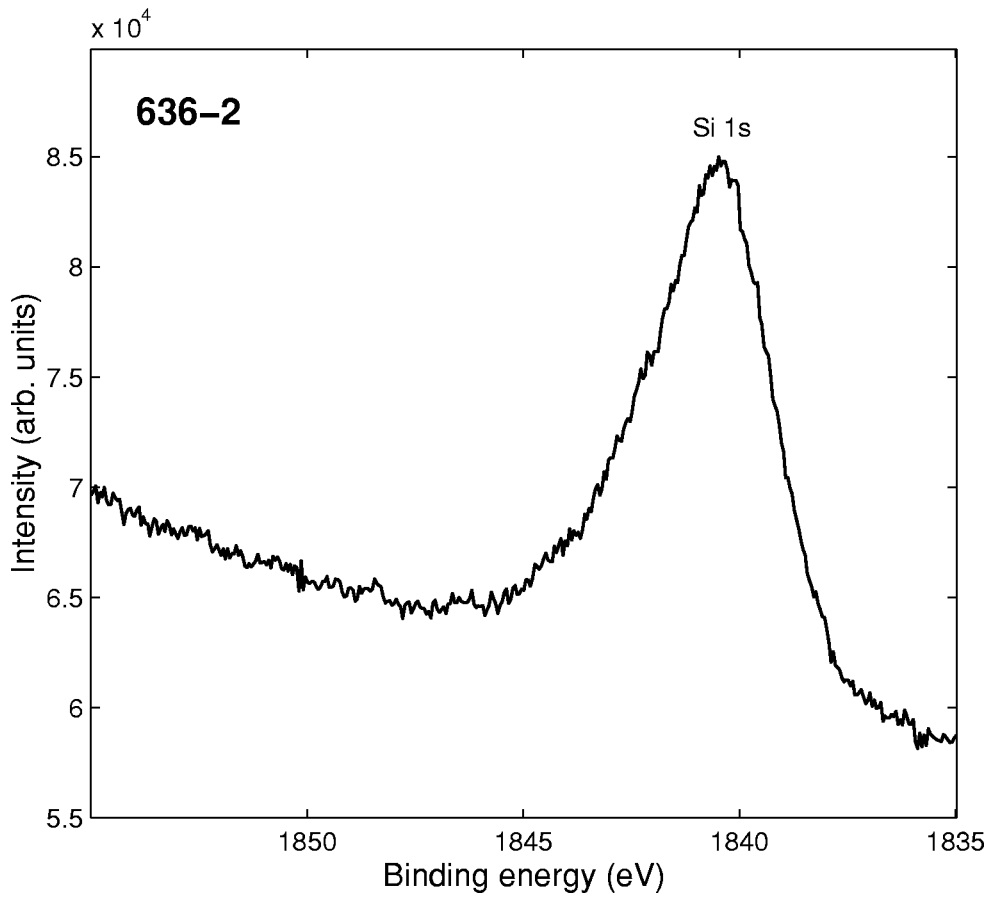
* Inferred sample potential relative to spectrometer ground due to charging, flood gun, or other phenomena.

