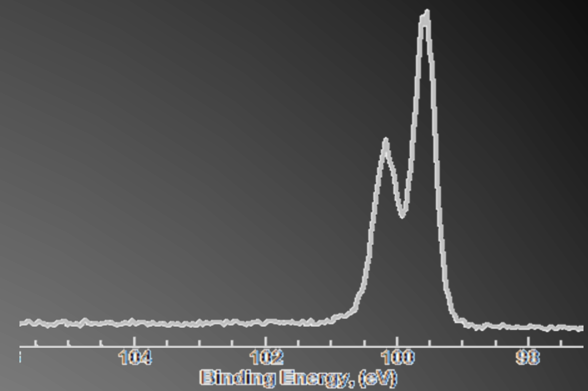
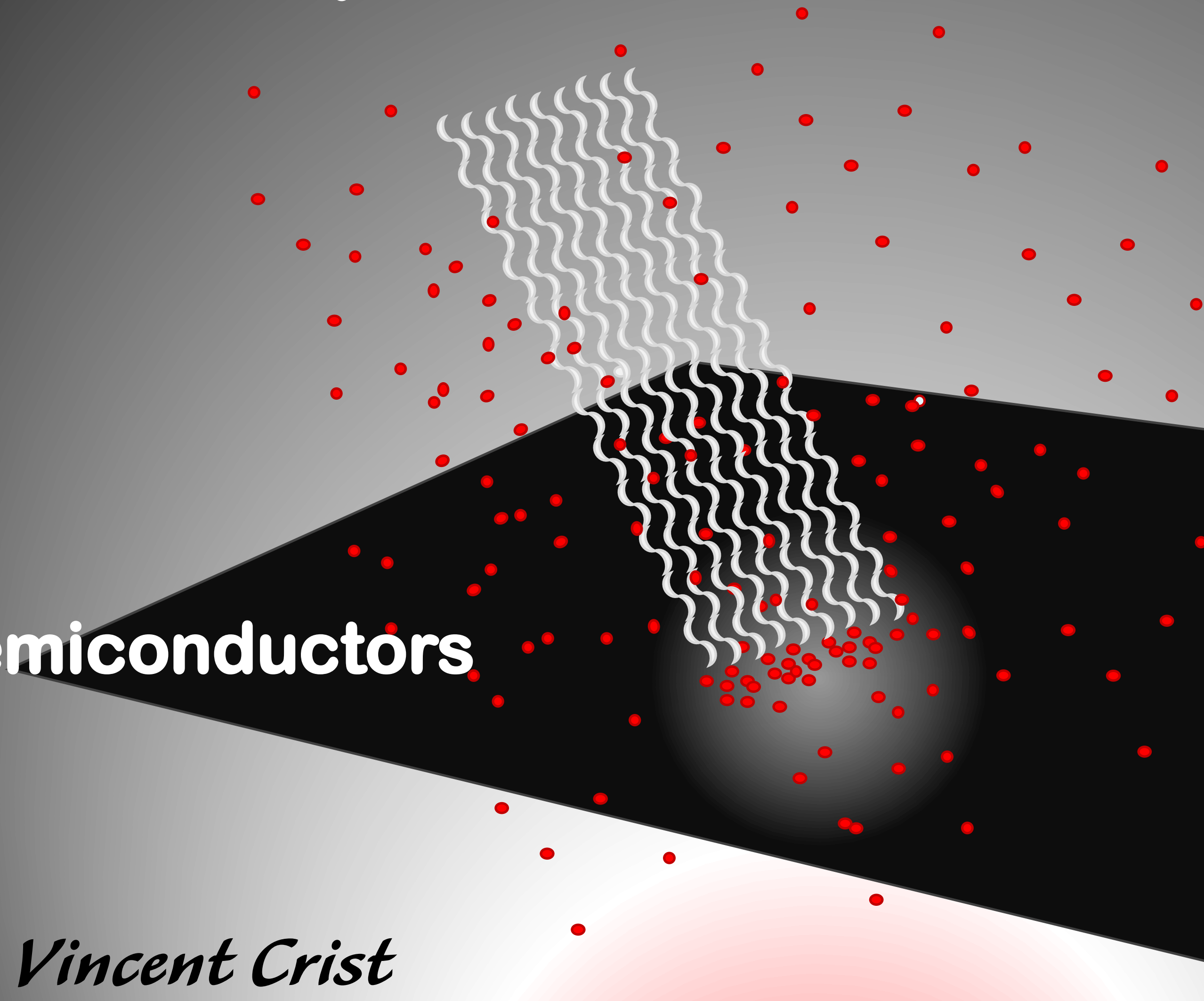
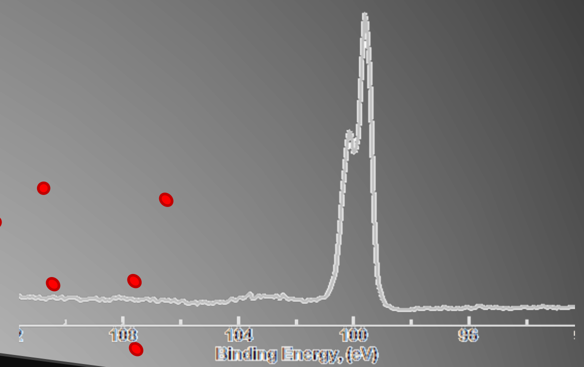
Monochromatic XPS Spectra







Semiconductors

B. Vincent Crist

XPS International, LLC
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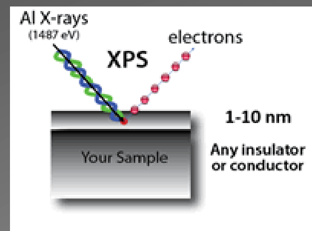
Monochromatic XPS Spectra

Semiconductors



1	H 1s	H_2°		LiH	
2	He 1s	He^+/Be		He^+/C	
3	Li 1s	LiOH	54.9 (1.65) 285.0 531.8 (1.6)	Li_2O	55.6 (1.6) 285.0 530.8 (1.5)
4	Be 1s	Be°	111.8 (0.79) 286.2 111.88 (0.69)	BeO*	113.6 (1.73) 285.0 531.2 (1.71)
5	B 1s	B°	187.5 (0.92) 285.2 187.8 (1.03)	B_2O_3	193.7 (1.30) 285.0 533.7 (1.6)
6	C 1s	HOPG	284.5 (0.42)	Black	284.4 (1.04)
7	N 1s	Kapton	400.9 (1.31) 285.0	BN	398.9 (1.10) 285.0 191.3 (1.03)
8	O 1s	CuO	529.6 (0.98) 284.7 934.0 (1.42)	SiO_2	532.4 (1.27) 285.0 103.1 (1.19)
9	F 1s	Teflon	689.2 (1.8) 285.0 292.0 (1.6)	CaF_2	685.1 (1.53) 285.0 348.1 (1.6)
10	Ne 1s	Ne^+/Be		Ne^+/C	863.1 (1.3)
11	Na 1s	Na°	1071.8 (1.1)	Na_2O	1072.6 (1.78) 285.0 530.6 (1.44)
12	Mg 2p	Mg°	49.7 (0.58) 286.5 49.77 (0.60)	MgO*	49.5 (1.25) 285.0 529.9 (1.38)
13	Al 2p	Al°	72.9 (0.62) 284.9 72.82 (0.41)	Al_2O_3*	74.4 (1.39) 285.0 530.8 (1.60)
14	Si 2p3	Si°	99.8 (0.57) 285.8 99.35 (0.45)	SiO_2*	103.1 (1.19) 285.0 532.4 (1.27)
15	P 2p3	P°	130.1 (0.67) 285.0	InP	128.8 (0.62) 285.5 444.7 (0.78)
16	S 2p	S°	164.0 (0.72) 285.0	MoS_2	162.7 (0.39) 229.7 (0.80)
17	Cl 2p3	PVC	199.8 (1.7) 285.0	NaCl	199.3 (1.19) 285.0 1072.0 (1.40)
18	Ar 2p3	Ar^+/B	241.8 (1.4) 285.2 188.1	Ar^+/HOPG	241.8 (0.89) 284.5
19	K 2p3	K°	294.4 (0.9)	K_2O	292.7 (1.37) 285.0 531.0 (1.6)
20	Ca 2p3	Ca°	346.5 (1.0) 284.6 346.5 (1.07)	$CaCO_3$	346.4 (1.67) 285.0 530.8 (1.64)
21	Sc 2p3	Sc°	398.5 (0.9) 285.9 398.46 (0.69)	Sc_2O_3*	401.9 (1.27) 285.0 530.0 (1.30)
22	Ti 2p3	Ti°	453.8 (0.90) 285.1 453.95 (0.62)	TiO_2	458.8 (1.02) 285.0 530.0 (1.20)
23	V 2p3	V°	512.2 (0.79) 285.0 512.22 (0.75)	V_2O_5	517.0 (0.99) 284.8 530.0 (1.33)
24	Cr 2p3	Cr°	574.2 (1.05) 284.8 574.37 (0.89)	Cr_2O_3	575.6 (1.10) 285.0 530.1 (1.27)
25	Mn 2p3	Mn°	638.7 (1.00) 286.3 638.74 (0.89)	MnO_2	641.4 (1.12) 284.6 529.0 (1.02)
26	Fe 2p3	Fe°	706.6 (0.90) 285.0 706.78 (0.99)	a-Fe_2O_3	709.8 (1.31) 285.0 529.9 (1.04)
27	Co 2p3	Co°	778.1 (0.99) 285.0 778.26 (0.85)	Co_3O_4*	779.5 (1.51) 285.0 530.0 (1.00)
28	Ni 2p3	Ni°	852.6 (1.14) 284.7 852.65 (1.02)	NiO*	853.7 (1.19) 284.8 529.3 (1.06)
29	Cu 2p3	Cu°	932.7 (1.22) 284.7 932.67 (0.92)	Cu_2O	932.7 (1.16) 285.0 530.5 (1.00)
30	Zn 2p3	Zn°	1021.8 (1.10) 284.8 1021.76 (0.97)	ZnO*	1021.7 (1.43) 285.0 530.5 (1.15)
31	Ga 3d5	Ga°	18.5 (0.70) 285.6 18.5 (0.60)	Ga_2O_3*	20.7 (1.28) 285.0 531.4 (1.51)
32	Ge 3d5	Ge°	29.3 (0.68) 285.1 29.28 (0.64)	GeO_2*	32.9 (1.28) 285.0 532.1 (1.40)
33	As 3d5	As°	41.8 (0.65) 284.8 41.69 (0.67)	As_2O_3	45.3 (1.26) 285.0 532.0 (1.71)
34	Se 3d5	Se°	54.8 (0.76) 284.2 54.90 (0.78)	SeO_x	59.3 (1.09) 284.6 532.6
35	Br 3d5			KBr	68.8 (0.92) 285.0 293.0 (1.31)
36	Kr 3d5	Kr^+/Be		Kr^+/C	86.9 (0.88) 285.0
37	Rb 3d5	Rb°	111.5 (0.8)	RbOAc	109.7 (1.40) 285.0 530.6 (1.9)
38	Sr 3d5	Sr°	134.3 (0.9)	$SrCO_3$	133.4 (1.56) 285.0 531.5 (1.9)
39	Y 3d5	Y°	155.9 (0.60) 286.0 155.92 (0.62)	Y_2O_3*	158.0 (1.18) 285.0 530.7 (1.30)
40	Zr 3d5	Zr°	178.9 (0.63) 285.5 178.80 (0.63)	ZrO_2*	182.5 (1.20) 285.0 530.4 (1.44)
41	Nb 3d5	Nb°	202.1 (0.78) 285.0 202.35 (0.57)	Nb_2O_5	207.2 (1.12) 285.0 530.3 (1.34)
42	Mo 3d5	Mo°	227.8 (0.66) 285.1 227.94 (0.57)	MoO_3	233.0 (1.03) 284.9 530.9 (1.23)
43	Tc 3d5	Tc°		TcO_2	256.8
44	Ru 3d5	Ru°	280.0 --- 284.7 280.11 (0.59)	RuO_2	280.7 (0.77) 284.6 529.3 (0.95)
45	Rh 3d5	Rh°	307.2 (0.73) 284.6 307.21 (0.69)	Rh_2O_3	308.6 (0.90) 284.7 530.2 (1.09)
46	Pd 3d5	Pd°	335.1 (0.80) 284.6 335.10 (0.77)	PdO*	336.9 (0.98) 284.9 530.6 (1.09)
47	Ag 3d5	Ag°	368.2 (0.64) 284.8 368.28 (0.62)	Ag_2O*	367.6 (1.00) 284.3 530.1 (1.20)
48	Cd 3d5	Cd°	405.0 (0.80) 285.0 405.04 (0.61)	CdO*	404.1 (1.42) 285.0 528.6 (1.28)
49	In 3d5	In°	443.8 (1.08) 285.0 443.87 (0.71)	In_2O_3*	444.3 (1.33) 285.0 529.8 (1.19)
50	Sn 3d5	Sn°	484.9 (0.81) 284.9 485.01 (0.68)	SnO_2	487.3 (1.32) 285.5 531.1 (1.14)
51	Sb 3d5	Sb°	528.1 (0.88) 284.8 528.26 (0.80)	Sb_2O_5	532.4 (1.6) 285.0 531.0 (1.6)
52	Te 3d5	Te°	572.7 (0.97) 284.3 572.97 (0.83)	TeO_2	576.6 (1.48) 284.9 530.8 (1.42)
53	I 3d5			KI	619.2 (1.30) 285.0 293.2 (1.11)
54	Xe 3d5	Xe^+/Be		Xe^+/C	669.6 (1.13) 285.0
55	Cs 3d5	Cs°	726.4 (1.3)	Cs_2O	724.7 (2.00) 285.0 198.9
56	Ba 3d5	Ba°	780.6 (1.4)	$BaCO_3$	779.9 (2.07) 285.0 531.4 (1.77)
57	La 3d5	La°	835.8 (1.3)	La_2O_3	834.4 (2.5) 285.0 529.0 (1.66)
58	Ce 3d5	Ce°	883.8 (3.2)	CeO_2	882.1 (2.0) 285.0 529.6 (2.00)
59	Pr 3d5	Pr°	929.4 (2.96)	Pr_2O_3	928.8 (3.2) 285.0 528.5 (1.2)
60	Nd 3d5	Nd°	980.8 (2.9) 285.6	Nd_2O_3	983.2 (2.7) 285.0 530.8 (1.3)
61	Pm 4d5	Pm°	Radioactive	Pm_2O_3	
62	Sm 4d5	Sm°	1081.1 --- --- 128.7 (2.5)	Sm_2O_3	1083.8 (4.3) 285.0 529.9 (1.6)
63	Eu 4d5	Eu°	128.2 --- 284.3 128.18 (1.08)	Eu_2O_3	136.2 (3.6) 285.0 530.5 (1.4)
64	Gd 4d5	Gd°	140.2 --- 281.4 140.31 (1.05)	Gd_2O_3	(1187.5) (5.4) 285.0 529.3 (1.5)
65	Tb 4d5	Tb°	145.9 --- --- 145.95 (1.16)	Tb_2O_3	(149.5) (?) 285.0 529.7 (1.5)
66	Dy 4d5	Dy°	152.4 --- --- 152.34 (0.90)	Dy_2O_3	(153.5) (1.9) 285.0 529.4 (1.7)
67	Ho 4d5	Ho°	159.8 --- --- 159.58 (0.98)	Ho_2O_3	160.9 (2.0) 285.0 529.3 (1.6)
68	Er 4d5	Er°	167.7 --- --- 167.25 (1.00)	Er_2O_3	168.5 (1.9) 285.0 529.7 (1.5)
69	Tm 4d5	Tm°	175.3 --- 285.3 175.37 (1.06)	Tm_2O_3	176.3 (1.1) 285.0 529.6 (1.6)
70	Yb 4d5	Yb°	182.4 --- 285.6 182.39 (0.61)	Yb_2O_3	185.0 (2.7) 285.0 529.2 (1.5)
71	Lu 4f7	Lu°	7.1 (0.46) 284.6 7.10 (0.69)	Lu_2O_3*	8.0 (2.5) 285.0 529.5 (1.4)
72	Hf 4f7	Hf°	14.4 (0.63) 285.7 14.32 (0.62)	HfO_2*	17.2 (1.31) 285.0 529.9 (1.71)
73	Ta 4f7	Ta°	21.8 (0.72) 285.1 21.78 (0.56)	Ta_2O_5*	26.3 (1.11) 285.0 530.4 (1.47)
74	W 4f7	W°	31.4 (0.58) 285.1 31.38 (0.53)	WO_3	35.8 (1.02) 285.1 530.6 (1.28)
75	Re 4f7	Re°	40.3 (0.67) 285.0 40.30 (0.54)	Re_2O_7	46.9 (1.47) 285.0 532.2 (1.49)
76	Os 4f7	Os°	50.7 (1.2)	OsO_2	53.8
77	Ir 4f7	Ir°	60.8 (0.80) 284.5 60.88 (0.82)	IrO_2	61.7 (0.84) 284.8 530.0 (0.99)
78	Pt 4f7	Pt°	71.1 (0.96) 284.4 71.15 (0.88)	PtO_2	75.1 (1.09) 284.9 531.3 (1.52)
79	Au 4f7	Au°	84.0 (0.66) 284.1 83.98 (0.68)	Au_2O_3	85.1 (1.37) 285.1 530.2 (1.13)
80	Hg 4f	Hg°	99.8 --- 285.0 99.81 (0.65)	HgO	100.9 (1.07) 285.0 530.0 (1.00)
81	Tl 4f7	Tl°	117.8 (0.97) 285.2 117.77 (0.66)	Tl_2O_3*	118.1 (1.1) 284.8 528.6 (1.07)
82	Pb 4f7	Pb°	136.9 (0.67) 285.0 136.95 (0.63)	PbO*	137.5 (1.17) 285.0 528.9 (1.09)
83	Bi 4f7	Bi°	157.0 (0.73) 284.9 157.05 (0.62)	Bi_2O_3*	158.9 (1.37) 285.0 529.6 (1.52)
84	Po 4f7		Radioactive		
85	At 4f7		Radioactive		
86	Rn 4f7		Radioactive		
87	Fr 4f7		Radioactive		
88	Ra 4f7		Radioactive		
89	Ac 4f7		Radioactive		
90	Th 4d5	Th°	333.2 (1.7)	ThO_2	334.5 (1.6)
91	Pa 4d5		Radioactive		
92	U 4f7	U°	377.3 (1.4)	UO_3	381.7
93	Np		Radioactive		
94	Pu		Radioactive		
95	Am		Radioactive		
96	Cm		Radioactive		
97	Bk		Radioactive		
98	Cf		Radioactive		
99	Es		Radioactive		
100	Fm		Radioactive		
101	Md		Radioactive		
102	No		Radioactive		
103	Lr		Radioactive		

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Handbooks of Monochromatic XPS Spectra

Volume 3 - *Semiconductors*

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LIST OF XPS SPECTRA IN VOLUME THREE

SEMICONDUCTORS

SEMICONDUCTORS (continued)

SEMICONDUCTORS (continued)

INTRODUCTION

This handbook contains wide scan spectra and narrows scan spectra from simple semiconductors and compound semiconductors. These materials have been analyzed under conditions that have maximized the accuracy of the binding energies. Please refer to section "F" (Energy Scale Reference Energies and Calibration Details) for more details about calibration.

The Semiconductors Section:

Includes wide scan spectra, principal metal signal high energy resolution spectra, some secondary metal signal high energy resolution spectra, carbon (1s) high energy resolution spectra, oxygen (1s) high energy resolution spectra, valence band spectra, and some Auger signal spectra obtained from the following semiconductors that were analyzed “as received” and “after freshly exposing the bulk” by fracturing in air. Some materials were analyzed “after ion etching” or “chemical cleaning”. Semiconductors analyzed include: AlGaAs, AlN, BeO, C^{o}, CdO, CdSe, CuCl, Cu_2O, Diamond, GaAs, GaInAs, GaP (100), GaP (111), GaSb, GeSe, $GeSe_2$, HgS, HgTe, HOPG, InP, InSb, InSnOx (ITO), PbO, PbO_2, Pb_2O_3, Pb_3O_4, PbS, SbTe, Se^{o}, n-Si^{o}, p-Si^{o}, p-Si^{o} (NIST), Si^{o} (un-doped), Si_3N_4, SnO_2, Te^{o}, WO_3, ZnO. Atomic percentage tables of surface composition, which reveal the chemical composition, the natural oxidative tendencies of the semiconductors, and the tendencies of these semiconductors to capture various gases from the air are provided.

ORGANIZATION AND DETAILS OF SPECTRAL SETS

Organization of Spectra

A set of spectra for a particular chemical is located by looking for the chemical formula abbreviation written in the upper right hand corner of each page. For the binary oxide called "aluminium oxide" the user will find the chemical abbreviation "Al_2O_3" in the upper right corner of the pages that belong to that set of data and spectra. The spectra are organized by using the chemical abbreviation. This means that "Antimony Oxide" spectra will be found by looking for the chemical formula: "Sb_2O_3".

Contents of Each Set of Spectra

The spectra are presented exactly as printed by the Spectral Data Processor software provided in each XI SpecMaster Data-Base system. The first page of a set includes the "Detailed Surface Composition Table" which reports the peak assignments, binding energies, relative sensitivity factors, and Atom % abundance of each major signal contained in the wide scan survey spectrum for that chemical. In the title line of this first page the user will find the full chemical name along with other basic information about the chemical, such as Formula Weight, Chemical Abstract Services number, common name, and a few key words about the analysis conditions.

The second page of each set is the wide scan survey spectrum with information about the experimental conditions used to collect the spectrum, the history of the sample, the source of the sample if known, and peak labels. Detailed information about the operating capabilities of the SSI systems and the instrument and analysis conditions used to collect these data are presented in the next section of this book.

The remaining pages of each set are the high energy resolution narrow scan spectra which were obtained by measuring the strongest signals found in the wide scan survey spectrum. These spectra normally contained detailed peak-fit results in a table and display the actual peak-fit results for each spectrum. The binding energies of insulating materials are reported without any charge correction because there is currently no standard method or standard reference energy for charge referencing spectra from insulating materials. The FWHM values for each peak of a high energy resolution spectrum is adjacent to the binding energy for that peak. The percentage numbers given for each peak is a relative percentage that is based on the intensity of that signal only (It is not an atom % value).

In this edition the spectra do not have labels which identify the XPS signal so the reader needs to refer to the energy range to determine which signal has been reported. In many cases valence band region spectra, Auger signal spectra, and spectra from weaker XPS signals are also included, but only for materials which were expected to be commercially pure.

Philosophy of Data Collection Methods

Our philosophy is to collect spectra under analysis conditions that are practical, readily reproduced, and typically used in laboratories that use monochromatic X-ray sources and work under real world practical analysis conditions. We have assumed that the most XPS laboratories need practical reference spectra and will not spend the time or money to produce and to analyze pure, clean surfaces under ultimate energy resolution conditions. However, we did spend extra time to collect data with above average signal to noise (S/N) ratios which reveal the presence of minor components that might otherwise be missed. In the production of these spectra we did not attempt to produce clean surfaces which would make charge referencing of insulators a difficult task. For practical reasons we used the C (1s) spectra from the naturally formed layer of adventitious hydrocarbons because that signal is the “de facto” standard for charge referencing insulating materials.

The spectral data contained within these handbooks are designed to assist engineers, scientists, analysts, theoreticians, and teachers who use XPS on an everyday basis under practical working conditions. We believe that these spectra will help XPS users to analyze industrial problems, gather reference data, perform basic research, test theories, and teach others.   Our spectra are designed to be practical tools for everyday use and were obtained under practical working conditions. We have not actually attempted to produce research grade spectra, but we have, in fact, produced research grade spectra because of our self-consistent methods.

In the production of these spectra no attempt to produce a pure, clean surface, but an effort was made to produce surfaces with a minimum amount of natural surface contamination.   When ion etching was used to clean a material that contained more than one element, then ion etching was done with conditions that should minimize preferential sputtering.

Peak-Fitting (Curve-Fitting) of High Energy Resolution Spectra

Peak-fitting was performed by using the software provided with the Surface Science Instruments XPS system. This software allows the user to control full width at half maxima (FWHM) value of any peak, the binding energy (BE) of any peak, peak areas, the ratio of two peak areas, the energy difference between two peak maxima, the shape of a peak as a sum-function of Gaussian and Lorentzian peak shapes in any peak, and the percentage of asymmetry in any peak..

By empirically peak-fitting the spectra from large sets of closely related materials in a trial and error method and analyzing the trends, it was possible to recognize several fundamental peak-shape and peak-fitting parameters for pure elements, binary oxides, polymers, and semiconductors. We used those empirical results to guide our efforts to peak-fit many of the spectra which had complicated peak shapes. In some cases we used the theoretical ratio of spin-orbit coupled signals to assist the peak-fitting of many spectra and also the energy interval between spin-orbit couple signals which were derived from pure element spectra. No attempt was made to fit the spectra in accordance with theoretical expectations or calculations.

The reduced “chi-squared” value, which indicates the goodness of a peak-fit, was used to determine if a peak-fit was reasonable or not. Based on practical experience a “chi-squared” value between 1 and 2 implies a relatively good peak-fit. A “chi-squared” value between 2 and 4 implies that the fit has not yet been optimized. A “chi-squared” value larger than 4 implies that one or more signals may be missing from the peak-fit effort.

A Shirley-type baseline was used for most peak-fits. Peak shapes for the main XPS signals from chemical compounds (e.g. oxides or polymers,)were typically optimized by using a Gaussian:Lorentzian ratio between 80:20 and 90:10. For pure metals Gaussian:Lorentzian ratio for the main XPS signals was normally between 50:50 and 70:30. For the main XPS signals from semi-conductor materials, the Gaussian:Lorentzian ratio was usually between 70:30 and 80:20.

From the peak-fitting of the binary oxides, we have observed that FWHM for the C (1s), O (1s) and the main metal signal from the binary oxide are usually in range 1.0-1.4 eV. This trend helped us to decide if we had good charge compensation.

Charge Compensation of Insulating Materials

Charge compensation of insulating materials was normally handled by using the patented SSI mesh-screen together with a low voltage flood gun of electrons which used an acceleration voltage that was adjusted to 2-4 eV for optimum results. The mesh-screen device uses a 90% transmission electro-formed mesh made of nickel metal that is supported above the surface of the sample by mounting the mesh on a conductive metal frame that is grounded to the sample mount. To achieve good charge compensation the mesh-screen is positioned so that the distance between the mesh and the surface of the sample is between 0.5 - 1.0 mm. When the distance between the mesh-screen and the surface of the sample is greater than 1.2 mm, the usefulness of the mesh screen flood gun system was null.

The mesh-screen is understood to function as a electron cut-off lens with some tendency to allow incoming flood gun electrons to focus on the area being irradiated with monochromatic X-ray beam because the X-ray beam does not have a uniform flux density of the area of the beam. In effect, the mesh-screen produces a nearly uniform electric potential at the surface of the sample and allows incoming flood-gun electrons to pass through whenever they are needed.

The mesh-screen was used on every insulating material except for a few materials that were analyzed before the mesh-screen method was developed.

Abbreviations Used

Due to the limited space provided to describe each sample in each electronic data-file, it was necessary to use various abbreviations. The abbreviations are:

scr = screen used for charge compensation
scrn = screen used for charge compensation
TOA = take-off-angle for the electrons
Aldr = Aldrich Chemical Co.

1mm =1 mm height used for the mesh-screen,
semi-con = semi-conductive behavior
conduc. = conductive behavior
Tech = technical grade purity,

INSTRUMENT AND ANALYSIS DETAILS USED TO MAKE XPS SPECTRA

A. Instrument Details

Manufacturer:	Surface Science Instruments (SSI)
Model:	X-Probe
	S-Probe (upgraded from M-Probe model 2703)
Software Version;	1.36.05 (Compiled in MS-DOS "C" version 6.0)
Analyzer Type:	Fixed Analyzer Transmission (FAT)
	Fixed (Constant) Pass Energy = Constant Analyser Energy (CAE)
	180° Hemi-spherical (truncated)
Input Lens Field of View:	30° for sample normal to lens axis (1" diameter port)
	(always larger than X-ray beam; retarding potential scanned)
X-ray Type:	Al° monochromatic (one 2 " diameter thin natural SiO2
	crystal wafer glued onto Zerodur substrate heated to 65° C)
X-ray kV and mA Emission:	10 KV, 1.5-22.0 mA (depending on spot size used)
X-ray Energy Defined as:	1486.7 eV (8.3393 Å), Bragg Angle=78.5°
Excitation Source Window:	0.6 μ aluminum in S-Probe (10μ mylar in X-Probe)
Angle of X-ray Incidence:	α = 71° (relative to sample normal)
Electron Emission Angle:	β = 0° (relative to sample normal)
Angle Between X-ray Axis and Electron Analyzer Axis:	ϕ =71° (fixed, non-variable)
Pass Energy of Analyzer:	150 V for Resolution 4 setting
	100 V for Resolution 3 setting
	50 V for Resolution 2 setting
	25 V for Resolution 1 setting
Type & Size of Input Slit:	Fixed (2 mm X 35 mm); magnetic compression
Type & Size of Output Slit:	None (dispersion limited by hemisphere voltages)
Electron Collection Lens Field of View:	~ 1 mm^2 for b = 0° at 1000 eV KE
Electron Collection Lens Efficiency:	7% over 2π steradians
Sample Surface to Tip of Electron Collection Lens Distance:	~33 mm
X-ray Crystal to Sample Surface Distance:	~190 mm
X-ray Crystal to X-ray Anode Distance:	~190 mm

True Background Count of Noise:	<10 electrons/second at -50 eV (shot noise limited)
Detector Type:	SSI Position Sensitive Detector, resistive anode, 40 mm X 40 mm
	electronically defined as 128 active channels with max ct rate 1,000,000
Dead Time:	normally zero (unless ion etching pure element while collecting XPS data)
Base Pressure:	4. x 10^{-10} torr
Normal Operating Pressure:	1.6 x 10^{-9} torr
FWHM of X-rays Diffracted by natural SiO2:	~0.25 eV
Power Settings:	200 Watts in a 250 x1100 μ X-ray beam
	100 Watts in a 150 x 800 μ X-ray beam
	45 Watts in a 80 x 350 μ X-ray beam
	15 Watts in a 40 x 250 μ X-ray Beam
X-ray Induced Current:	1.1 x 10^{-9} amps for a 600 μ spot in X-Probe
Converted from amps to watts	
Approximate True X-ray Power :	~6 x 10^{-6} W in a 600 μ spot
Approximate True X-ray Irradiance:	~8 W/m^2
Approximate True X-ray Photon Flux:	~7 x 10^9 photons/sec

B. Experimental Details

Electron Take-Off-Angle:	90° relative to sample surface (unless otherwise reported)	
Pass Energies Used:	Wide scans were done at PE = 150 eV	
	Narrow scans were normally done at PE = 50 eV	
	Valence band scans were done at PE=150 eV	
X-ray Beam Size Used:	Wide scans:	250 x 1500 μ ellipse (at 90° TOA)
(for S-Probe)		250 x 1100 μ ellipse (at 35° TOA)
	Narrow Scans:	250 x 1500 μ ellipse (at 90° TOA)
		150 x 1000 μ ellipse (at 90° TOA)
SSI Mesh-Screen:	A 90% transmission (20 μ diameter wire with 200 μ spacing) nickel metal mesh screen was adhered to a small 25 mm x 25 mm x 1.5 mm (W x L x H) aluminum plate over a 20 mm x 20 mm aperture. This mesh-screen was placed over all oxide samples so that the distance between the sample surface and the mesh-screen was <1.0 mm but >0.3 mm.	
Dwell Time (counting time):	200 milliseconds/channel (usual setting)	
Data Transfer Time:	4 milliseconds	
Max. Number of Channels:	5000 (channels = data points)	
Scan Time for One Wide Scan:	~ 3.5 minutes (using 1024 data points)	
Scan Time for One Narrow Scan:	~100 seconds (using 256 data points)	

Energy Range:	-100 to +1400 eV (BE range)
Typical Step Size:	0.1 eV/step (i.e. 0.1 eV/data point)

C. Data Processing Details

Baseline Subtraction:	None, unless S/BG gave a small display. When the baseline was removed, the intensity of the lowest point was subtracted from all points.
Data Smoothing:	None
Energy Shifting:	None
Intensity Scaling:	None

D. Sample Details

The "Description" given on each XPS spectrum reports the empirical elemental formula for the oxide, purity, source, production lot number, a note, if appropriate, about being conductive or semi-conductive, the abbreviation "scrn" which means that the SSI mesh-screen was used, and a number, e.g. 90 which reports the electron take-off-angle used to collect the data for that sample. Abbreviations used in the description and their full meaning include: Aldr = Aldrich Chemical Co., RMC = Rare Metallics Co., semi-con = semi-conductive behavior, scrn = SSI mesh-screen used, TOA = electron Take-Off-Angle, Tech = technical grade purity, pellet = sample pressed into pellet form, plt = pellet, pel = pellet, MS Co. = Metal Samples Company in Munford, Alabama USA (Tel 205-358-4202), SPP = Scientific Polymer Products Inc. in Ontario, New York state, USA (Tel 716-265-0413)

Sources of Elements and Chemical Compounds Used for Element Series

The pure element samples were obtained from various sources without any specific information about sample purity so pure element samples must be assumed to be pure at the 99% level. The "halide" salts used to produce spectra from gaseous or highly reactive elements were also obtained from various sources. These halide samples were obtained as crystalline "windows" which are normally used in Infrared spectroscopy and have purities at the 99% level. The Boron Nitride (BN) sample was a white ceramic standoff which was fractured in air. The copper foil material, which was always used to determine reference energies, were obtained as 99% pure foil which was designed as a multiple purpose foil for use around the home. The gold ingot material, which was also used to determine reference energies was obtained as a 99.999% pure sample from Aldrich Chem. Co..

Source of Polymer Materials

A special kit (#205) of the 100 polymer materials was obtained from Scientific Polymer Products, Inc. which is located at 6265 Dean Parkway, Ontario, New York, USA 13519 (Tel 716-265-0413).

Source of Alloys

A special kit of 54 metallic alloys was obtained from the Metal Samples Co., which is located at Route #1, Box 152, Munford, Alabama, USA, 36268 (Tel 205-358-4202). This kit includes a materials analysis report on each alloy in weight percents. The National Research Institute for Metals in Tsukuba Japan has provided a series of various binary alloys made of AuCu and CoNi alloys.

Sources of Semi-Conductor Materials

Over the course of many years, many people in the Japanese semi-conductor business have given samples of various semi-conductor materials in crystalline wafer form. Various samples were donated by the Oki Electric Company, Mitsubishi Materials, Canon, and various universities. The source of each material is included with the individual sample descriptions whenever that information was provided.

Sources of Binary Oxide Samples

Most of the commercially pure binary oxides were purchased from the Aldrich Chem. Co.. Many packages from the Aldrich Chemical Co. included an "Analytical Information" sheet which described an ICP or AA analysis summary, a production lot number, the Aldrich product number, sample purity number (e.g. 99+%), sample appearance (color and physical form), date of chemical analysis, formula weight and a label on the bottle that reports the melting point, toxicity, Chemical Abstracts registry number and density. The samples from Aldrich were generally quite pure at the surface. Other oxide samples were obtained from either Cerac Inc. (USA) or Rare Metallics Co., Ltd. (Japan). The packages from Cerac Inc. included a "Certificate of Analysis" with an ICP or AA analysis summary, a production lot number, a product number, purity (e.g. 99+%),and mesh size. The packages from Rare Metallics Co. did not include analytical data reports, but instead had stock numbers and a purity statement. Two samples (i.e. SiO2 natural crystal and Al2O3 fused plate) were obtained from in-house sources and do not have any purity reports.

Powdered Samples Pressed into 3mm Diameter Pellet

Until analyzed, all finely powdered samples were kept stored in their original glass or plastic containers, which were packaged inside of plastic-lined aluminum bags. Just prior to XPS analysis, each bottle was opened in the normal air of the room where the XPS system was kept, and a small 50-100 mg portion of the sample was removed via a clean nichrome spatula and placed in the compression chamber of a hand-operated, stainless steel pellet press. All finely powdered samples were compressed without any chemical treatments, which, if done, may have introduced unusual contamination or produced some change in the samples. The resulting pellets varied in thickness from 0.3 - 0.8 mm. To avoid iron and /or chromium contamination from the anvil, a thin sheet of paper was placed over the sample in the compression chamber. Any powders, which were clumped together, were very gently pressed into a powder just prior to compression. To avoid unnecessary heat-induced oxidation, those samples which were hard and granular were very gently ground into a fine powder in a agate marble mortar and pestle. As soon as each sample was removed from the compression chamber, it was mounted onto silver (Ag°) paint inside of a 5mm wide round brass boat which was 1.3 mm in height. Silver paint was used so that conductive oxides could behave as true conductors thereby providing true electron binding energies for those oxides that were indeed conductive. In general, each oxide was exposed to room air for <15 min..

Benefits of Pressing Powders into Pellets (increased counts and simple charge control)

A comparison of the electron counts obtained from powdered samples pressed onto double-sided adhesive tape and positioned at a 35° electron take-off-angle with the electron counts obtained from hand-pressed glossy or semi-glossy pellets positioned at a 90° electron take-off-angle (TOA) revealed that a pellet at a 90° electron TOA produces 3-5 times higher electron counts than a powdered sample pressed onto double-sided tape at a 35° electron TOA.

By pressing the finely powdered oxides into pellets, it was also found the surface charging behavior of these glossy or semi-glossy samples was very easy to control by using the mesh-screen electron flood-gun combination with the flood gun set to 4-6 eV acceleration energy and approximately 0.5 mA filament current.

Problems Caused by Pressing Samples into Pellets

By pressing the finely powdered oxides into pellets, the surface of the resulting samples were usually smooth enough to appear glossy or semi-glossy, but some samples had iron or chromium contamination which indicated that the oxide had undergone a pressure induced reaction with the stainless steel anvil. Very strong hand pressure caused some oxides to react with the stainless steel anvil, but medium hand pressure usually did not produce undesired iron and chromium contamination. All analyses that showed any unexpected contamination were repeated. Other forms of accidental contamination (chlorine or previously analyzed oxides) were caused by insufficient cleaning of the stainless steel anvil, which was normally cleaned with a metal polishing solution (Pikal) and rinsed with distilled water and isopropanol. All analyses that showed any unexpected contamination were repeated.

Solution to Pressure Induced Contamination of Pellets

Experiments on ways to avoid the pressure-induced iron or chromium contamination, produced pellets with semi-smooth non-glossy surfaces which required more effort to produce good charge control. These non-glossy surfaces also gave electron count rates that were about 10-50% lower than the glossy or semi-glossy surfaces. As a result, it appears that very smooth surfaces, which appear glossy or semi-glossy, greatly simplify efforts to control surface charging under the charge-control mesh-screen and also enhance the electron count rate by 10-50% more than a pellet that has a semi-rough non-glossy appearance.
Extensive experiments on different methods to avoid contamination of the pellets revealed that contamination is minimized or avoided by using freshly cleaned aluminum foil as a "buffer" between the oxide powders and the metals in the steel anvil components. The aluminum foil, which is sold as a kitchen wrap material, is cleaned with 100% isopropanol (isopropyl alcohol) just prior to use. The foil is cut to a size that is readily useful with the pellet press device after it is cleaned. Alternately, we have also used a type of "glycine" paper which is commonly used to as a paper to hold powders when weighing a powdered sample. This "weighing" paper is common in many chemical laboratories and can be substituted for the aluminum foil whenever the pressing results with the aluminum foil produce undesired binding results. The glycine paper method sometimes introduces very small amounts of contaminants which produce a N (1s) and C (1s) signals. The amount of these contaminants is much smaller than the amount of contaminants that occur by simply pressing the powder without any sort of paper or aluminum foil buffers.

Source of Pellet Press Equipment

"Qwik Handi-Press" from Barnes Analytical Division, Spectra-Tech, Inc.652 Glenbrook Road, Stamford, Connecticut, 06906 (FAX 203-357-0609) Kit: Part # 0016-111 to 0016-121 contains 1,3, and 7 mm die sets. Originally purchased through Aldrich Chem. Co. in 1989.

E. Energy Resolution Details

Table 1: Experimentally Observed Relation Between Energy Resolution (FWHM) and Resolution Variables

Element (XPS signal)	Resulting FWHM	Resolution Setting	Pass Energy	X-ray Spot Size
Si ($2p_{3/2}$) crystal - fractured edge	0.38 eV	5	10 eV	40 x 250μ
Si ($2p_{3/2}$) crystal - fractured edge	0.43 eV	1	25 eV	80 x 350μ
Au ($4f_{7/2}$) foil - ion etched clean	0.64 eV	5	10 eV	250 x 1000μ
Au ($4f_{7/2}$) foil - ion etched clean	0.79 eV	1	25 eV	250 x 1000μ
Au ($4f_{7/2}$) foil - ion etched clean	0.86 eV	2	50 eV	250 x 1000μ
Au ($4f_{7/2}$) foil - ion etched clean	1.40 eV	4	150 eV	250 x 1000μ
Ag ($3d_{5/2}$) foil - ion etched clean	0.42 eV	5	10 eV	40 x 250μ
Ag ($3d_{5/2}$) foil - ion etched clean	0.64 eV	1	25 eV	40 x 250μ
Ag ($3d_{5/2}$) foil - ion etched clean	0.75 eV	2	50 eV	40 x 250μ
Ag ($3d_{5/2}$) foil - ion etched clean	1.00 eV	3	100 eV	40 x 250μ
Ag ($3d_{5/2}$) foil - ion etched clean	1.30 eV	4	150 eV	40 x 250μ
Cu ($2p_{3/2}$) foil - ion etched clean	0.85 eV	5	10 eV	250 x 1000μ
Cu ($2p_{3/2}$) foil - ion etched clean	0.94 eV	1	25 eV	250 x 1000μ
Cu ($2p_{3/2}$) foil - ion etched clean	1.06 eV	2	50 eV	250 x 1000μ
Cu ($2p_{3/2}$) foil - ion etched clean	1.60 eV	4	150 eV	250 x 1000μ
Cu ($2p_{3/2}$) foil - ion etched clean	0.85 eV	5	10 eV	150 x 800μ
Cu ($2p_{3/2}$) foil - ion etched clean	0.96 eV	1	25 eV	150 x 800μ
Cu ($2p_{3/2}$) foil - ion etched clean	1.05 eV	2	50 eV	150 x 800μ
Cu (3s) foil - ion etched clean	2.35 eV	2	50 eV	250 x 1000μ

Table 2: Theoretical Analyzer Resolution versus Pass Energy Settings

Theoretical Analyser Resolution	Pass Energy	Effective Detector Width
0.25 eV	25.0 eV	3.5 eV
0.50	50	7.0
1.00	100	14.0
1.50	150	21.0

F. Energy Scale Reference Energies and Calibration Details

From May 1986 to January 1993

Energy Scale Reference Energies: 932.47 eV for Cu ($2p_{3/2}$) signal
122.39 eV for Cu (3s) signal
83.96 eV for Au ($4f_{7/2}$) signal
Binding Energy Uncertainty: less than ±0.08 eV
Digital-to-Analog (DAC) Conversion Setting: 163.88

After January 1993

Energy Scale Reference Energies: 932.67 <±0.05 eV for Cu ($2p_{3/2}$) signal
122.45 <±0.05 eV for Cu (3s) signal
83.98 <±0.05 eV for Au ($4f_{7/2}$) signal
Observed Reference Energy: 75.01 <±0.05 eV for Cu (3p3) signal
Binding Energy Uncertainty: less than ±0.08 eV
Digital-to-Analog (DAC) Conversion Setting: 163.87

Reference Energies of Adventitious Hydrocarbon Contaminants

From May 1986 to January 1993 the electron binding energy of adventitious hydrocarbons was assumed to occur at 284.6 eV based on SSI and C. D. Wagner's research and recommendations. Publications by P.Swift (Surface and Interface Analysis **4**, 47 (1982), S. Kohiki and K. Oki (J. Electron Spectrosc. Related Phenom. 33, 375-380 (1984), and G. Barth, R. Linder and C. E. Bryson, III (Surface and Interface Analysis **11**, 307-311 (1988) have shown that the electron binding energy for various hydrocarbon contaminants and polymers is not necessarily a constant number. Research by this author indicates that the electron binding energy for adventitious hydrocarbons lies somewhere between 284.4 and 287.0 eV depending on the underlying oxide materials. By taking a simple average of all available binding energies, the author has found that 285.0 eV is preferred for hydrocarbons on ion etched metals where the hydrocarbon is many hours old. For naturally-formed native oxides the preferred binding energy is 285.2 eV. Oxide based materials at the far left of the periodic element table (columns 1-4) tend to have higher values (285.2-287.0 eV, while most of the transition metal oxides center around 285.0 eV. Near the far right of the periodic table, the binding energy again rises to a 285.2-286.5 eV range (columns 12-14). In routine practice, this author prefers to use the 285.0 eV number. Some potential factors that may cause this rather large range of electron binding energies for adventitious hydrocarbon contamination includes the dipole moment at the surface of the oxide material, which is expected to be much stronger than the dipole moment of a pure metal, and also, in the case of naturally formed native oxide films, the thickness of the native oxide, any physical or chemical treatments, the thickness of the adventitious hydrocarbon layer, and the type of instrument used to analyze the sample. The type of instrument being used may cause different shifts in the observed binding energy of the adventitious hydrocarbon contamination because the source may or may not generate different amounts of low energy secondary electrons from the window that protects the X-ray source. The heat from the source and contamination that degases from a just turned on source may also influence the observed binding energy. Electron flood guns may or may not influence the binding energy as well.