** [NP] signifies not published; digital spectra are archived in SSS database but not reproduced in the printed journal.

1. Zr L_α excitation source
2. Mg K_α excitation source
3. Calibration spectrum

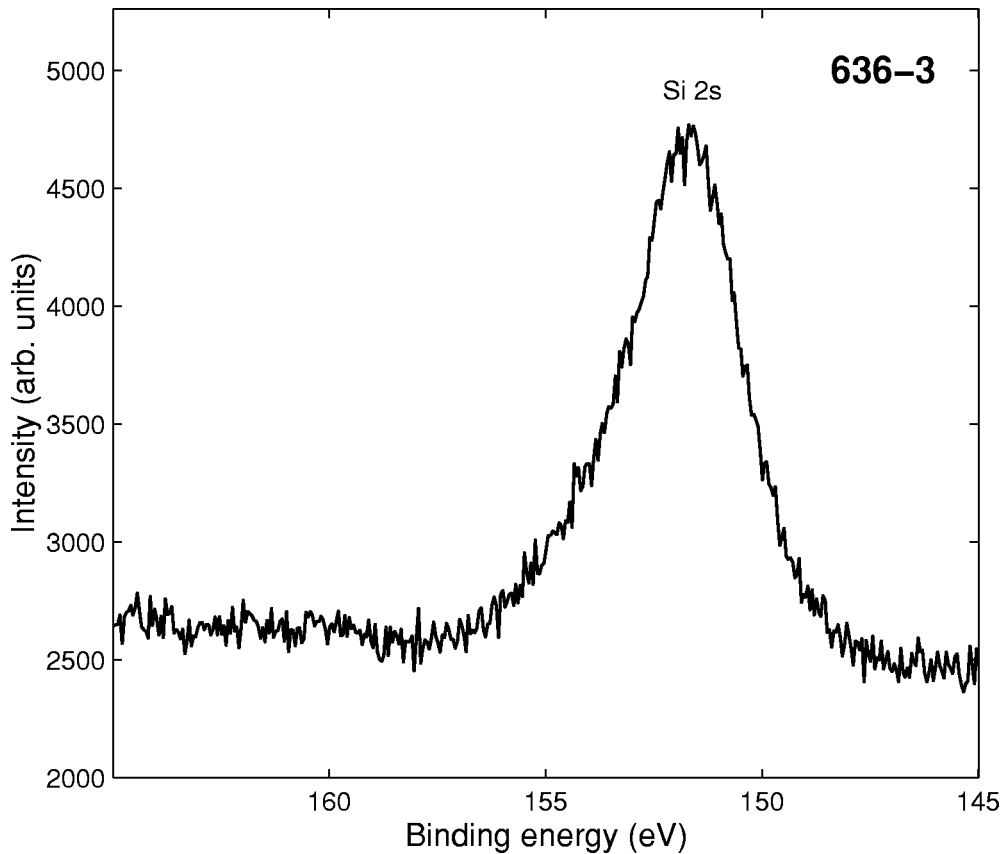


Accession #	00636-01
Host Material	SiC free-standing film (0001)
Technique	XPS
Spectral Region	survey
Instrument	Physical Electronics 5100 ESCA System
Excitation Source	Zr L_{α}
Source Energy	2042.4 eV
Source Strength	300 W
Source Size	25 mm \times 25 mm
Analyzer Type	spherical sector
Incident Angle	9°
Emission Angle	45°
Analyzer Pass Energy	89.45 eV
Analyzer Resolution	0.89 eV
Total Signal Accumulation Time	532.14 s
Total Elapsed Time	585.35 s
Number of Scans	7
Effective Detector Width	0.5 eV



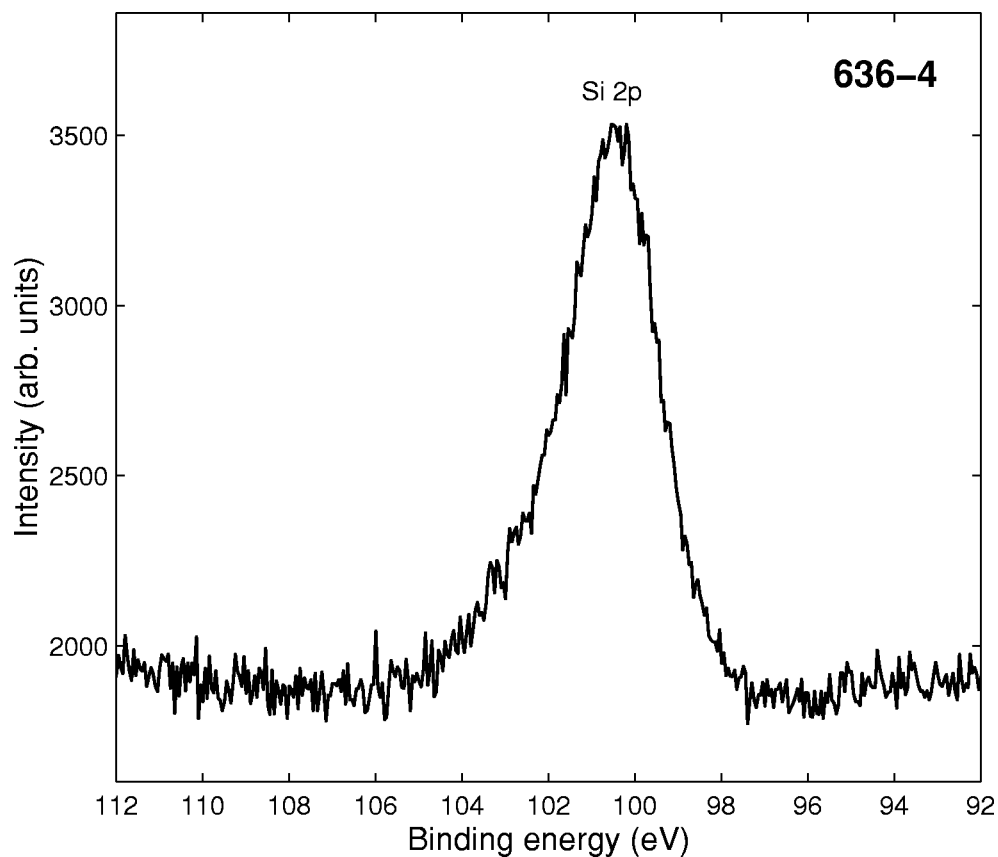
■ **Accession #:** 00636-02
 ■ **Host Material:** SiC free-standing film (0001)
 ■ **Technique:** XPS
 ■ **Spectral Region:** Si 1s

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Zr L_{α}
 Source Energy: 2042.4 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV



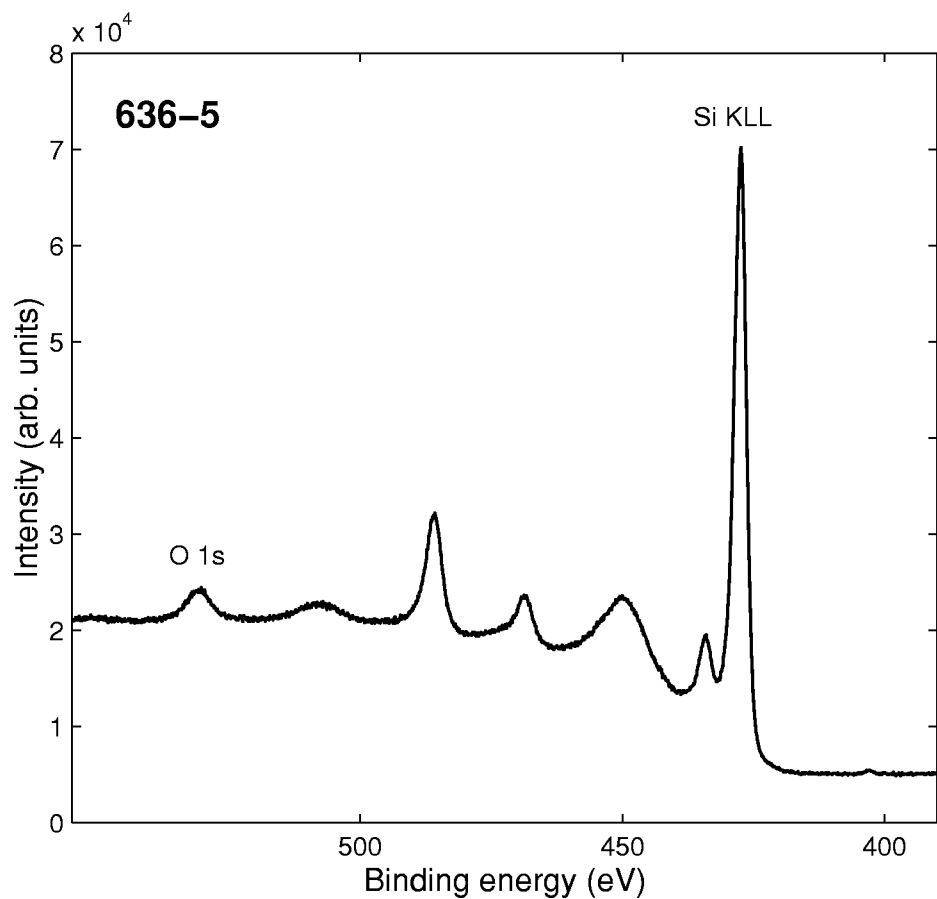
■ **Accession #:** 00636-03
 ■ **Host Material:** SiC free-standing film (0001)
 ■ **Technique:** XPS
 ■ **Spectral Region:** Si 2s

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Zr L_{α}
 Source Energy: 2042.4 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV



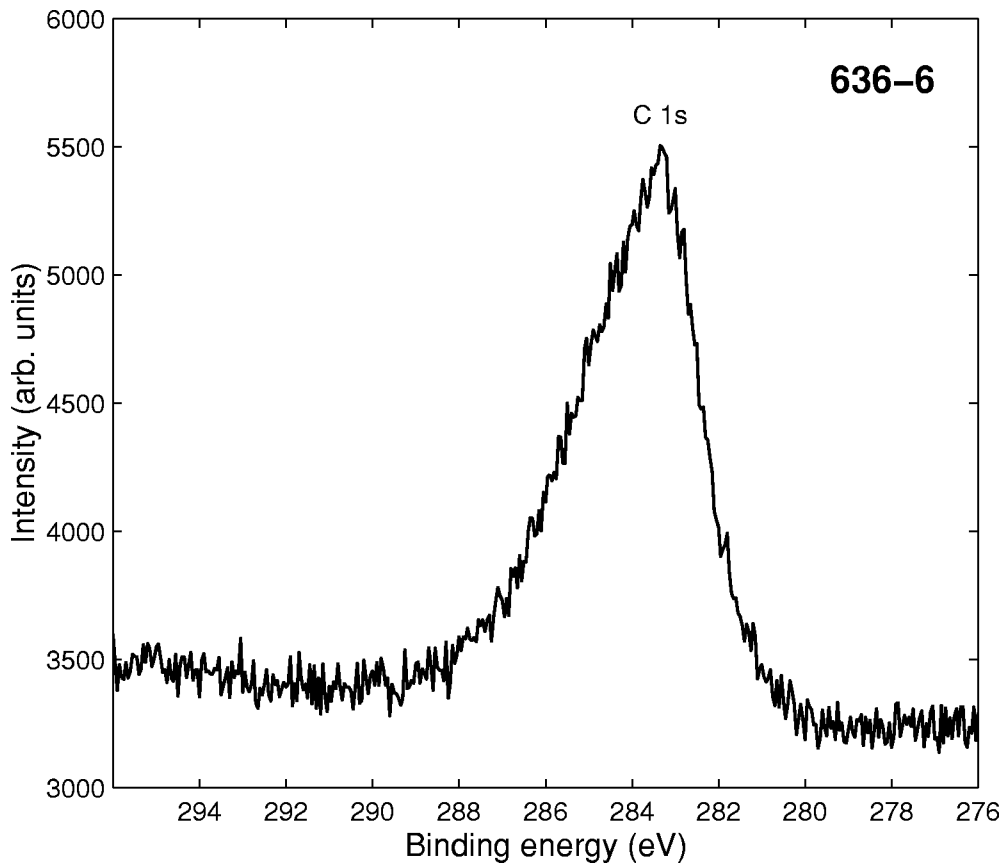
- **Accession #:** 00636-04
- **Host Material:** SiC free-standing film (0001)
- **Technique:** XPS
- **Spectral Region:** Si 2p