Instrument Stability and Long Term Calibration

Initially each of the three SSI systems, that we have used, was calibrated 2-3 times per week because its ability to maintain accurate voltage settings was unknown. Once it was determined that the systems could maintain reliable voltage settings for 1-3 months, it was decided that good calibration could be maintained by checking and, if necessary, correcting the pass energies of the system on a 2-4 week basis. Each of the three SSI XPS instruments, that we have used, have been calibrated on a routine basis every 2-4 weeks by using SSI's reference energies. By using this method over several years time, it was found that the maximum uncertainty (error in pass energies) was normally <±0.10 eV, but a few times rose to ±0.15 eV or less. In a very rare case, the uncertainty rose to 0.20 eV. Long term use of the SSI systems has shown that the DAC circuit does not change enough to be observed unless the room temperature changes by more than 10 deg Centigrade. If the room temperature changes within a few hours time by more than 10 deg or the temperature of the DAC chip is changed by more than 10 deg, then a >0.1 eV shift, which is much smaller than the reliability of almost all literature BEs, can be observed. Variables, which seem to cause pass energy settings to change slightly, include building line-voltages, ion etching conditions, and the addition or removal of some electrical device.

G. Electron Counting and Instrument Response Function Details (for the X-Probe System only)

Instrument Response Functions

Instrument Response Function: $Q(E)=E^{+0.27}$ for 150 eV PE (ref.3)
Instrument Response Function: $Q(E)=E^{+1.0}$ for 50 eV PE (ref.3)

Signal/Background Ratios for Ion Etched Silver using a 250x1000 µ Spot*

Pass Energy	25 eV	50 eV	100 eV	150 eV
S/BG ratio**	>140	>110	>70	>50

* Using a 90° electron take-off-angle and a smooth Ag°/mylar film.
** The S/BG ratio is a simple numerical ratio of electrons counts at the peak maximum relative to the average electron counts observed at approximately 10 eV lower BE.

Lens Voltage Settings Available via Software under Instrument Calibration

Pass Energy*	29.6-29.8	54.7-54.9	105.1-105.3	155.9-156.2
Detector Widths	3.743	7.486	14.954	22.297
Sensitivity Exponent	0.7	1.1	1.3	1.5
V1 Offset	30	55	105	155
V1 Slope	0.600	0.611	0.676	0.709

* These pass energies include corrections for instrument work function. True pass energies were set to 25, 50, 100, and 150 eV ±0.1 eV.

H. Effects of Poorly Focussing the Distance between the Sample and the Electron Lens

If the focus distance between the sample surface and the electron collection lens is poorly adjusted, then the number of electron counts drops very quickly. A 0.5mm error in focus produces a >300% decrease in counts, but does not produce any observable error in binding energies, which is a common problem with many other instruments. A 0.1mm error in focus produces a 15% decrease in peak area counts and is easily observed as a horizontal displacement in the static (un-scanned mode) XPS signal as observed on the standard CRT display of the detector response. Such a decrease in signal intensity generally causes the operator to correct the focus error so as to maximize the electron count rate. In this manner, the operator has avoided any chance of obtaining false BE readings and has accurately reproduced a nearly absolute focus point which greatly increases the quantitative accuracy of any unknown sample. Experiments with the Bragg angle alignment of the crystal indicated that the maximum error due to an unusual bad alignment of the crystal would be <0.1 eV. To observe an error greater than 0.1 eV, the electron counts were found to decrease by >50%.

I. Quantitation Details and Choice of "Sensitivity Exponents"

By default, the SSI software uses a 0.7 number as the sensitivity exponent factor for each pass energy setting which are used in an equation that modifies theoretically calculated atomic photo-ionization cross-sections (John H. Scofield) to generate relative sensitivity factors that are valid for this XPS systems and which can be used to generate valid atomic percentages. The 0.7 value produces a ±10% accuracy in quantitative results for XPS signals obtained by using a 150 eV pass energy and occur within the 0-700 eV BE range. For signals that occur at higher BEs, it is generally necessary to change the sensitivity exponent factor to a 1.1 or higher value. To measure signals obtained by using other pass energies for quantitation, it is necessary to use other sensitivity exponent factors, if the user desires to maximize quantitative accuracy. To determine useful sensitivity exponents, it is possible to use freshly ion etched poly-crystalline copper foil to test the validity of the sensitivity exponent for larger BE ranges and different pass energies. By integrating the peak areas of the Cu (2p1), Cu (2p3), Cu (3s), Cu (3p) and Cu (3d) signals with a modest amount of attention to baseline end points it is possible to perform trial and error choices of the sensitivity exponents until a useful number is determined. Once a useful number has been entered into the computer software routine, then the software can generate fictional atomic percentages for each of the integrated copper signals which will generate 20 atom % values with a uncertainty of ±1-2 atom %. If the exponent factor is severely wrong then the atomic percentages will generate numbers such as 10%, 11%, 26%, 24%, and 29% or perhaps 31%, 28%, 14%, 13%, and 14%. This trial-and-error approach may require 1-2 hours time and can be done on either wide scan data or more preferably narrow scan data for each of the 4-5 pass energies. This method, in effect, assumes that all five of the relative sensitivity factors for copper are reasonably correct. If wide scan data are used, this method requires a little extra effort to avoid the satellites associated with the Cu (2p) signals. This method, in effect, pretends that the pure copper sample is a standard material that is composed of 5 components which are present in 20 atomic % concentration. The objective is to change the sensitivity exponent until the software generates a 20 atom % result for each of the five copper signals. After useful sensitivity exponents are found, they are tested by analyzing freshly exposed bulk regions of crystalline materials such as SiO_2, Al_2O_3, and NaCl.

The high and low BE signals of the NaCl crystal are especially useful to test the validity of the sensitivity exponents. As further checks, the freshly exposed bulk of common polymers (e.g. mylar or PMMA) or a thin film of high purity silicone oil can also be analyzed. Teflon has repeatedly given slightly larger than desirable error by comparison to the other materials listed above. For that reason Teflon is a less desirable material to test the sensitivity exponents.

J. Crude Tests of the Reliability of Relative Sensitivity Factors

Crude testing of Scofield's numbers are included in atomic percentage composition tables that give atomic percentages for only one element. This testing used the software's automatic peak area integration software that is reasonably accurate. The results indicate that some of the relative sensitivity factors for some of the weaker signals are less reliable. If, however, all factors are taken into account, then Scofield's numbers are reliable to a 95% accuracy level for truly homogeneous materials.

K. Traceability Details

The definition of traceability reported by Martin P. Seah and Cedric J. Powell in the J. Vac. Soc. Technol. Vol 8, p.736 (1990) publication is: "The property of a result of a measurement whereby it can be related to appropriate standards, generally international or national standards, through an unbroken chain of comparisons."

Traceability of Reference Binding Energies (Calibration)

At this time, there are no international standards for binding energies or reference energies. Numbers which are considered to be standard binding energies (BE), which would lead to traceability in BEs, include (a) those provided by Martin P. Seah at the National Physical Laboratory (NPL) in the United Kingdom (England), and (b) those provided by the ASTM in the USA "Standard Practice for Checking the Operating Characteristics of XPS Spectrometers" designated as "E 902-88". Other nations also have similar national standards, which tend to imitate those set by the USA and the UK. Recently, many people in the world have been using NPL's reference energies, which have become "de facto" standards but have not yet been accepted by the International Standards Organization (ISO). There are still many workers and researchers using various numbers provided by the instrument makers. The author of this book was using Surface Science Instruments (SSI) Co. reference energies until December 1992 and then switched to NPL BEs in January 1993. SSI reference energies came from Hewlett-Packard (HP). SSI and HP both used high precision voltage meters from HP to calibrate their ESCA machines (i.e. X, M, and S-Probe and HP-5950 A-type and B-type, resp.). Hewlett Packard was the first company to offer a commercial ESCA system, which used reference energies developed in cooperation with Kai Siegbahn at Uppsala, who effectively developed ESCA into a useful science and received the Nobel Prize. In a recent effort to improve the accuracy of BEs obtained from pure elements, the S-Probe pass energies were checked and corrected, if needed, almost every work-day for two months to obtain high precision and high accuracy BEs for the pure elements that are metals. This study used the NPL reference energies with Cu (2p3) at 932.67 eV with +/- 0.02 uncertainty and Au (4f7) 83.98 eV with +/-0.02 uncertainty by using 0.02 eV/pt. steps for the calibrations. To determine the "true" BE of each of the pure elements, which were scraped clean in air and then ion etched in vacuum, a 0.05 eV/pt. step was used. A repetitive ion etching (depth profile) style was used to collect wide scan, valence (Fermi edge) band, and narrow scans of the main signals for each metal at 50, 25 and 10 eV pass energies. Each repetitive experiment run lasted about 4 hours. Therefore, if NPL's BE numbers are accepted as "de facto" international standards, then the ultimate traceability of BEs in this data collection can be related to NPL BE numbers for Cu (2p3) and Au (4f7). In a different, but similar manner, the BEs used to calibrate the S-Probe are traceable to Siegbahn's work and HP's high precision, high voltage meters.

Traceability Transfer from Pure Metals to Non-conductive Binary Oxides

A question that should be posed is traceability to the oxide BEs. Traceability begins with NPL's BEs for pure copper and gold as state above. Traceability then transfers to pure element BEs which are based on NPL reference BEs. Traceability then transfers to pure element BEs based on SSI's reference BEs, and then the naturally formed native oxide data published in Volume 2 of our XPS Spectral Handbook series where BEs were measured from pure element signals and also the naturally formed native oxide signals. Naturally formed native oxides typically have thin oxide films (10-80Å) which, in general, behave as good or true electrical conductors, which allows a direct measure of the true binding energy of many, but not all, binary oxides. To determine if traceability can indeed be transferred to true binary oxides, it was necessary to study the behavior of the naturally formed native oxides by applying various flood gun settings with the samples grounded and insulated. The results from that study can be used to transfer traceability to the experimentally observed BEs of pure binary oxides. The most difficult transfer of traceability occurs for the naturally formed native oxide systems. If the flood gun study was not done, then it is difficult to transfer traceability in a reliable manner from a conductive metal to one of its corresponding non-conductive binary oxides.

Traceability of Instrument Response (Throughput) Function

Copper, gold and silver data obtained from the M-Probe system were submitted to Martin P. Seah at the NPL for a round robin test on transmission function; the results of which were published in Surface and Interface Analysis, p.243 (1993). In that publication, M-Probe data, which we contributed, were attributed to group #35. That paper reported that instrument has a $Q(E) = E^{0.27}$ for Res 4 pass energy (PE=150 V) and a $Q(E) = E^{1.0}$ for the Res 2 pass energy (PE=50 V). If the NPL method is accepted as a "de-facto" standard, even though it is not an internationally recognized standard, then the transmission function and quantitation results of the S-Probe system are traceable to the "metrology spectrometer" at NPL.

Traceability of Relative Sensitivity Factors used for Quantitation

Scofield's theoretically calculated photo-ionization cross-sections are internationally used as the "de-facto" standard theoretical numbers, except in Russia and a few other places, where Band's numbers are preferred but are almost identical to Scofields. The SSI system uses a very simple equation that modifies Scofield's numbers to generate relative sensitivity factors that are used by the SSI software to calculate atom %s. That equation corrects for pass energy differences, transmission function differences, and inelastic mean free path versus kinetic energy dependency. The SSI system relies on Scofield numbers and that simple equation. Other instrument makers prefer to blend Scofield's numbers and experimentally determined numbers.

Traceability of Sample Purity

The purity of the commercially pure (99+%) binary oxides can be traced to Aldrich's ICP or AA analyses performed by Aldrich. Copies of their results are included in the handbook at the beginning of each group of spectra. Similar data sheets were also obtained for samples bought from Cerac. A set of gold, copper, and silver samples, i.e. "Reference Metal Samples SCAA90" set, kit #367, was obtained from the NPL and used to test the instrument response function of the M-Probe system. Binding energies obtained from those gold, copper, and silver samples were identical to binding energies obtained from our commonplace gold, copper, and silver samples within the expected uncertainty of ±0.08 eV used for routine instrument calibration.

L. Reference Papers Describing Capabilities of X-Probe, M-Probe, and S-Probe XPS systems

1. Robert L. Chaney, *Surface and Interface Analysis*, **10,** 36-47 (1987) [re: X-Probe]
2. Noel H. Turner, *Surface and Interface Analysis*, **18,** 47-51 (1992) [re: Quantitation]
3. M. P. Seah, *Surface and Interface Analysis*, **20,** 243-266 (1993) [re: Response Function]
4. L.T. Weng et al, *Surface and Interface Analysis*, **20,** 179-192 (1993) [re: Response Function]
5. L.T. Weng et al, *Surface and Interface Analysis*, **20,** 193-205 (1993) [re: Response Function]
6. B. Vincent Crist, *Surface Science Spectra*, **1**, 292-296 (1993) [re: KBr spectra]
7. B. Vincent Crist, *Surface Science Spectra*, **1**, 376-380 (1993) [re: Ar/C spectra]

Spectra of Semiconductors

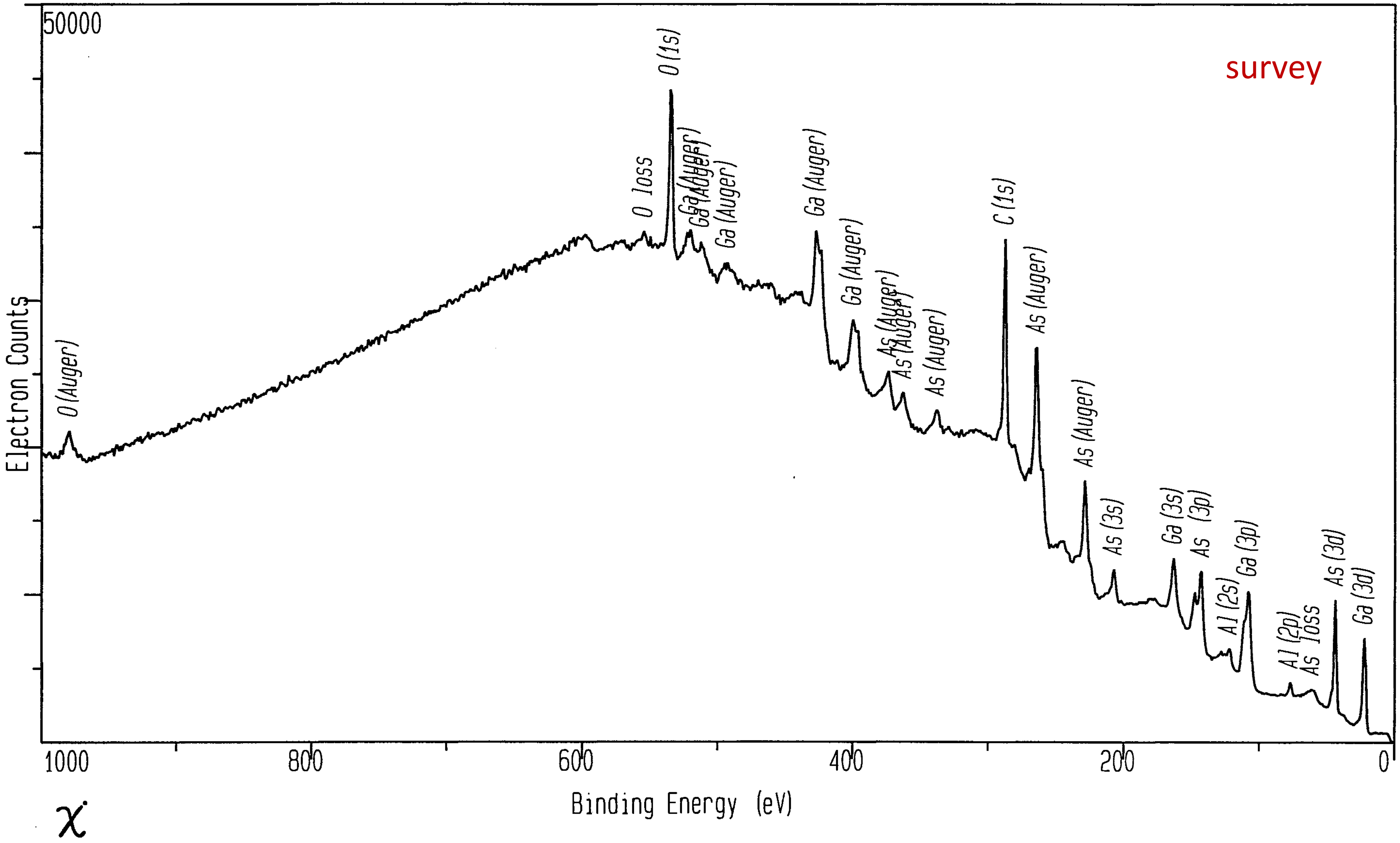
Detailed Surface Composition Table

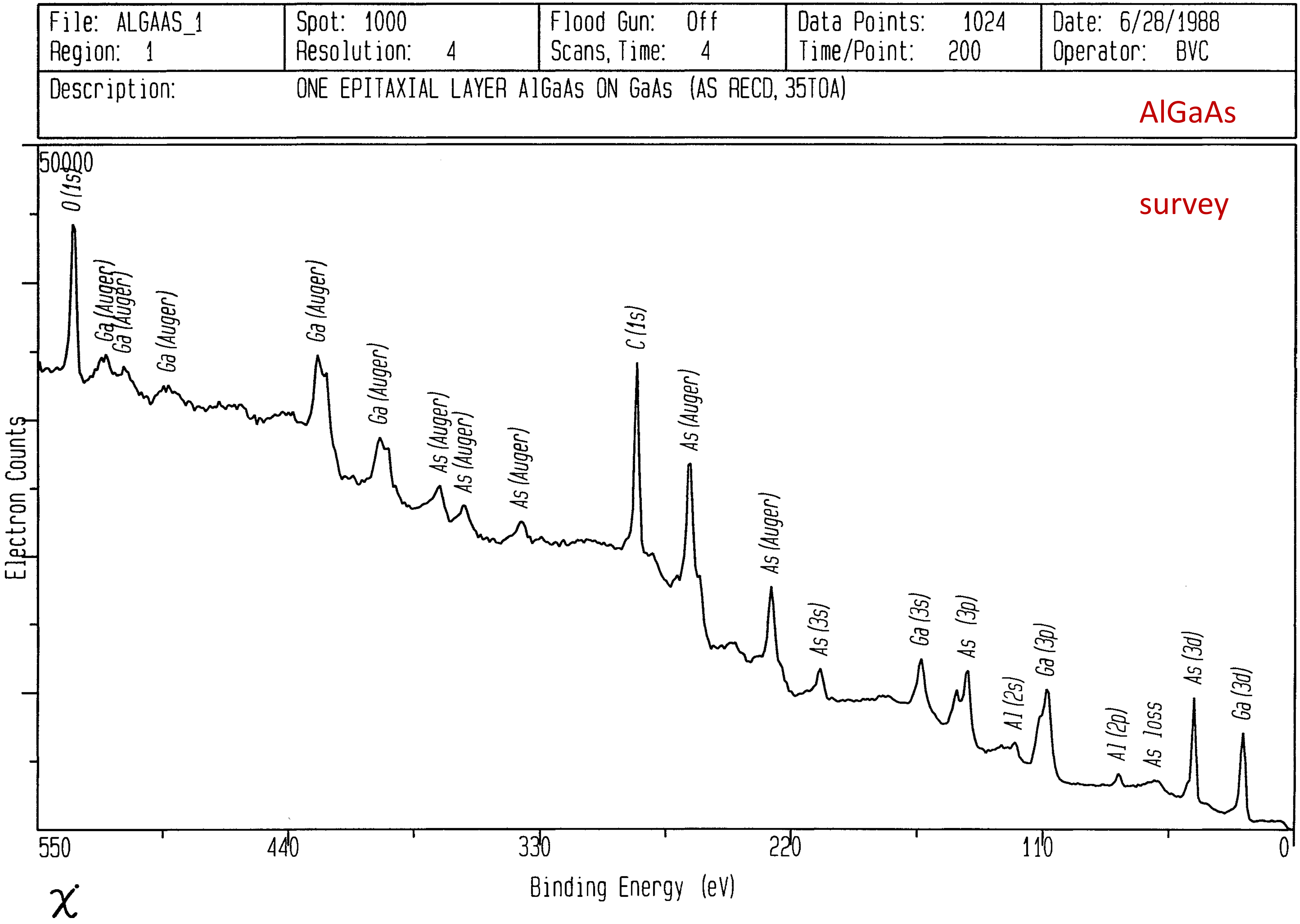
File name: ALGAAS_1.MRS
Region: 1
Description: ONE EPITAXIAL LAYER AlGaAs ON GaAs Wafer(AS RECEIVED,35 TOA)

Operator: BVC
Date: Tues Jun 28 1998

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	979.6	979.6	0.00	14884	0	
O loss	553.8	553.8	0.00	7282	0	
* O 1s	533.8	533.8	2.22	46992	21196	22.08
GaAuger	519.5	519.5	0.00	12076	0	
GaAuger	511.6	511.6	0.00	4721	0	
GaAuger	492.0	492.0	0.00	10678	0	
GaAuger	426.4	426.4	0.00	64583	0	
GaAuger	399.1	399.1	0.00	41300	0	
AsAuger	373.1	373.1	0.00	16674	0	
AsAuger	362.5	362.5	0.00	10697	0	
AsAuger	337.4	337.4	0.00	14694	0	
* C 1s	286.8	286.8	1.00	45211	45312	47.21
AsAuger	263.7	263.7	0.00	75758	0	
AsAuger	227.9	227.9	0.00	42038	0	
As3s	206.7	206.7	1.42	12674	8904	
Ga3s	162.6	162.6	1.27	24395	19224	
* As (3p)	142.3	142.3	3.07	37799	12332	12.85
Al2s	121.4	121.4	0.88	10789	12299	
* Ga3p	107.3	107.3	3.79	45020	11890	12.39
* Al2p	76.1	76.1	0.65	3413	5256	5.48
As loss	60.5	60.5	0.07	7778	111149	
As3d	43.1	43.1	2.27	25422	11213	
Ga3d	21.6	21.6	1.38	23856	17340	

File: ALGAAS_1 Region: 1	Spot: 1000 Resolution: 4	Flood Gun: Off Scans, Time: 4	Data Points: 1024 Time/Point: 200	Date: 6/28/1988 Operator: BVC
Description:	ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)			AlGaAs

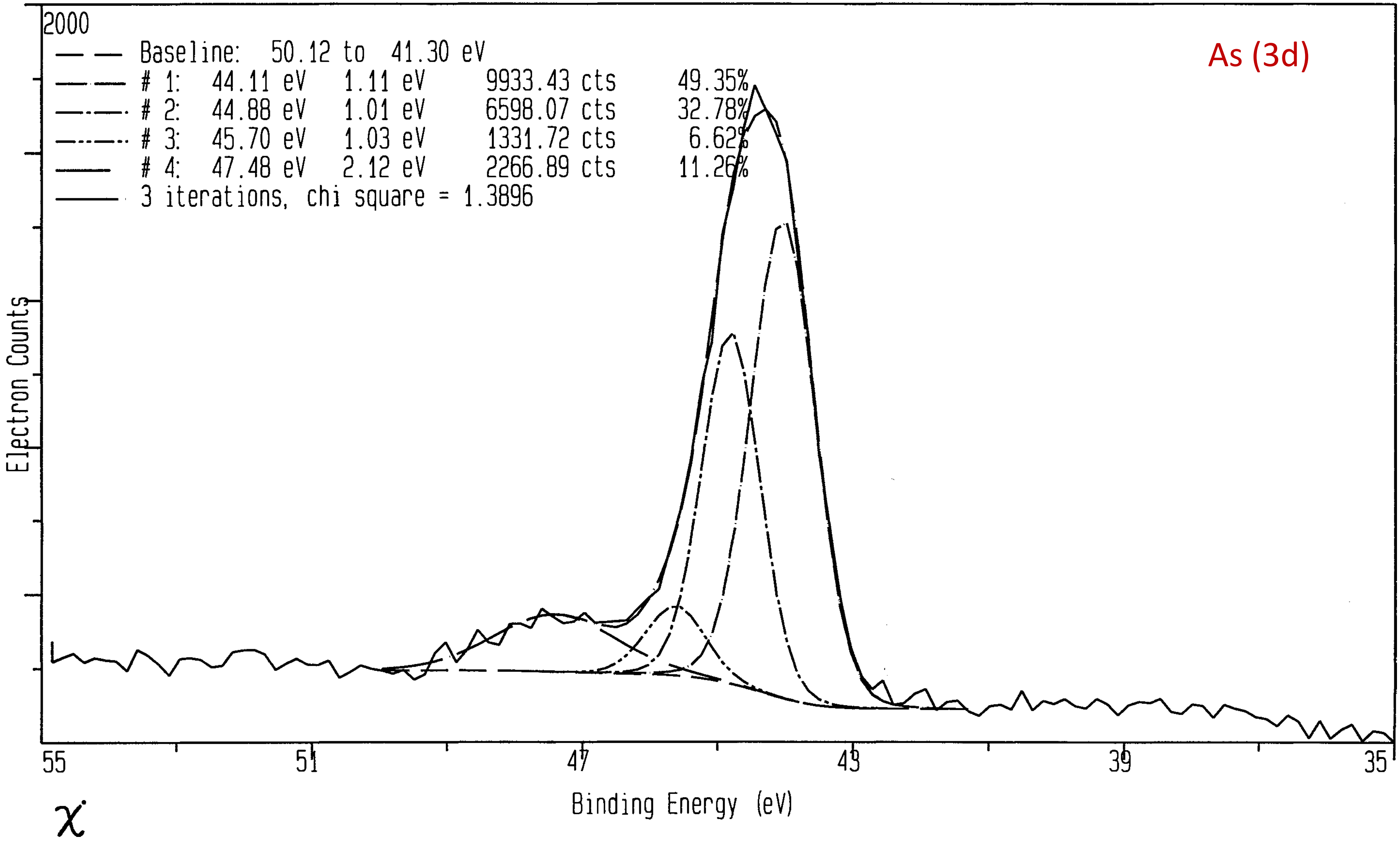



File: ALGAAS_1
Region: 1
Spot: 1000
Resolution: 4
Flood Gun: Off
Scans, Time: 4
Data Points: 1024
Time/Point: 200
Date: 6/28/1988
Operator: BVC
Description: ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)
AlGaAs
survey
50000
O (1s)
Ga (Auger)
Ga (Auger)
Ga (Auger)
Ga (Auger)
Ga (Auger)
As (Auger)
As (Auger)
As (Auger)
C (1s)
As (Auger)
As (Auger)
As (3s)
Ga (3s)
As (3p)
Al (2s)
Ga (3p)
Al (2p)
As loss
As (3d)
Ga (3d)
Electron Counts
550
440
330
220
110
0
Binding Energy (eV)

File: ALGAAS_1	Spot: 600	Flood Gun: Off	Data Points: 128	Date: 6/28/1988
Region: 3	Resolution: 2	Scans, Time: 10	Time/Point: 200	Operator: BVC

Description: ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)

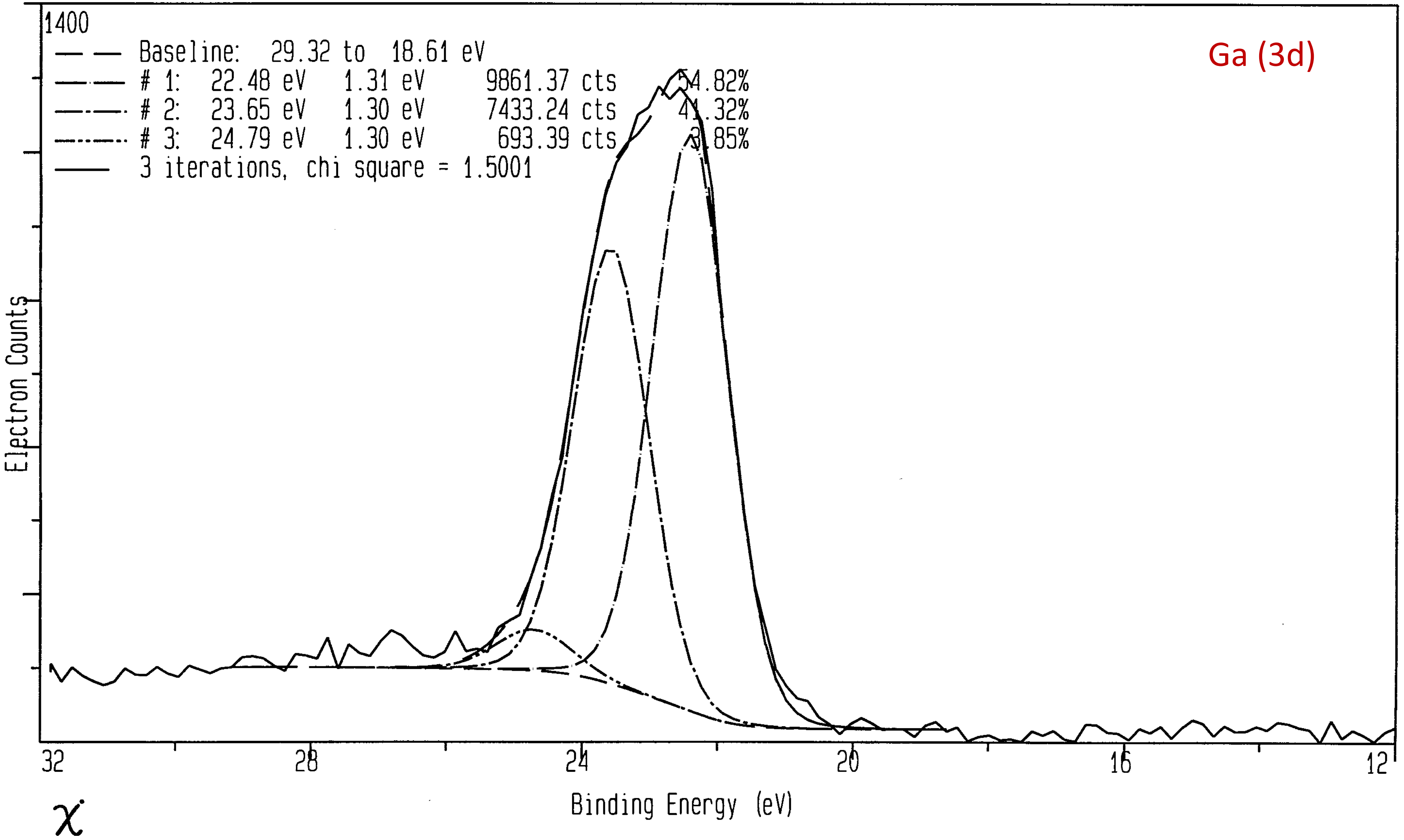
AlGaAs



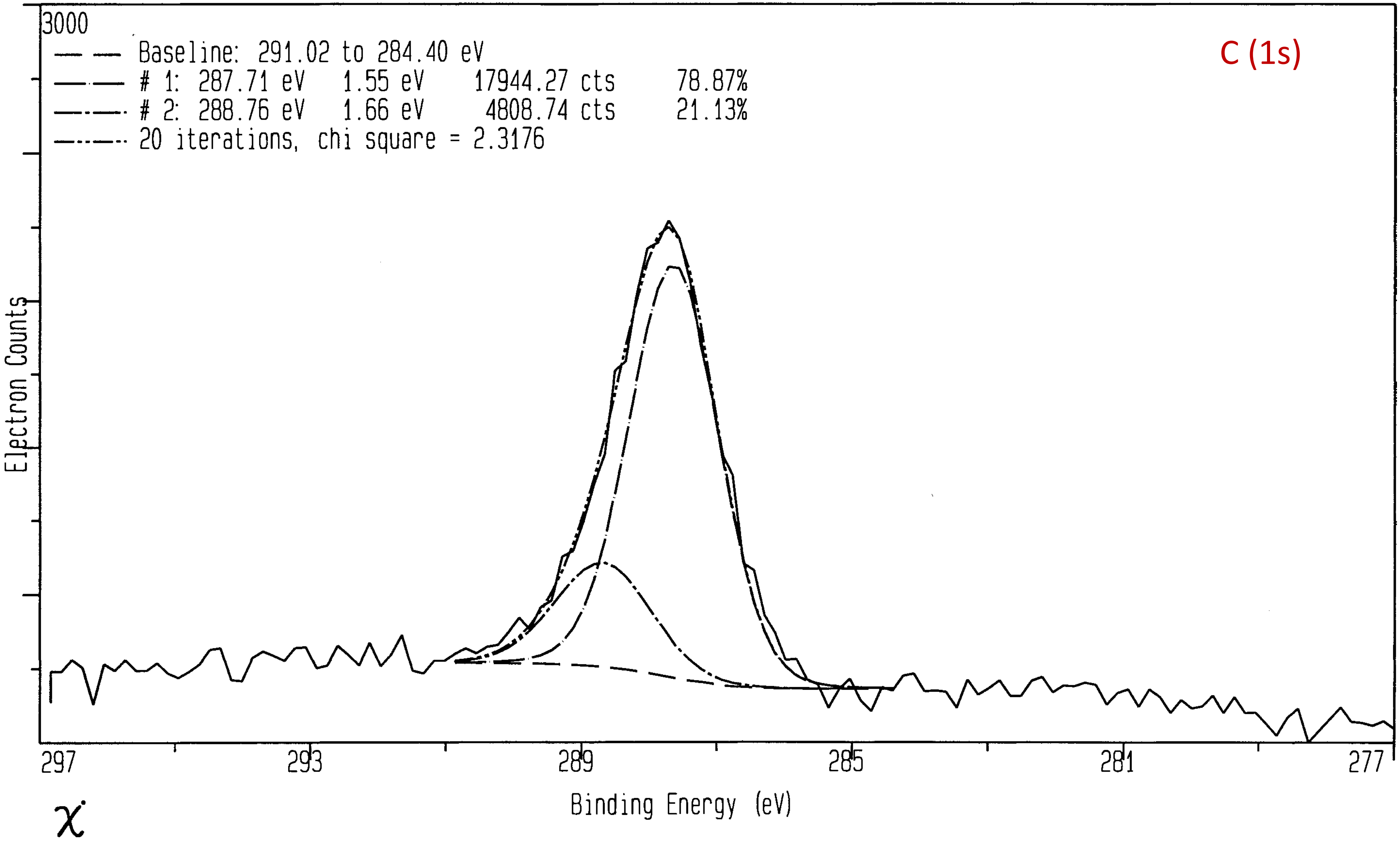
File: ALGAAS_1	Spot: 600	Flood Gun: Off	Data Points: 128	Date: 6/28/1988
Region: 4	Resolution: 2	Scans, Time: 10	Time/Point: 200	Operator: BVC

Description: ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)

AlGaAs



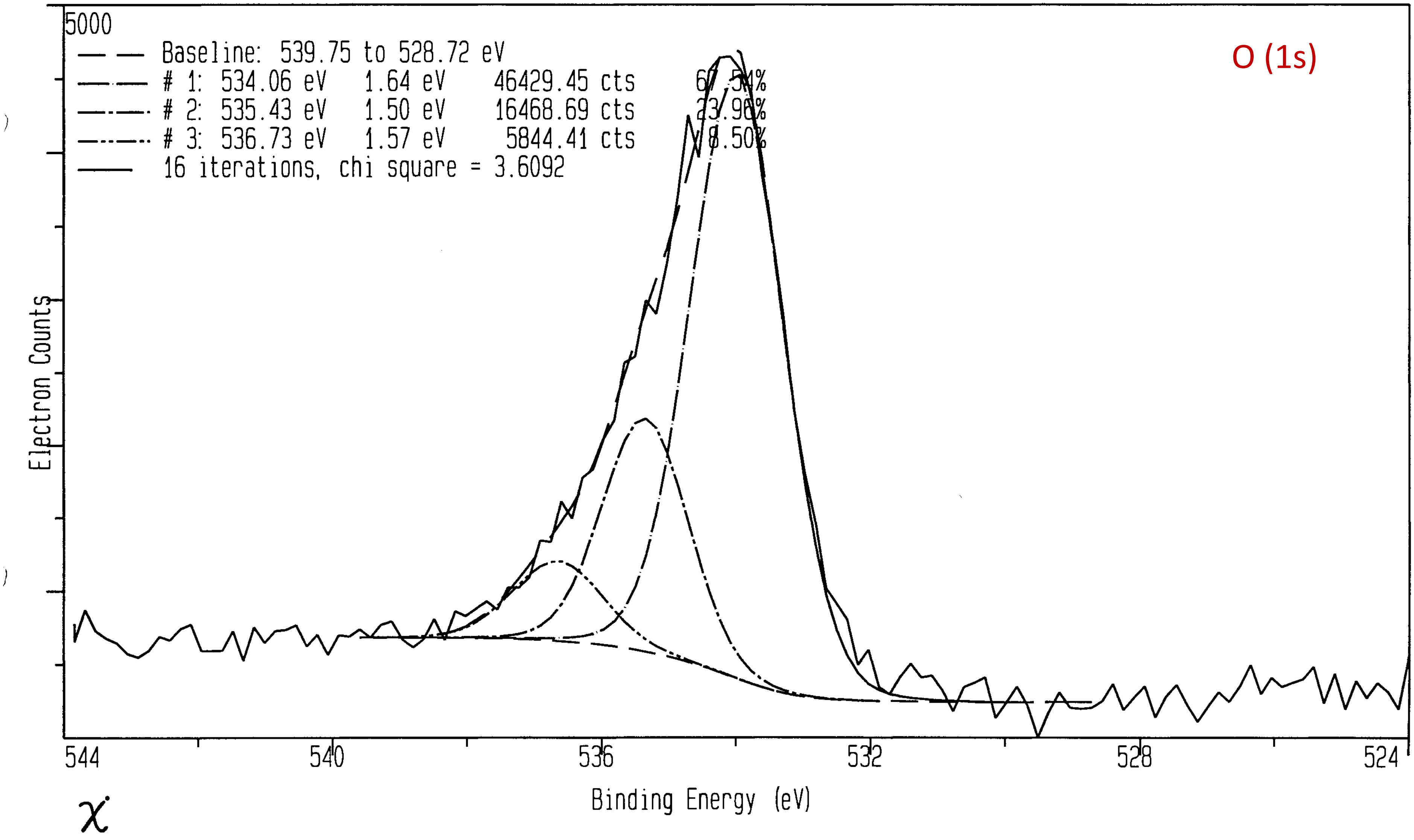
File: ALGAAS_1 Region: 2	Spot: 600 Resolution: 2	Flood Gun: Off Scans, Time: 4	Data Points: 128 Time/Point: 200	Date: 6/28/1988 Operator: BVC
Description:	ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)			AlGaAs



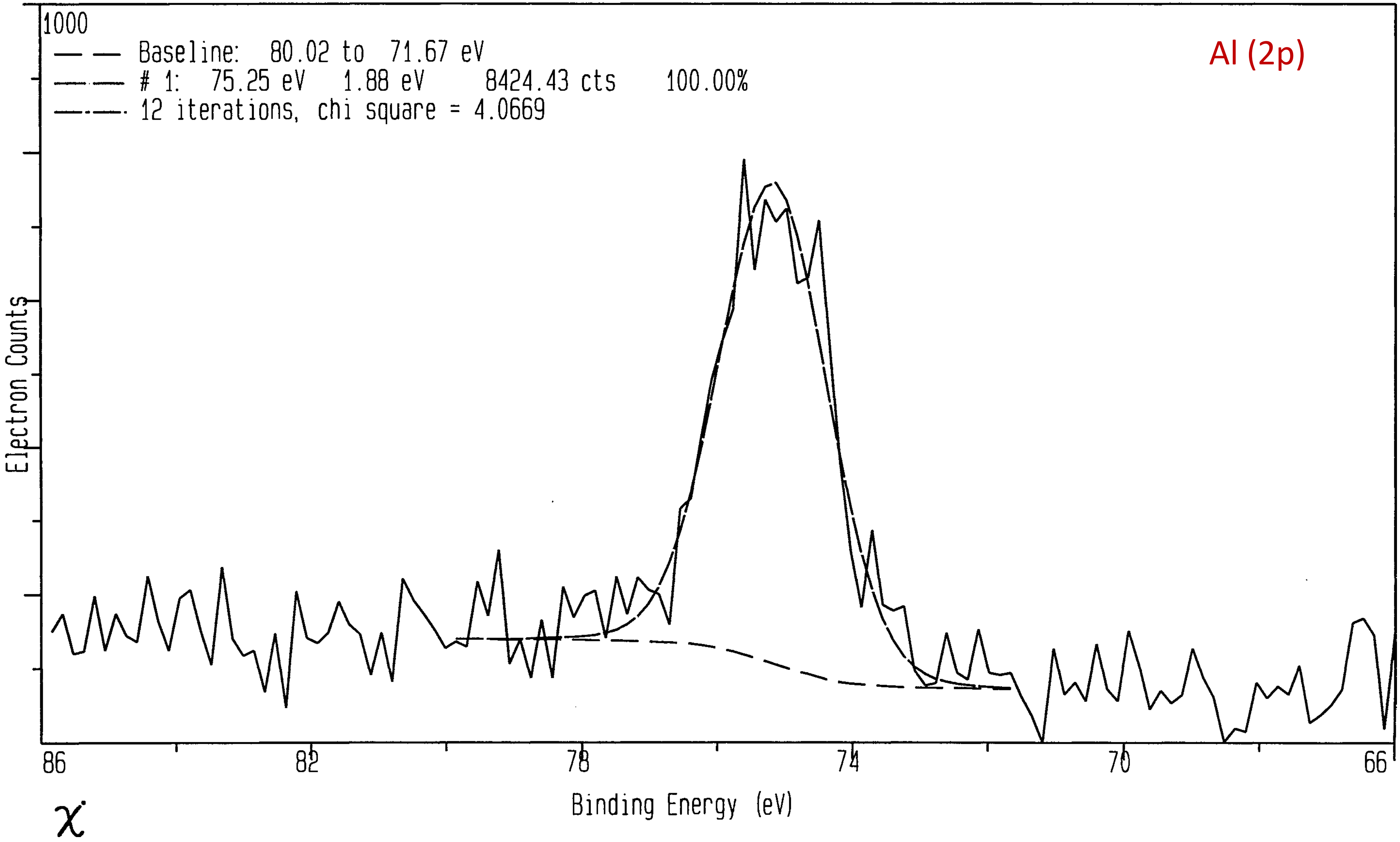
File: ALGAAS_1	Spot: 600	Flood Gun: Off	Data Points: 128	Date: 6/28/1988
Region: 5	Resolution: 2	Scans, Time: 10	Time/Point: 200	Operator: BVC

Description: ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)

AlGaAs



File: ALGAAS_1 Region: 10	Spot: 600 Resolution: 2	Flood Gun: Off Scans, Time: 40	Data Points: 128 Time/Point: 200	Date: 6/28/1988 Operator: BVC
Description:	ONE EPITAXIAL LAYER AlGaAs ON GaAs (AS RECD, 35TOA)			AlGaAs