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Zr L_{α}
 Source Energy: 2042.4 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV



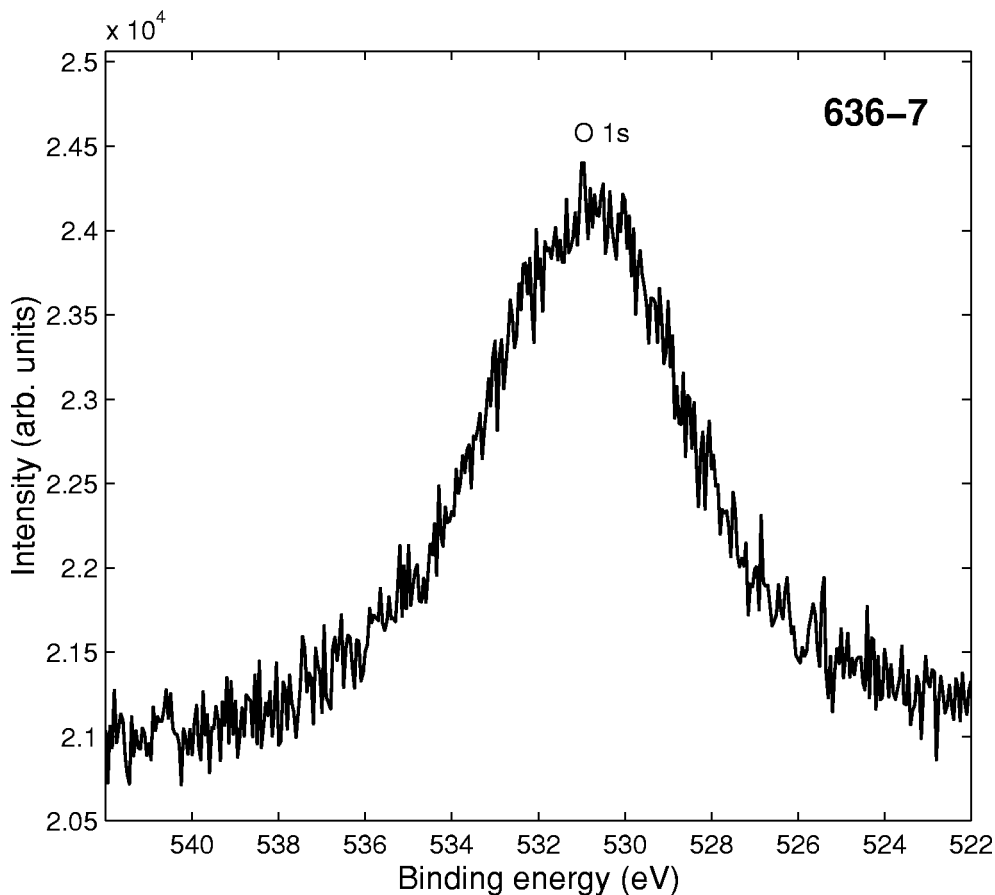
- **Accession #:** 00636-05
- **Host Material:** SiC free-standing film (0001)
- **Technique:** XPS
- **Spectral Region:** Si KLL

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Zr L_{α}
 Source Energy: 2042.4 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 4956 s
 Total Elapsed Time: 5451.6 s
 Number of Scans: 30
 Effective Detector Width: 0.1 eV



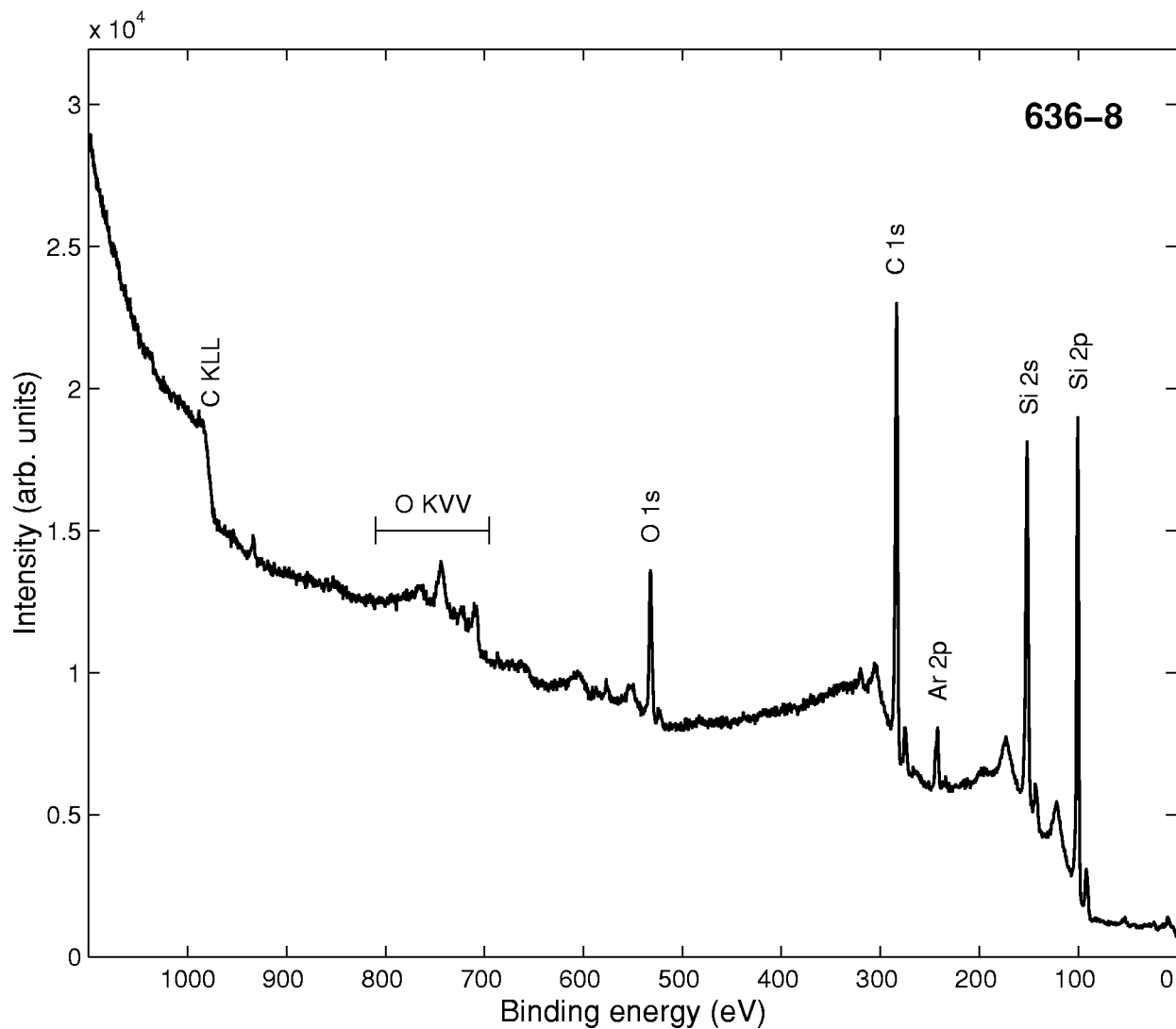
- Accession #: 00636-06
- Host Material: SiC free-standing film (0001)
- Technique: XPS
- Spectral Region: C 1s

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Zr L_{α}
 Source Energy: 2042.4 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV

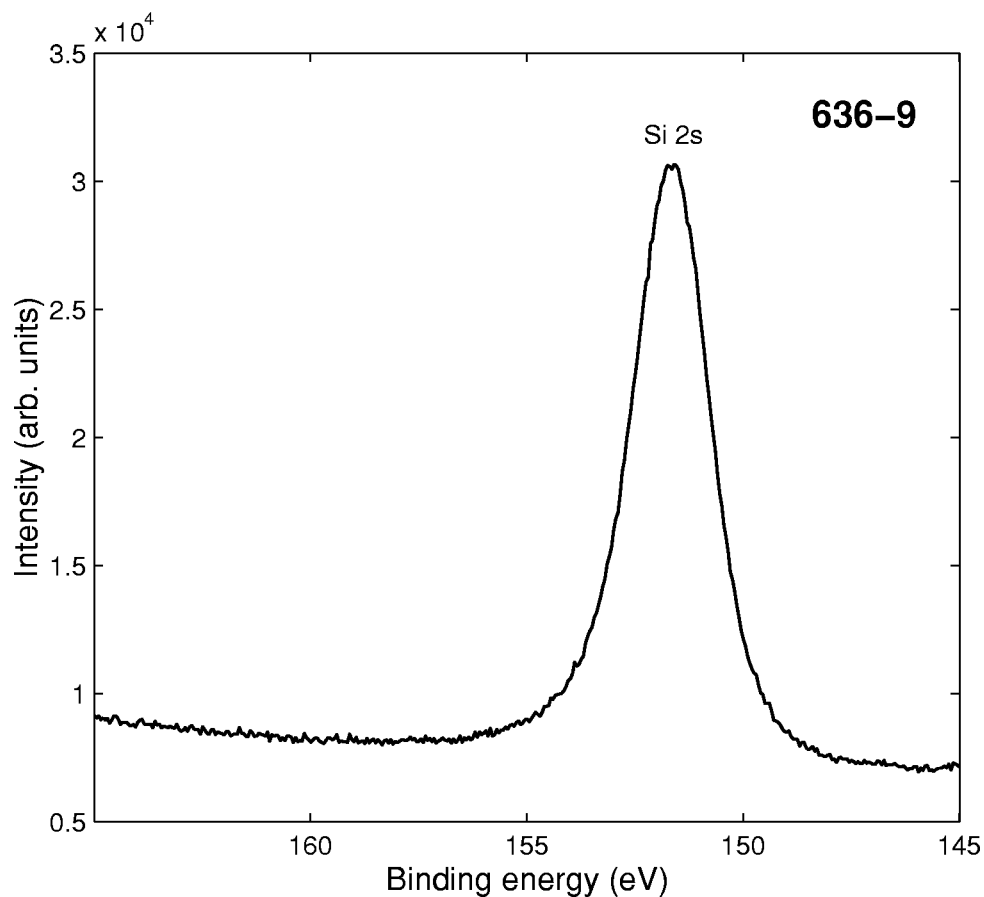


- Accession #: 00636-07
- Host Material: SiC free-standing film (0001)
- Technique: XPS
- Spectral Region: O 1s