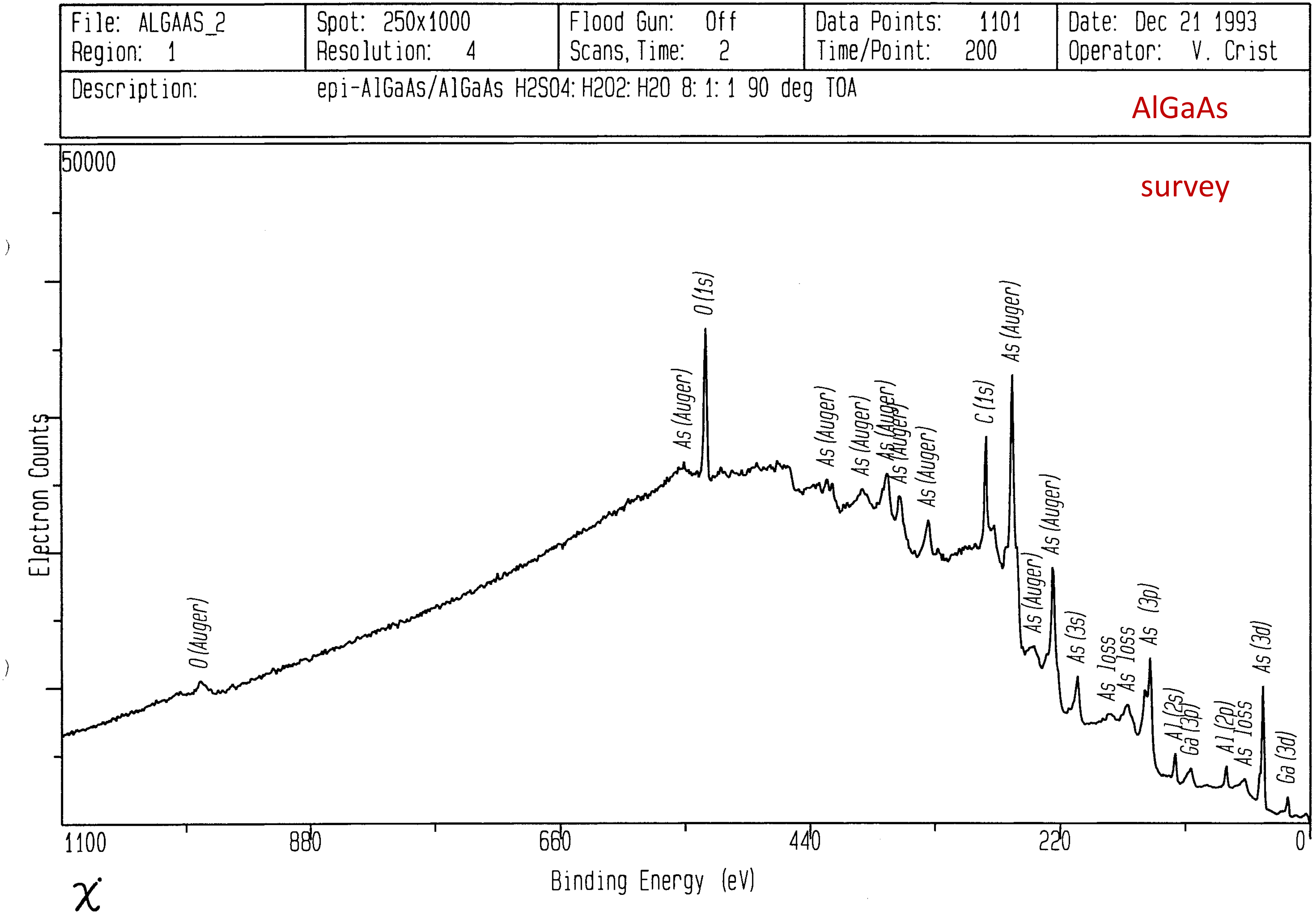


Detailed Surface Composition Table

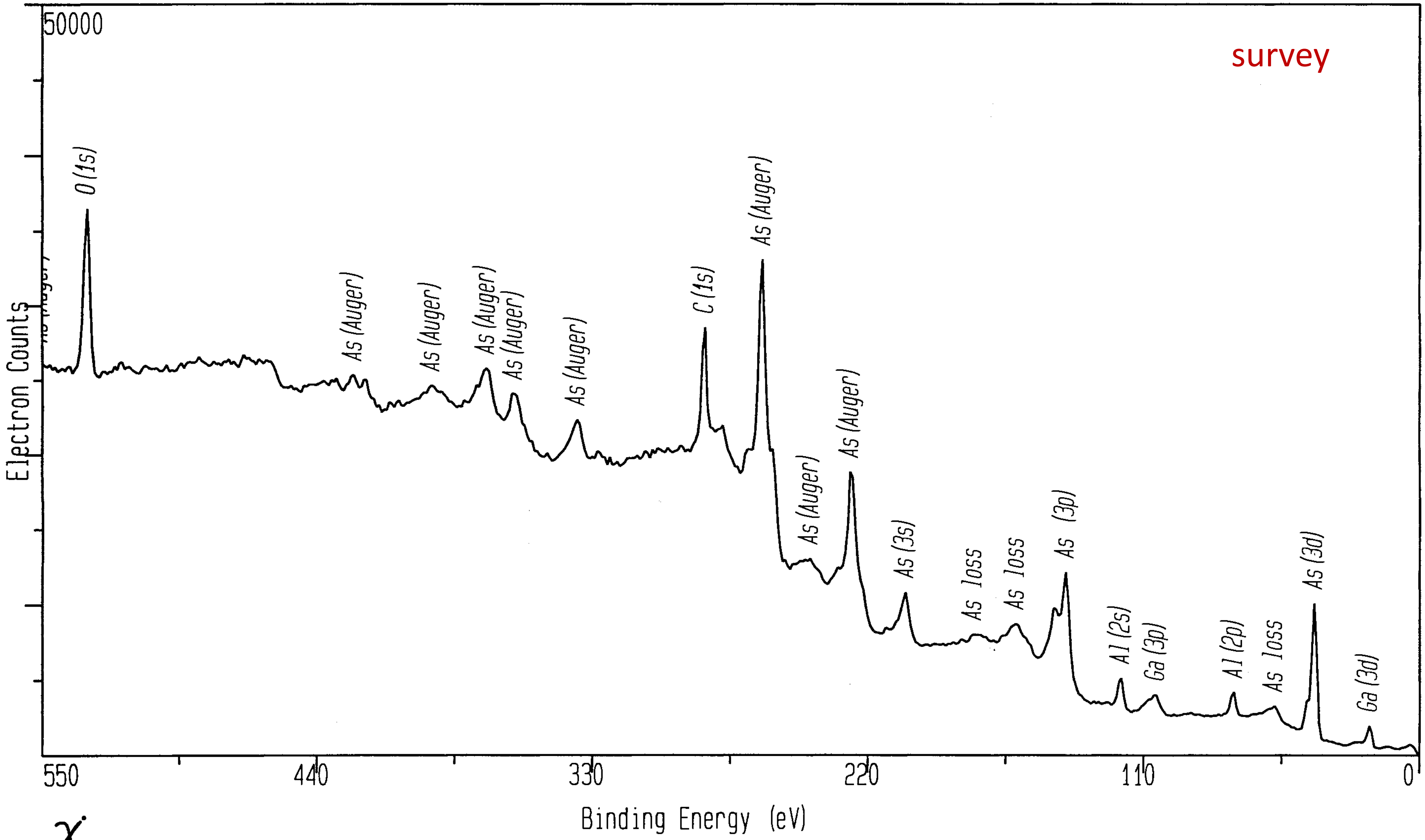
File name: ALGAAS_2.MRS
Region: 1
Description: epi-AlGaAs/AlGaAs H2SO4:H2O2:H2O 8:1:1 90 deg TOA

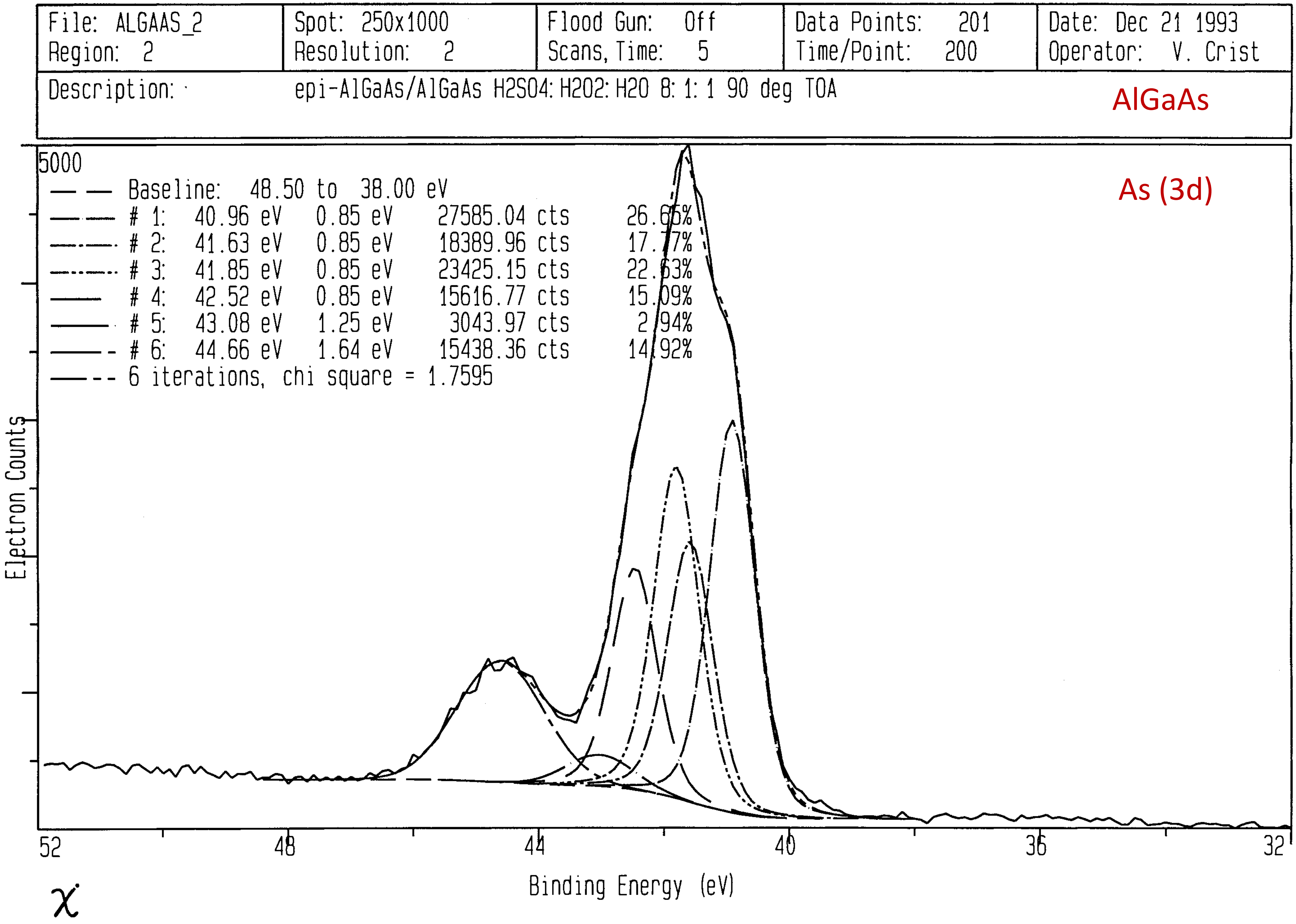
Operator: V. Crist
Date: Tue Dec 21 14:07 1993

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	977.5	977.5	0.00	12643	0	
AsAuger	550.5	550.5	0.09	11148	130742	
* O 1s	531.7	531.6	2.12	87544	41230	31.23
AsAuger	424.8	424.7	0.10	15011	147570	
AsAuger	393.4	393.3	0.11	24991	235855	
AsAuger	371.5	371.4	0.00	52607	0	
AsAuger	360.8	360.8	0.00	34063	0	
AsAuger	335.3	335.3	0.00	36352	0	
* C 1s	285.1	285.0	1.00	37536	37553	28.45
AsAuger	261.5	261.4	0.00	230007	0	
AsAuger	242.4	242.4	0.13	19230	151428	
AsAuger	225.9	225.8	0.00	124807	0	
As3s	204.4	204.3	1.45	40026	27699	
As loss	177.0	177.0	0.00	8993	0	
As loss	160.2	160.1	0.00	34239	0	
As (3p)	140.3	140.3	4.70	114331	24326	
Al2s	118.5	118.4	0.90	16532	18315	
Ga3p	104.6	104.6	3.90	18981	4867	
* Al2p	73.4	73.3	0.67	11398	16920	12.82
As loss	57.2	57.2	0.07	21597	297270	
* As3d	41.0	41.0	2.36	65627	27848	21.10
* Ga3d	19.0	19.0	1.43	12097	8462	6.41

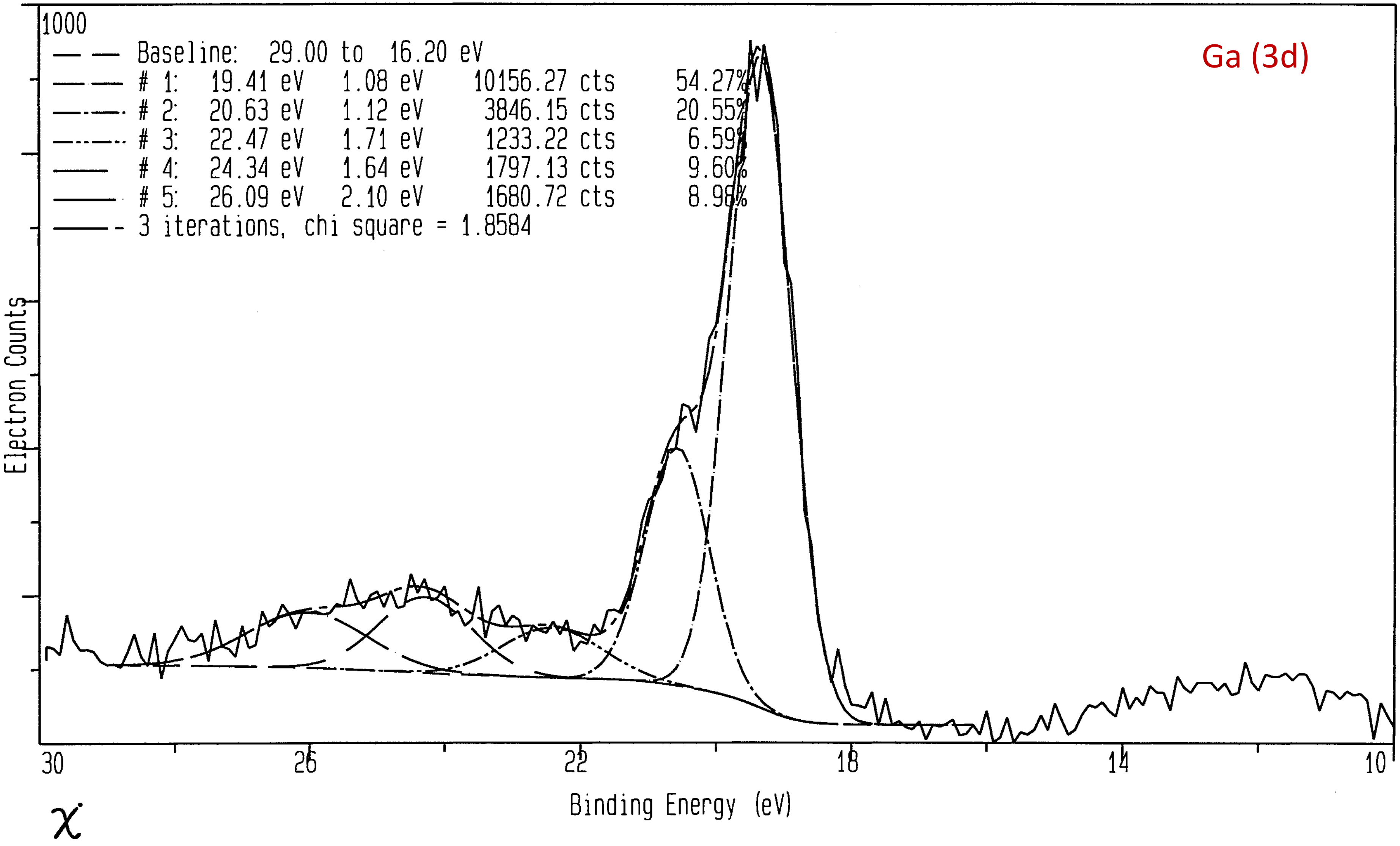

File: ALGAAS_2
Region: 1
Spot: 250x1000
Resolution: 4
Flood Gun: Off
Scans, Time: 2
Data Points: 1101
Time/Point: 200
Date: Dec 21 1993
Operator: V. Crist
Description: epi-AlGaAs/AlGaAs H2SO4: H2O2: H2O 8: 1: 1 90 deg TOA
AlGaAs
survey
50000
Electron Counts
O (Auger)
As (Auger)
O (1s)
As (Auger)
As (Auger)
As (Auger)
As (Auger)
As (Auger)
C (1s)
As (Auger)
As (Auger)
As (Auger)
As (3s)
As loss
As loss
As (3p)
Al (2s)
Ga (3p)
Al (2p)
As loss
As (3d)
Ga (3d)
1100
880
660
440
220
0
Binding Energy (eV)

File: ALGAAS_2 Region: 1	Spot: 250x1000 Resolution: 4	Flood Gun: Off Scans, Time: 2	Data Points: 1101 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs H2SO4: H2O2: H2O 8: 1: 1 90 deg TOA			AlGaAs

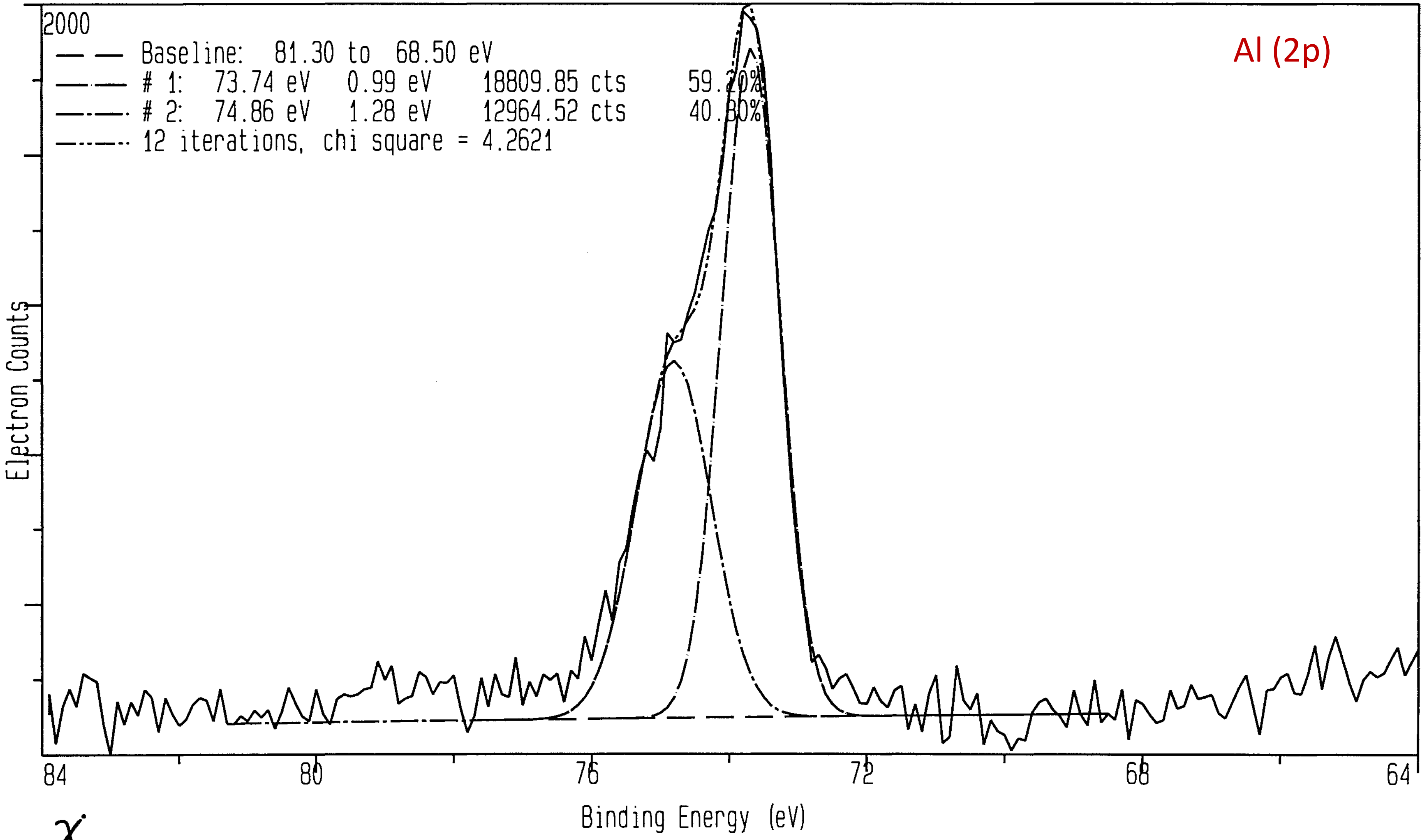



File: ALGAAS_2
Region: 2
Spot: 250x1000
Resolution: 2
Flood Gun: Off
Scans, Time: 5
Data Points: 201
Time/Point: 200
Date: Dec 21 1993
Operator: V. Crist
Description: epi-AlGaAs/AlGaAs H2SO4: H2O2: H2O 8: 1: 1 90 deg TOA
AlGaAs
As (3d)
5000
Baseline: 48.50 to 38.00 eV
1: 40.96 eV 0.85 eV 27585.04 cts 26.65%
2: 41.63 eV 0.85 eV 18389.96 cts 17.77%
3: 41.85 eV 0.85 eV 23425.15 cts 22.63%
4: 42.52 eV 0.85 eV 15616.77 cts 15.09%
5: 43.08 eV 1.25 eV 3043.97 cts 2.94%
6: 44.66 eV 1.64 eV 15438.36 cts 14.92%
6 iterations, chi square = 1.7595
Electron Counts
52
48
44
40
36
32
Binding Energy (eV)

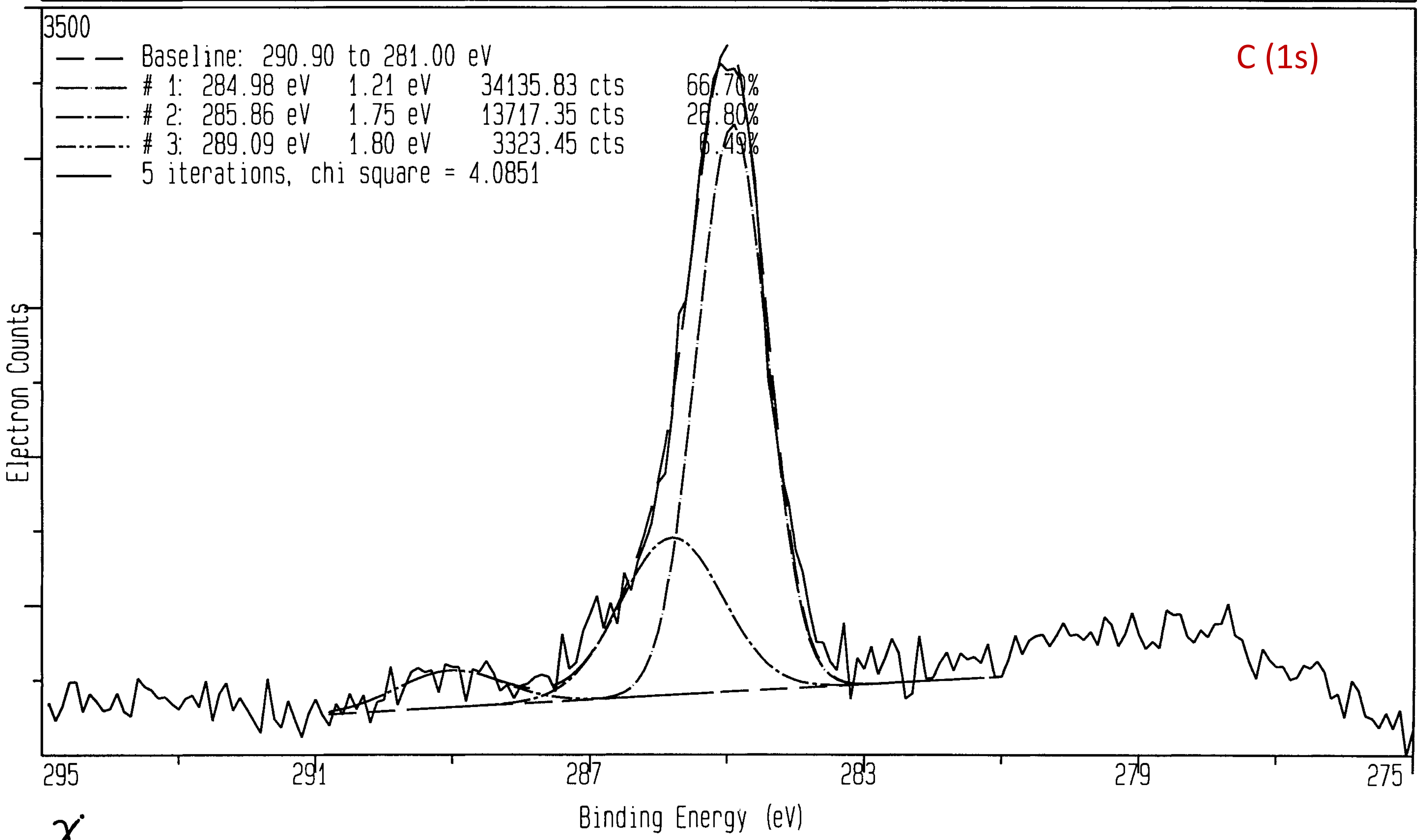
File: ALGAAS_2	Spot: 250x1000	Flood Gun: Off	Data Points: 201	Date: Dec 21 1993
Region: 3	Resolution: 2	Scans, Time: 5	Time/Point: 200	Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs H2SO4: H2O2: H2O 8: 1: 1 90 deg TOA			AlGaAs