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Zr L_{α}
 Source Energy: 2042.4 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV

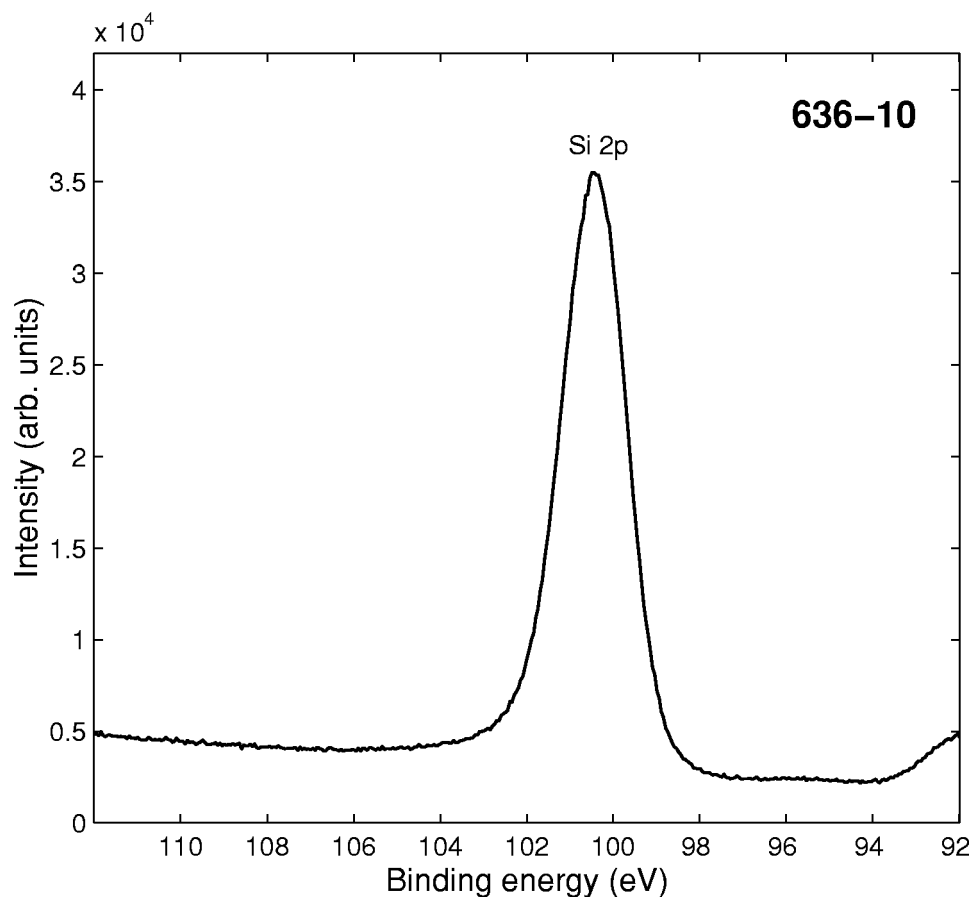


Accession #	00636-08
Host Material	SiC free-standing film (0001)
Technique	XPS
Spectral Region	survey
Instrument	Physical Electronics 5100 ESCA System
Excitation Source	Mg K_{α}
Source Energy	1253.6 eV
Source Strength	300 W
Source Size	25 mm \times 25 mm
Incident Angle	9°
Analyzer Type	spherical sector
Analyzer Pass Energy	89.45 eV
Analyzer Resolution	0.89 eV
Emission Angle	45°
Total Signal Accumulation Time	264.12 s
Total Elapsed Time	290.33 s
Number of Scans	6
Effective Detector Width	0.5 eV



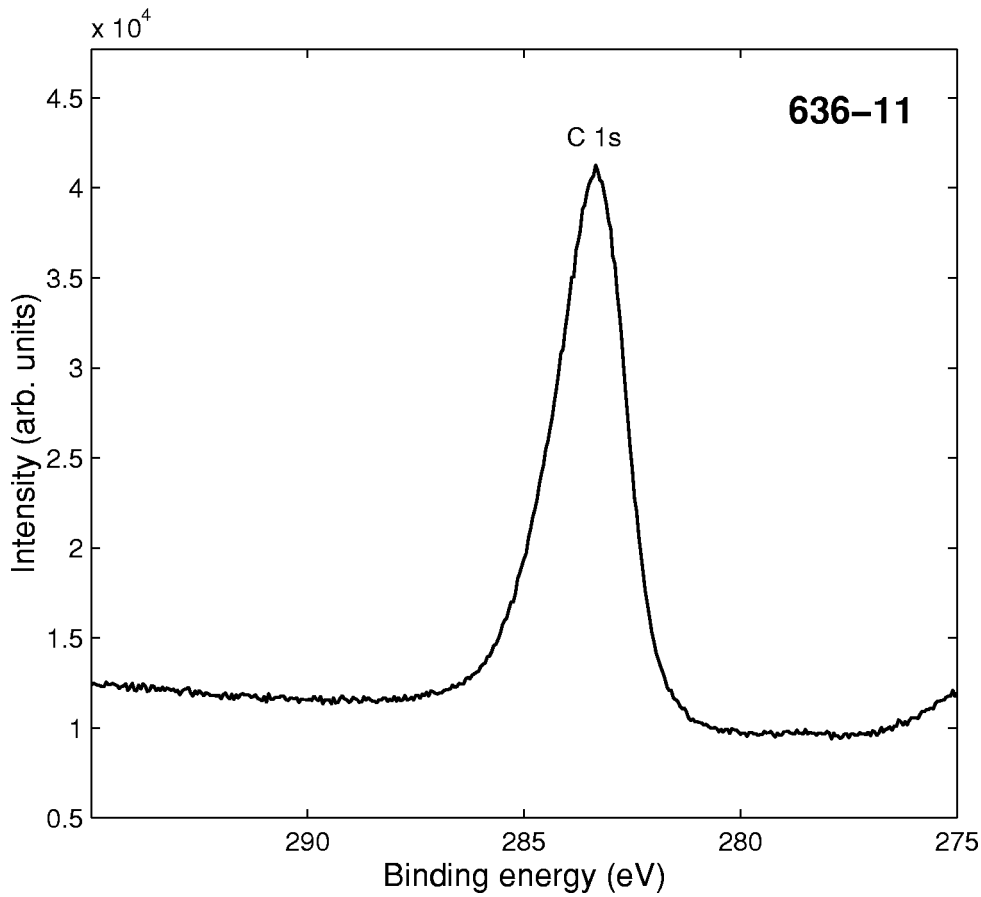
■ **Accession #:** 00636-09
 ■ **Host Material:** SiC free-standing film (0001)
 ■ **Technique:** XPS
 ■ **Spectral Region:** Si 2s

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Mg K_{α}
 Source Energy: 1253.6 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV



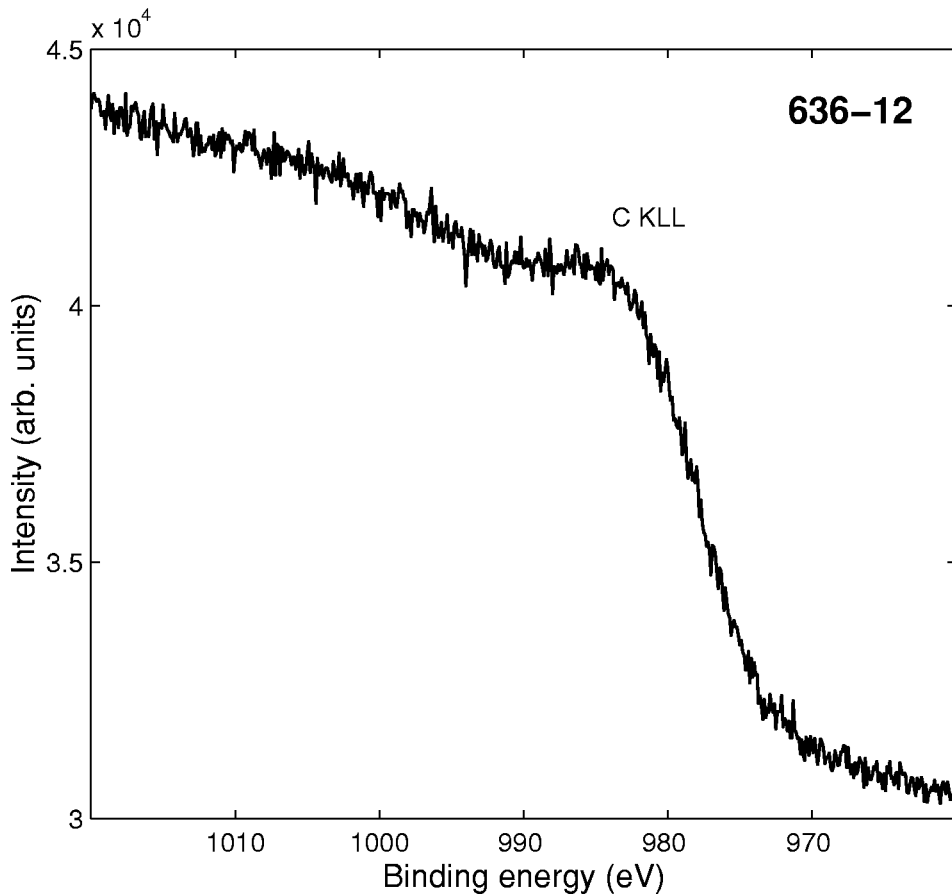
■ **Accession #:** 00636-10
 ■ **Host Material:** SiC free-standing film (0001)
 ■ **Technique:** XPS
 ■ **Spectral Region:** Si 2p