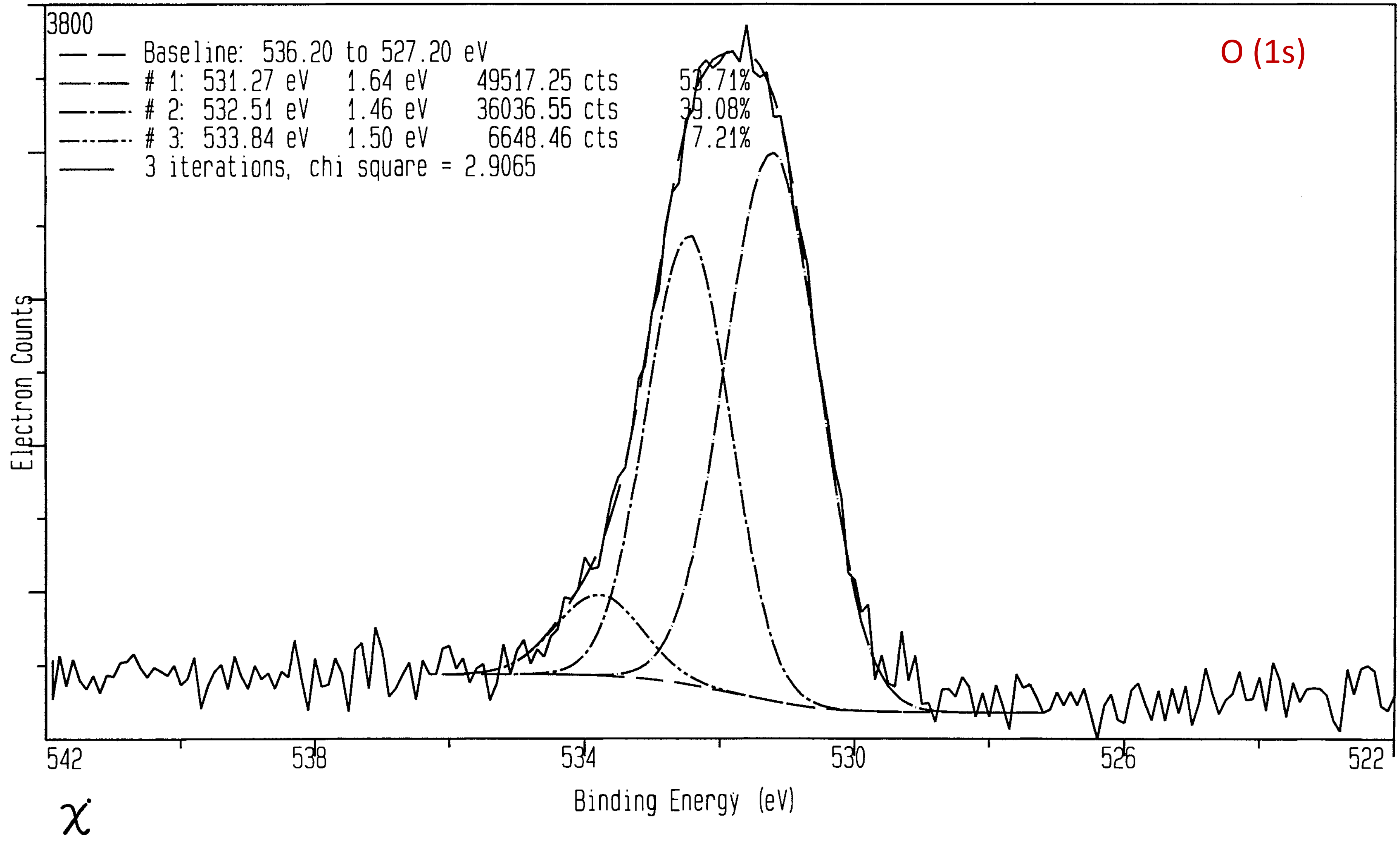
File: ALGAAS_2 Region: 4	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs H2SO4: H2O2: H2O 8: 1: 1 90 deg TOA			AlGaAs



File: ALGAAS_2 Region: 5	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 3	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs H2SO4: H2O2: H2O 8: 1: 1 90 deg TOA			AlGaAs



File: ALGAAS_2 Region: 6	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 3	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs H2SO4: H2O2: H20 8: 1: 1 90 deg TOA			AlGaAs



epi-Aluminium Gallium Arsenide (2 hr at 380 C in air)

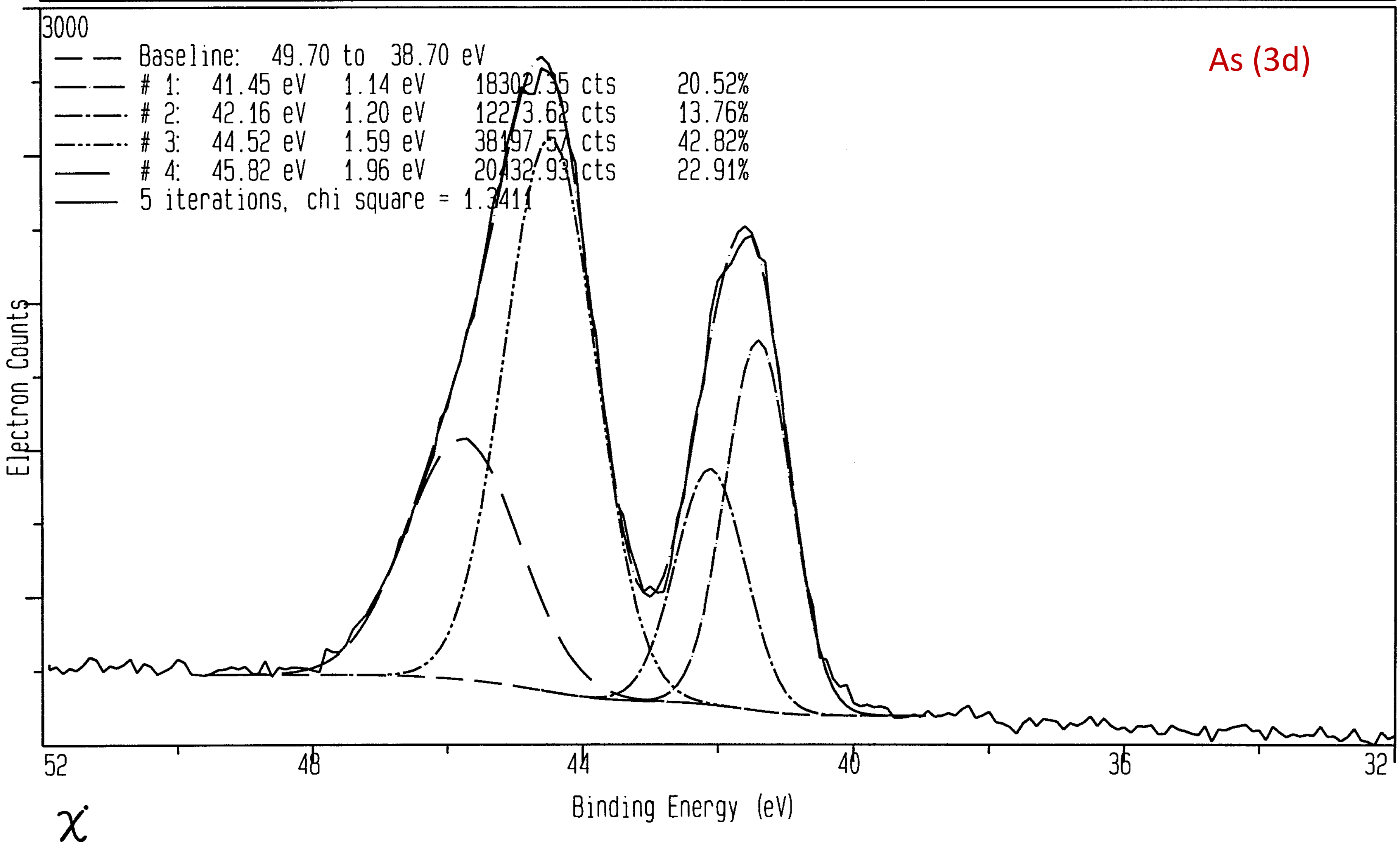
Detailed Surface Composition Table

File name: ALGAAS_3.MRS
Region: 1
Description: epi-AlGaAs/AlGaAs: AlGaAs_2 after 2h 380 C in air

Operator: V. Crist
Date: Tue Dec 21 14:41 1993

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
* As3d	41.5	41.5	1.89	1825	966	1.23
* As3d	42.2	42.2	1.89	1217	645	0.82
* As3d	44.5	44.5	1.89	3796	2011	2.56
* As3d	45.8	45.8	1.89	2021	1071	1.36
* Ga3d	19.5	19.5	1.13	467	414	0.53
* Ga3d	20.6	20.6	1.13	2332	2066	2.63
* Ga3d	22.9	22.9	1.13	843	747	0.95
* Ga3d	24.5	24.5	0.02	580	30984	39.45
* Ga3d	26.4	26.4	0.02	218	11649	14.83
* Al2p	74.4	74.4	0.55	2659	4795	6.10
* Al2p	75.4	75.4	0.55	315	568	0.72
* C 1s	285.0	285.0	1.00	6919	6920	8.81
* C 1s	286.5	286.5	1.00	1094	1094	1.39
* C 1s	289.0	289.0	1.00	619	619	0.79
* O 1s	531.2	531.2	2.80	29851	10667	13.58
* O 1s	532.4	532.4	2.80	9308	3327	4.24

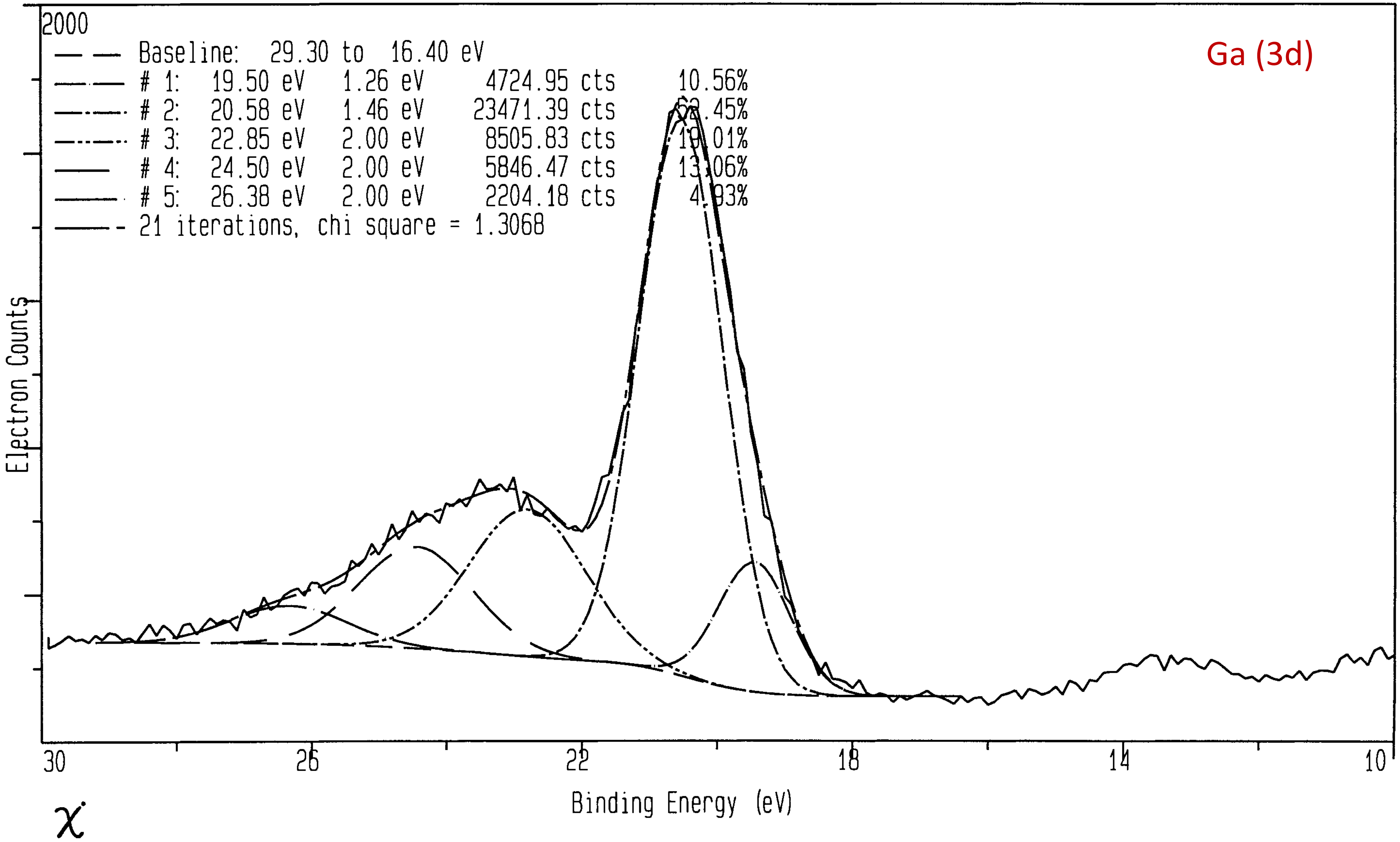
File: ALGAAS_3 Region: 1	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 5	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs: AlGaAs_2 after 2h 380 C in air			AlGaAs



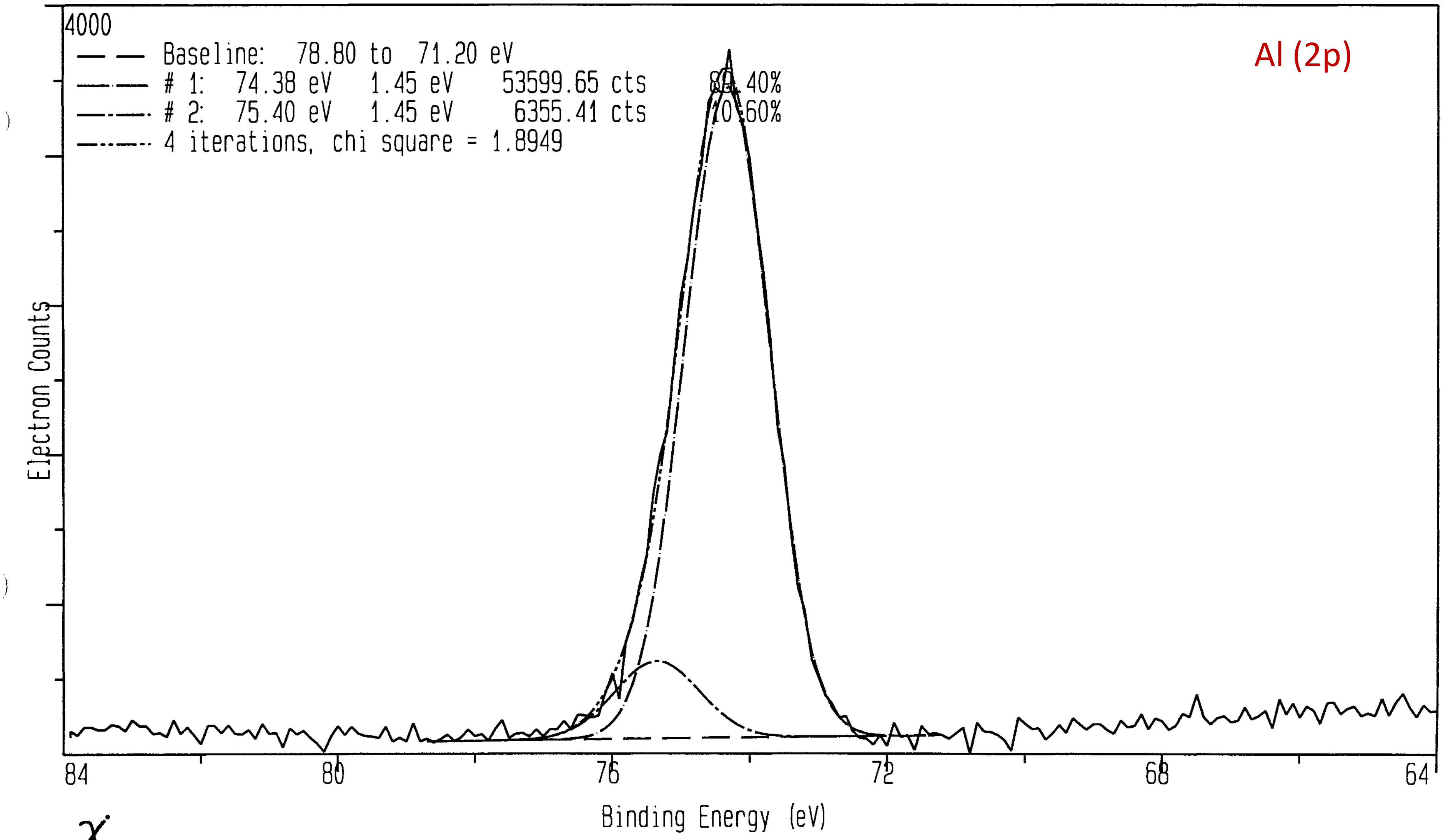
File: ALGAAS_3	Spot: 250x1000	Flood Gun: Off	Data Points: 201	Date: Dec 21 1993
Region: 2	Resolution: 2	Scans, Time: 5	Time/Point: 200	Operator: V. Crist

Description: epi-AlGaAs/AlGaAs: AlGaAs_2 after 2h 380 C in air

AlGaAs



File: ALGAAS_3 Region: 3	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs: AlGaAs_2 after 2h 380 C in air			AlGaAs



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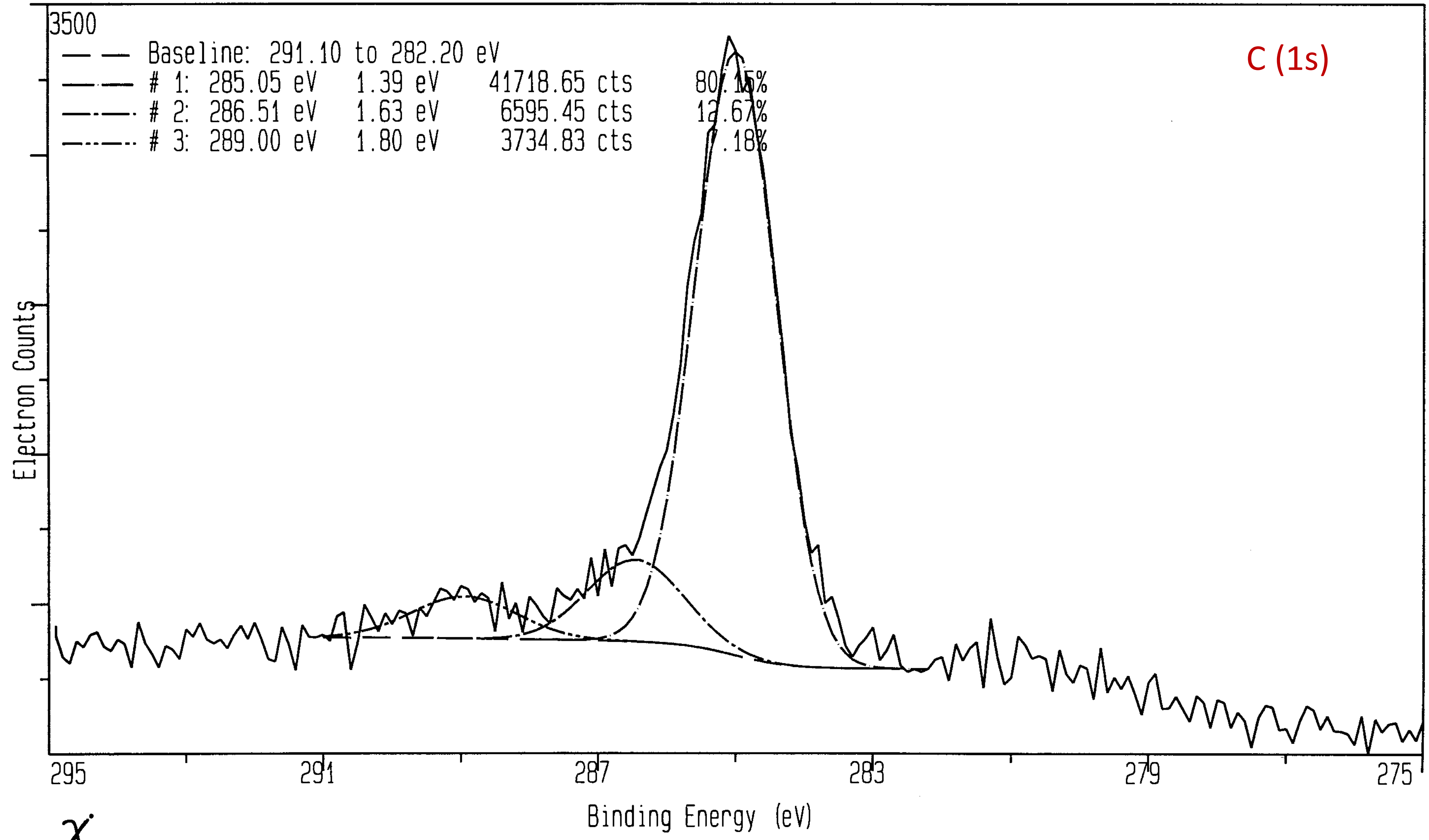
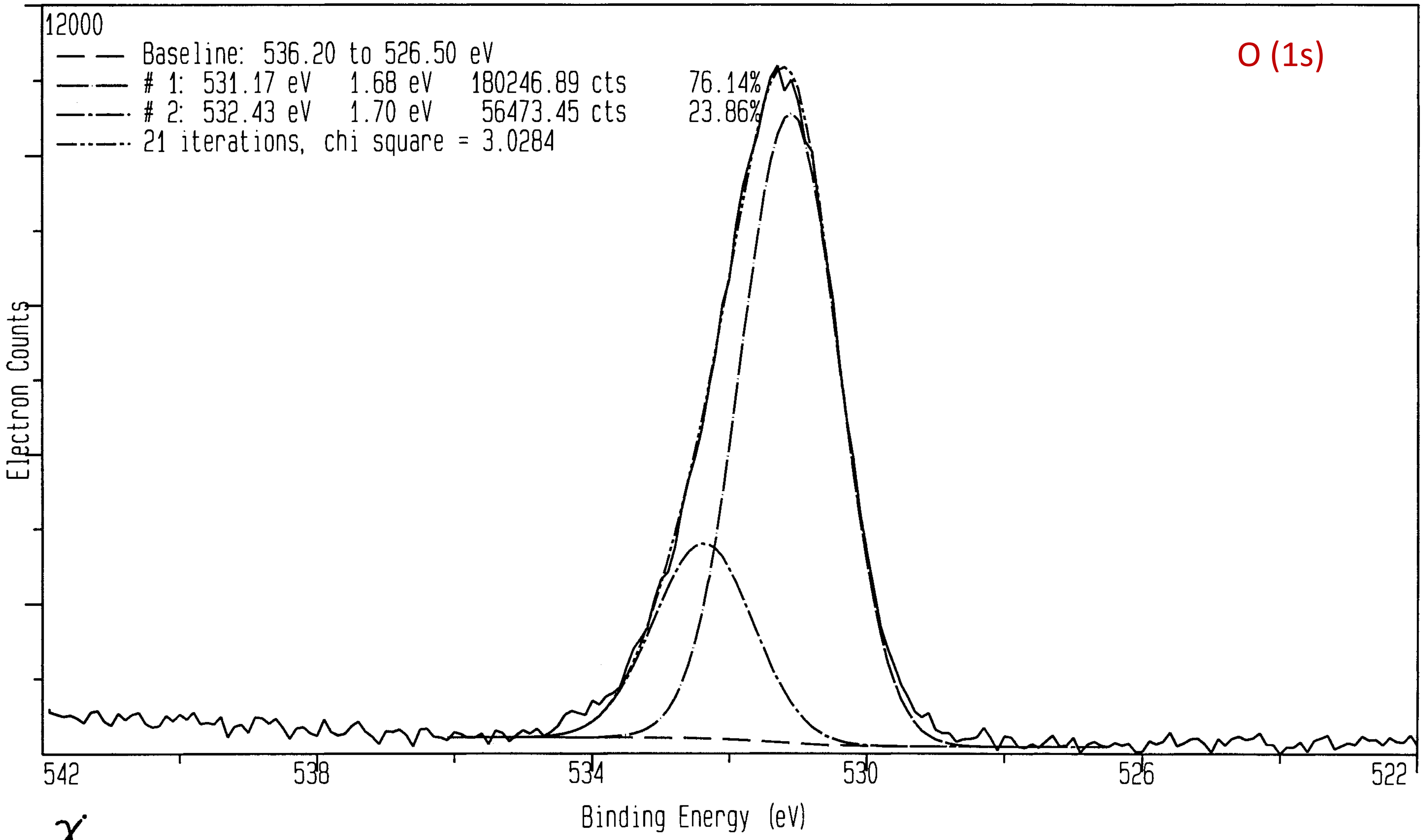
File: ALGAAS_3 Region: 4	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 3	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs: AlGaAs_2 after 2h 380 C in air			AlGaAs



File: ALGAAS_3 Region: 5	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 3	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs: AlGaAs_2 after 2h 380 C in air			AlGaAs



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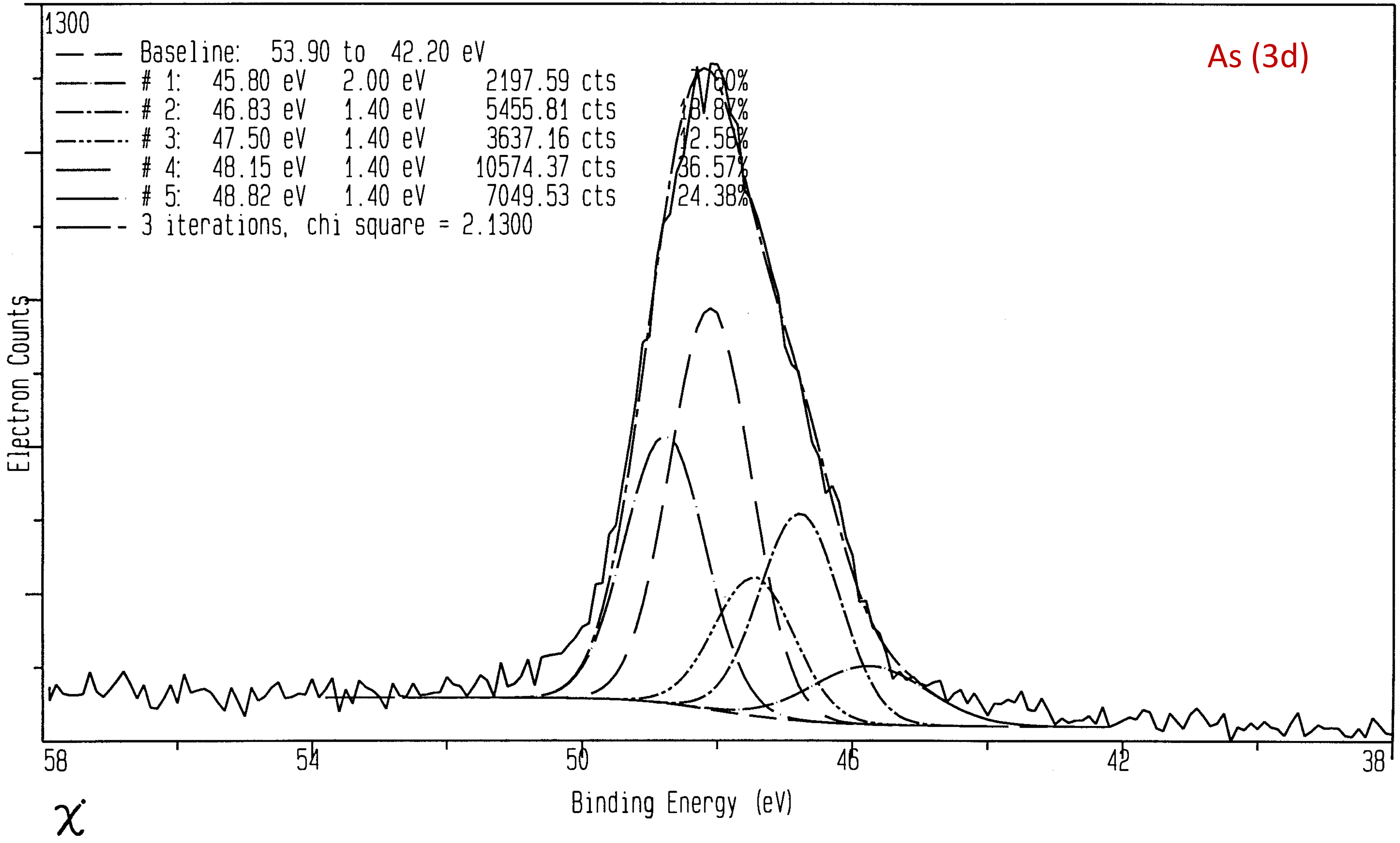
File: ALGAAS_5 Region: 1	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 5	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist

Description: epi-AlGaAs/AlGaAs: AlGaAs_3 after 2hr in Ar at 380

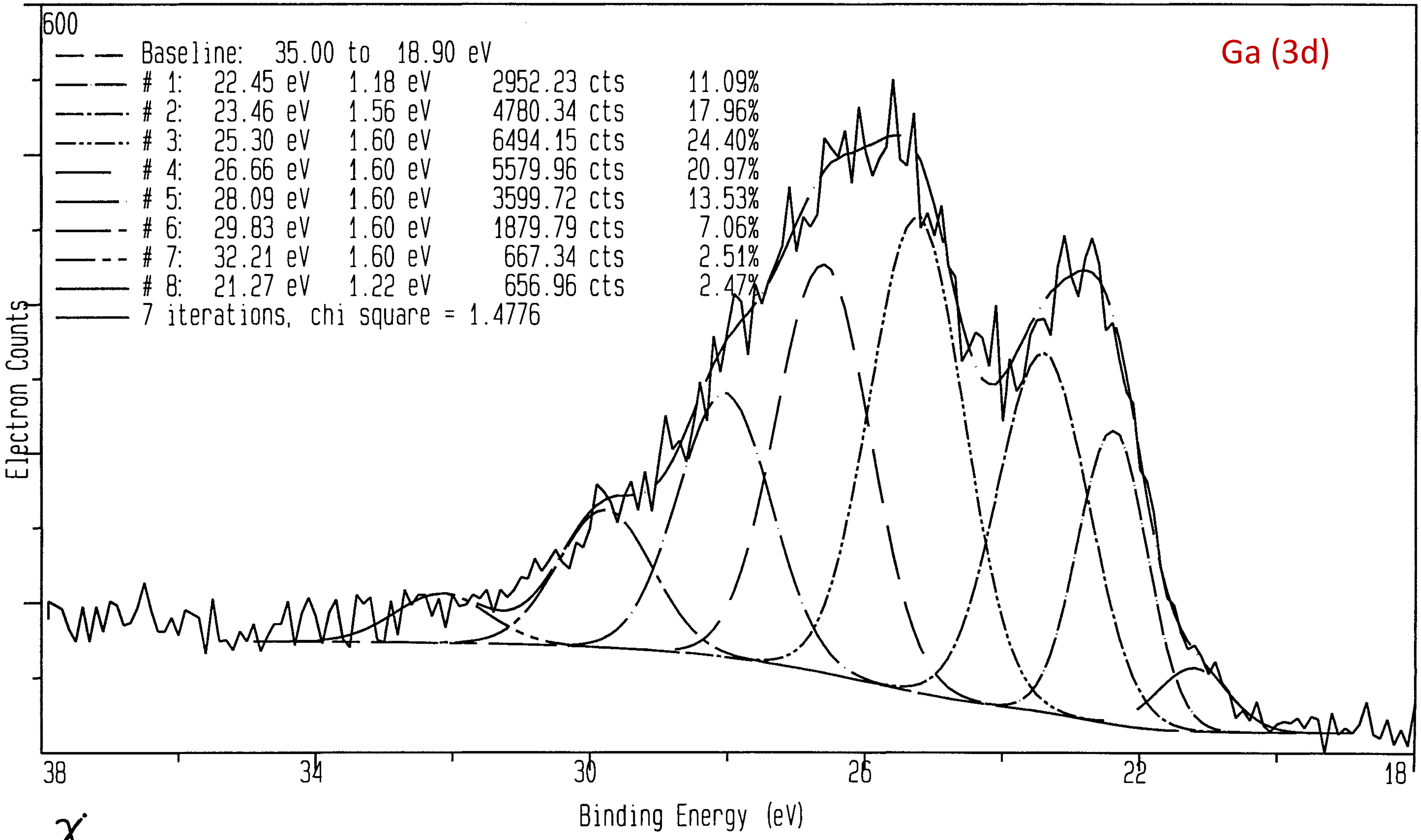
AlGaAs



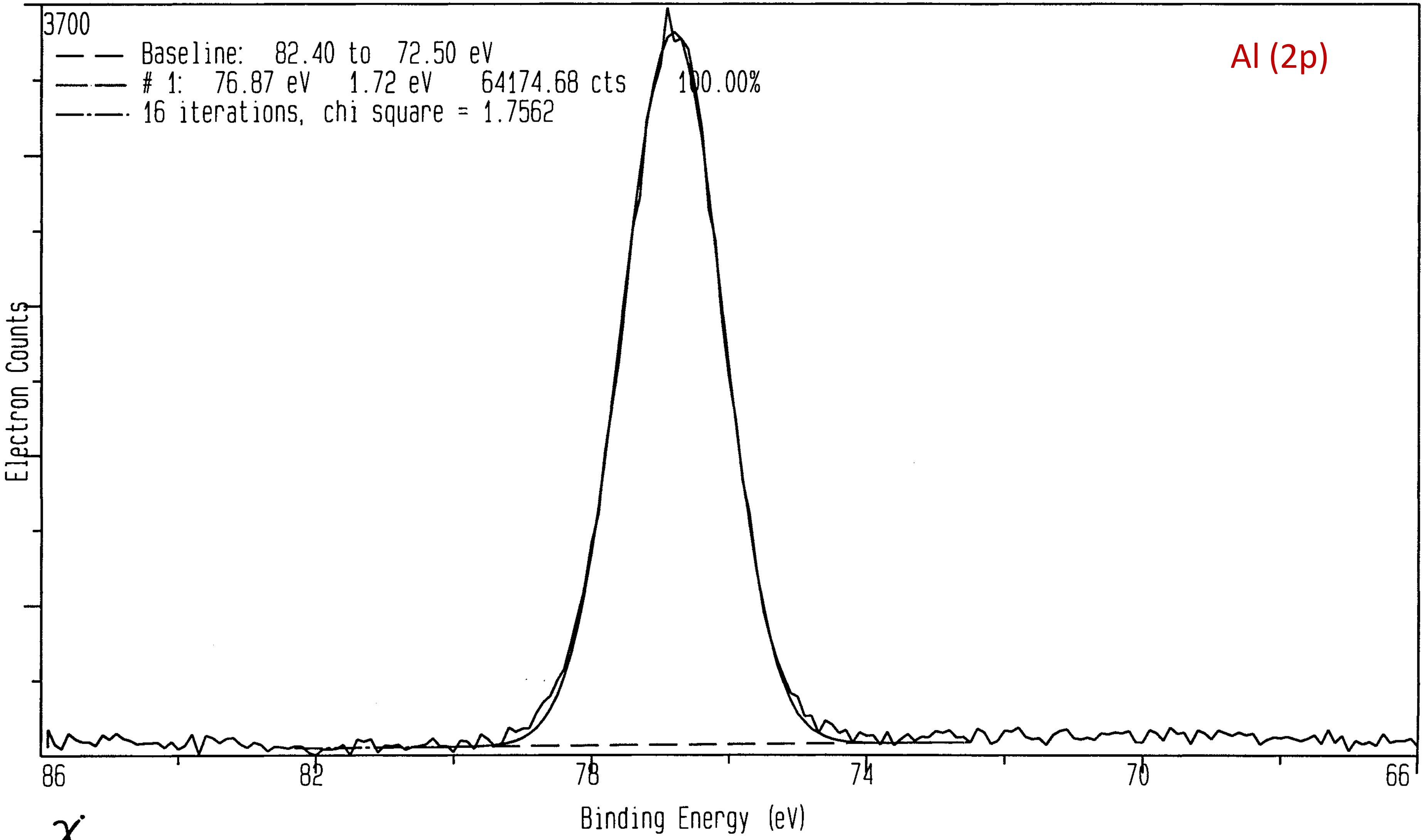
File: ALGAAS_5	Spot: 250x1000	Flood Gun: Off	Data Points: 201	Date: Dec 21 1993
Region: 2	Resolution: 2	Scans, Time: 5	Time/Point: 200	Operator: V. Crist

Description: epi-AlGaAs/AlGaAs: AlGaAs_3 after 2hr in Ar at 380

AlGaAs



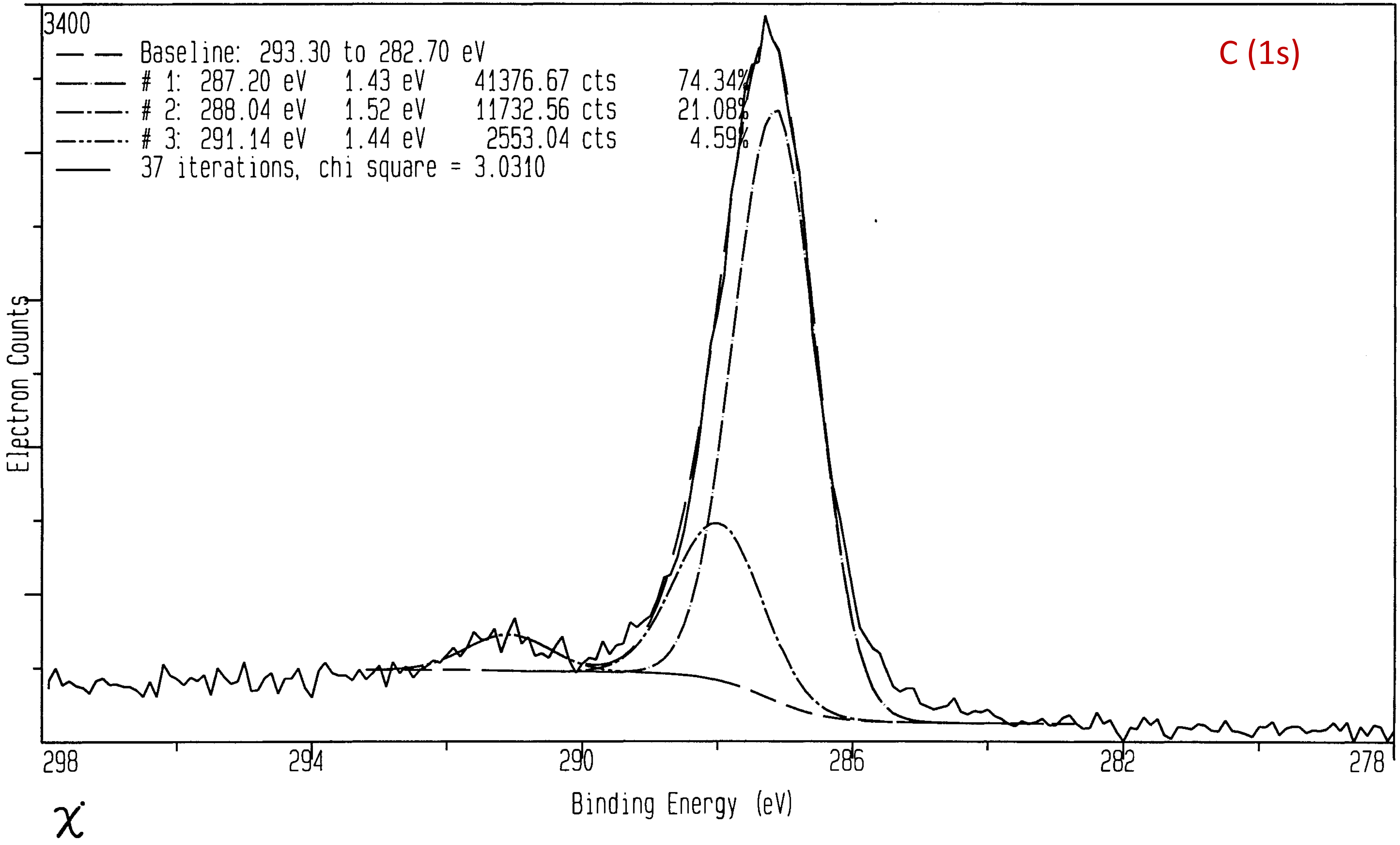
File: ALGAAS_5 Region: 3	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 8	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist
Description:	epi-AlGaAs/AlGaAs: AlGaAs_3 after 2hr in Ar at 380			AlGaAs

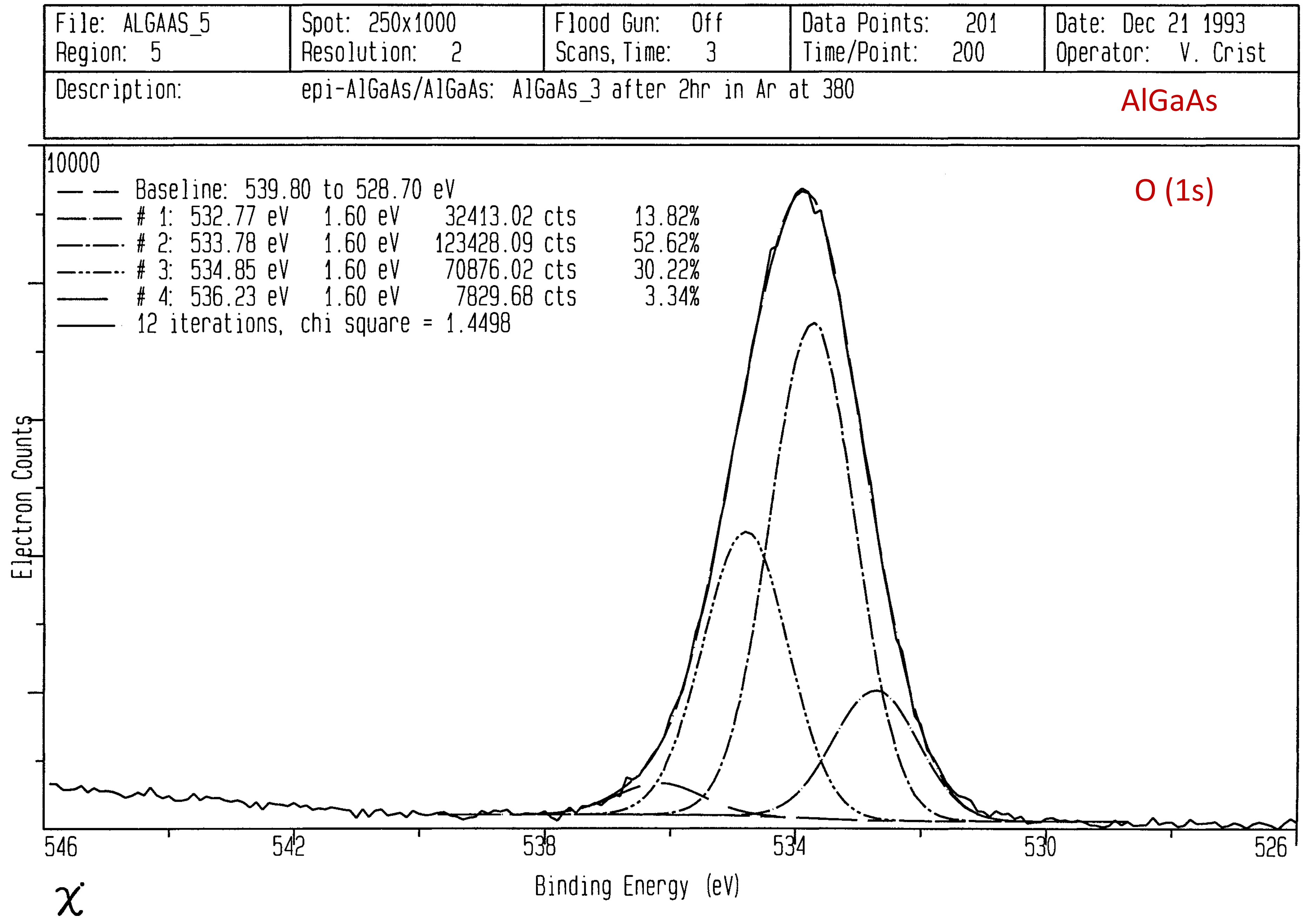


File: ALGAAS_5 Region: 4	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 3	Data Points: 201 Time/Point: 200	Date: Dec 21 1993 Operator: V. Crist