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Mg K_{α}
 Source Energy: 1253.6 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV



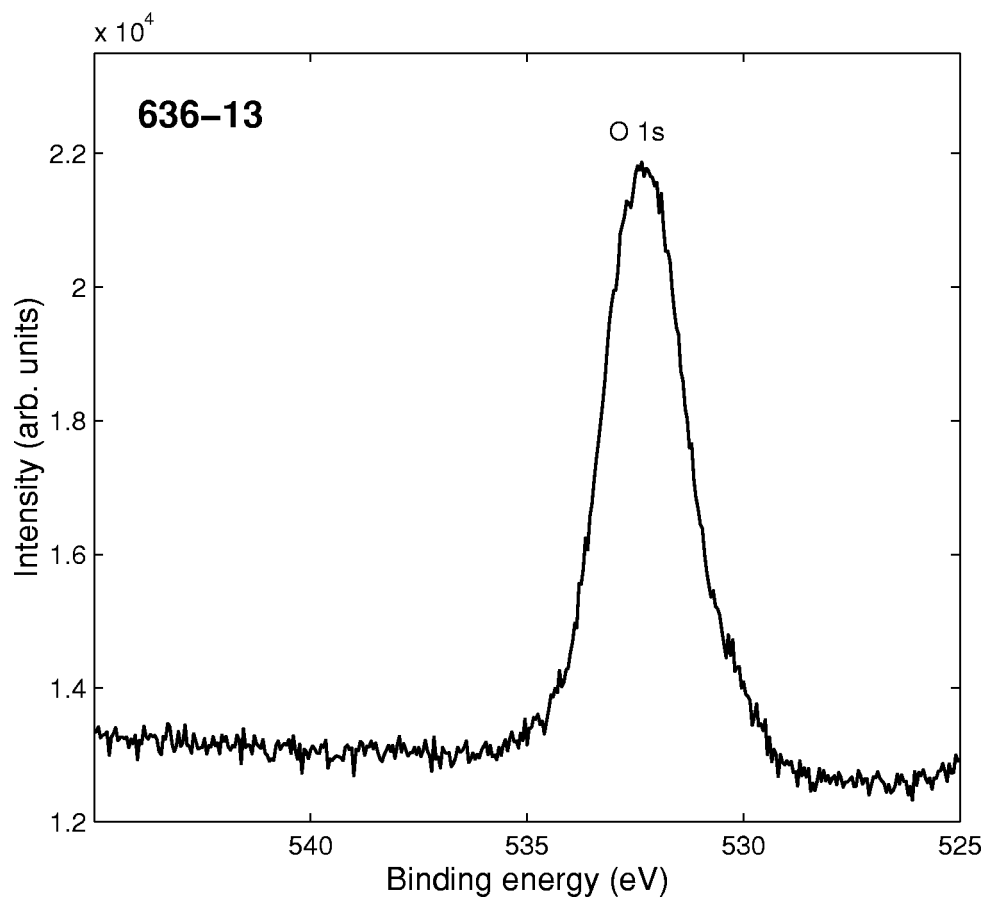
- **Accession #:** 00636-11
- **Host Material:** SiC free-standing film (0001)
- **Technique:** XPS
- **Spectral Region:** C 1s

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Mg K_{α}
 Source Energy: 1253.6 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1203 s
 Total Elapsed Time: 1323.3 s
 Number of Scans: 30
 Effective Detector Width: 0.05 eV



- **Accession #:** 00636-12
- **Host Material:** SiC free-standing film (0001)
- **Technique:** XPS
- **Spectral Region:** C KLL

Instrument: Physical Electronics 5100 ESCA System
 Excitation Source: Mg K_{α}
 Source Energy: 1253.6 eV
 Source Strength: 300 W
 Source Size: 25 mm \times 25 mm
 Incident Angle: 9°
 Analyzer Type: spherical sector
 Analyzer Pass Energy: 17.9 eV
 Analyzer Resolution: 0.18 eV
 Emission Angle: 45°
 Total Signal Accumulation Time: 1803 s
 Total Elapsed Time: 1983.3 s
 Number of Scans: 30
 Effective Detector Width: 0.10 eV



■ **Accession #:** 00636-13
■ **Host Material:** SiC free-standing film (0001)
■ **Technique:** XPS
■ **Spectral Region:** O 1s

Instrument: Physical Electronics
5100 ESCA System

Excitation Source: Mg K_α

Source Energy: 1253.6 eV

Source Strength: 300 W

Source Size: 25 mm × 25 mm

Incident Angle: 9°

Analyzer Type: spherical sector

Analyzer Pass Energy: 17.9 eV

Analyzer Resolution: 0.18 eV

Emission Angle: 45°

Total Signal Accumulation Time:
1203 s

Total Elapsed Time: 1323.3 s

Number of Scans: 30

Effective Detector Width: 0.05 eV