Description: epi-AlGaAs/AlGaAs: AlGaAs_3 after 2hr in Ar at 380

AlGaAs




File: ALGAAS_5
Region: 5
Spot: 250x1000
Resolution: 2
Flood Gun: Off
Scans, Time: 3
Data Points: 201
Time/Point: 200
Date: Dec 21 1993
Operator: V. Crist
Description: epi-AlGaAs/AlGaAs: AlGaAs_3 after 2hr in Ar at 380
AlGaAs
10000
Baseline: 539.80 to 528.70 eV
1: 532.77 eV 1.60 eV 32413.02 cts 13.82%
2: 533.78 eV 1.60 eV 123428.09 cts 52.62%
3: 534.85 eV 1.60 eV 70876.02 cts 30.22%
4: 536.23 eV 1.60 eV 7829.68 cts 3.34%
12 iterations, chi square = 1.4498
O (1s)
Electron Counts
546
542
538
534
530
526
Binding Energy (eV)

Aluminium Nitride (as received) (FW=40.99)

Detailed Surface Composition Table

File name: ALN_2.MRS
Region: 1
Description: AlN Coating (as received, 35 deg TOA) Conductive

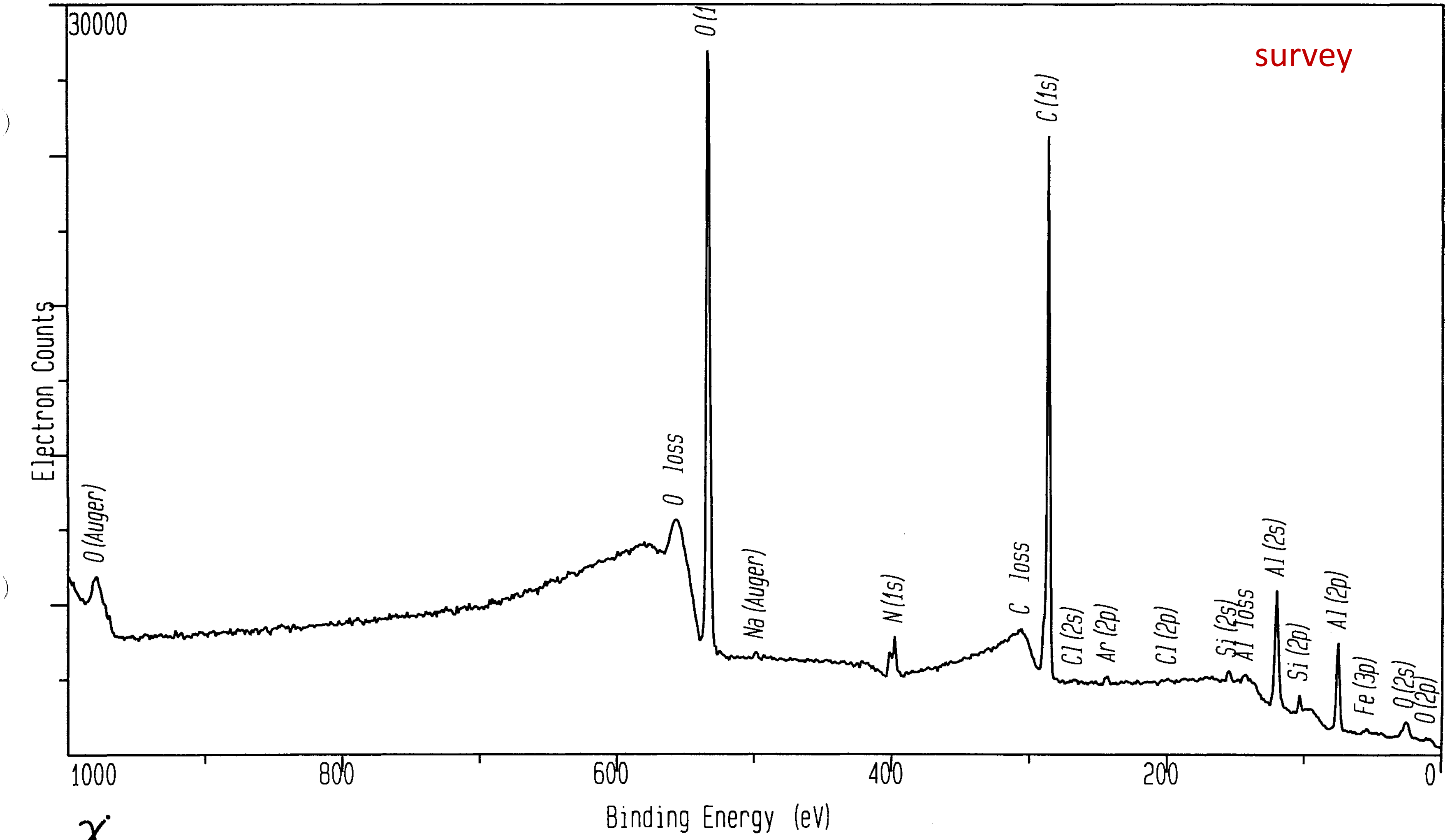
Operator: Vince Crist
Date: Tue Jun 11 12:04 1991

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	979.1	979.1	0.00	12938	0	
O loss	556.4	556.4	0.00	37500	0	
* O 1s	532.8	532.8	2.27	63459	27934	29.93
* NaAuger	498.5	498.5	2.74	863	315	0.34
* N 1s	397.3	397.3	1.62	5699	3528	3.78
C loss	305.4	305.4	4.02	7588	1888	
* C 1s	285.7	285.7	1.00	44772	44816	48.02
Cl2s	267.8	267.8	1.72	806	470	
* Ar2p	242.8	242.8	3.16	1034	327	0.35
* Cl2p	199.4	199.4	2.46	754	306	0.33
* Si2s	154.2	154.2	1.07	1143	1069	1.15
Al loss	141.8	141.8	0.00	4812	0	
* Al2s	119.4	119.4	0.87	12813	14769	15.83
Si2p	103.6	103.6	0.95	1171	1228	
Al2p	74.6	74.6	0.64	8231	12839	
* Fe3p	53.6	53.6	2.03	521	257	0.28
O 2s	25.0	25.0	0.17	3506	20196	
O 2p	10.1	10.1	0.02	973	40831	

File: ALN_2	Spot: 250x1000	Flood Gun: Off	Data Points: 1024	Date: Jun 11 1991
Region: 1	Resolution: 4	Scans, Time: 6	Time/Point: 200	Operator: Vince Cri

Description: AlN coating (as rec'd, 35 deg TOA) Conductive
(null)

AlN



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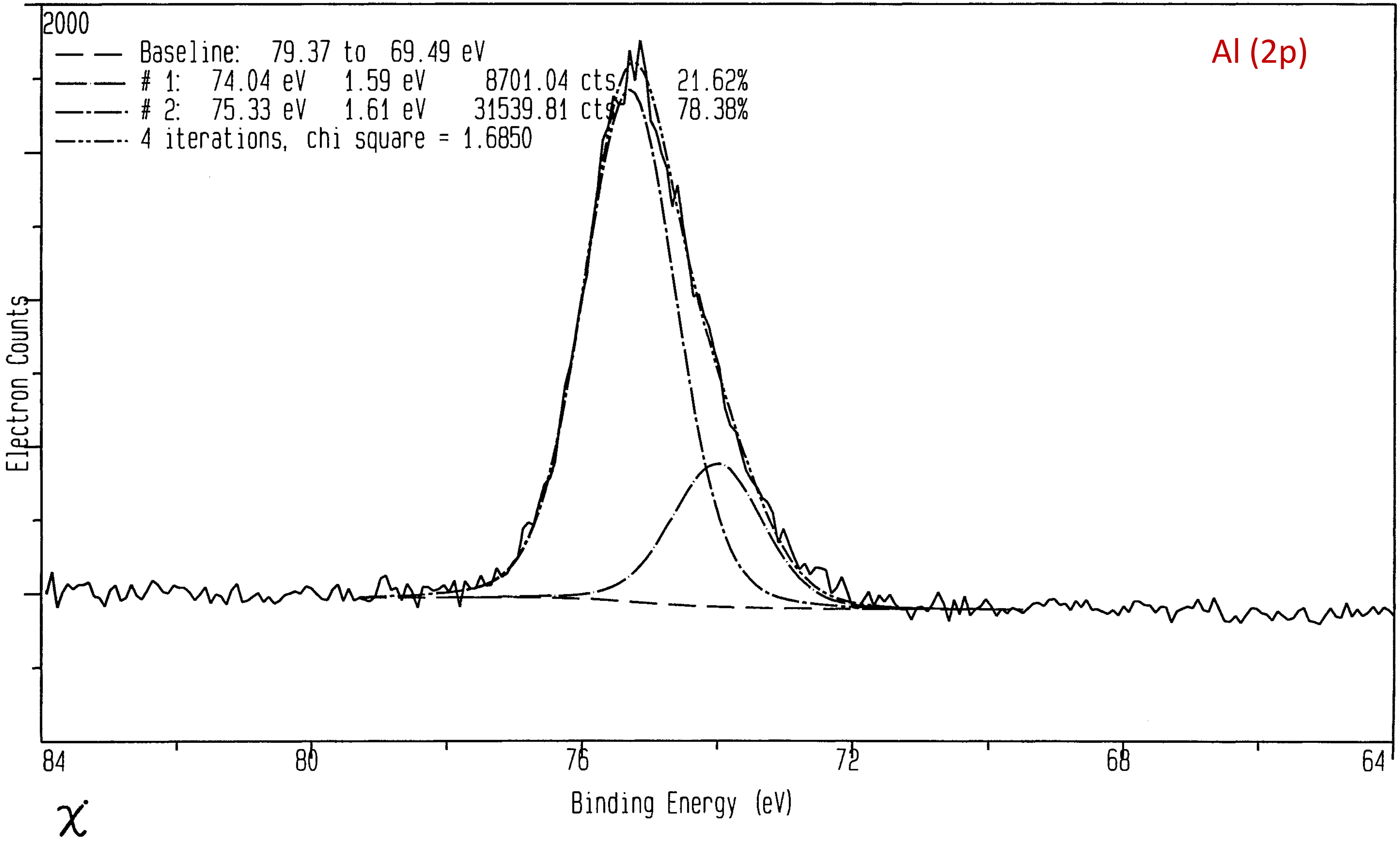
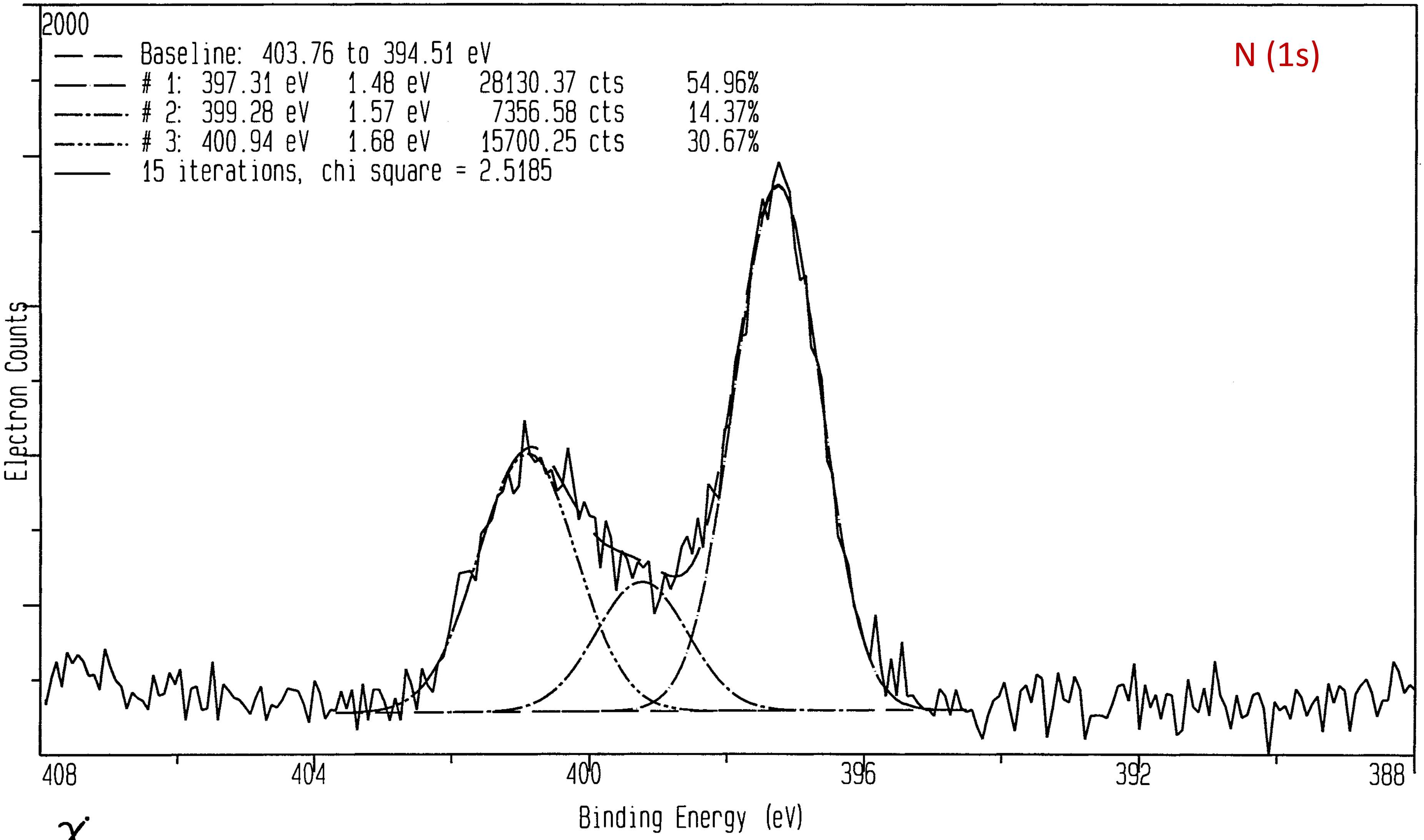
File: ALN_2 Region: 4	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 256 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri

Description: AlN coating (as rec'd, 35 deg TOA) Conductive
(null)

AlN



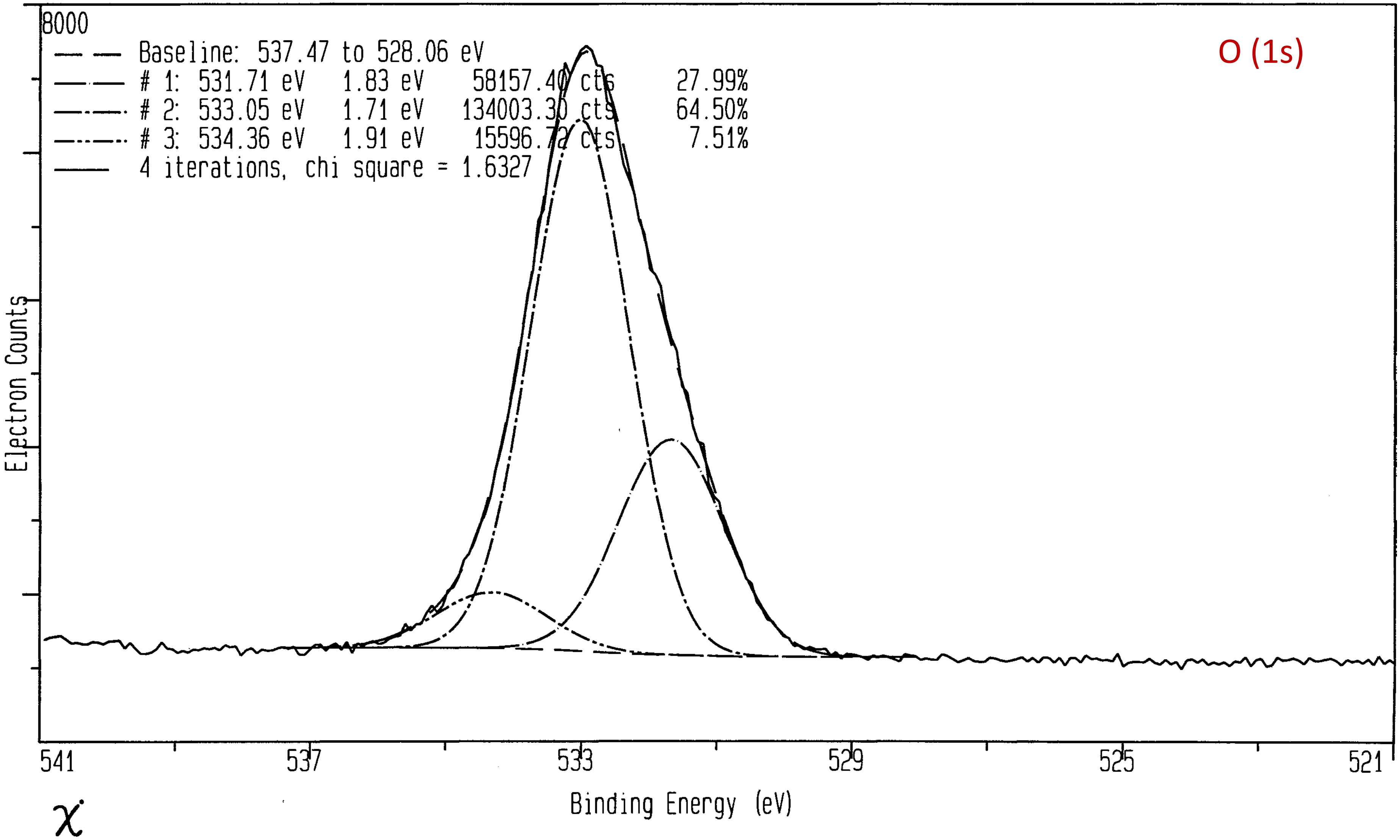
File: ALN_2 Region: 5	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 20	Data Points: 256 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	AlN coating (as rec'd, 35 deg TOA) Conductive (null)			AlN



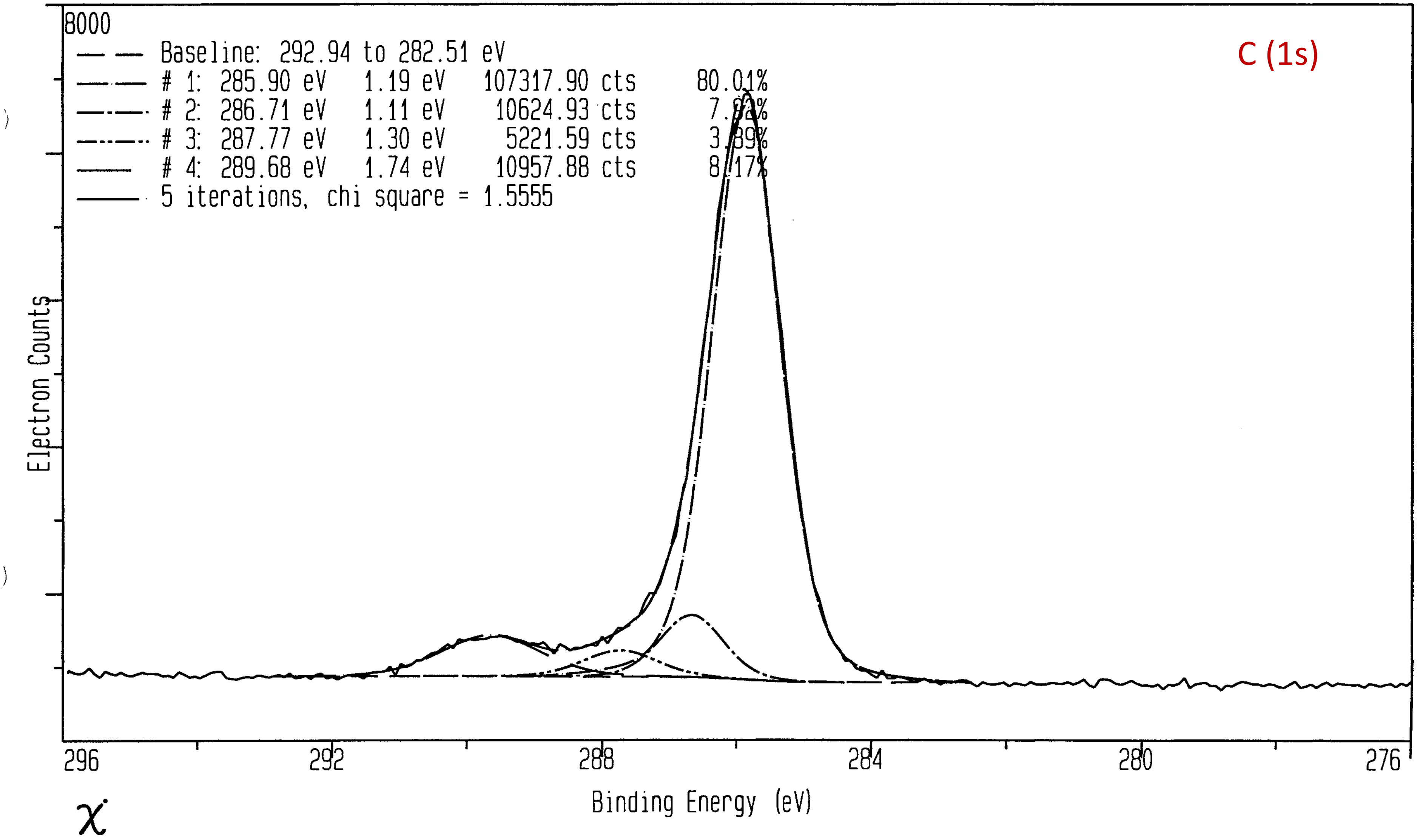
File: ALN_2 Region: 3	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 6	Data Points: 256 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri

Description: AlN coating (as rec'd, 35 deg TOA) Conductive
(null)

AlN



File: ALN_2 Region: 2	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 6	Data Points: 256 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	AlN coating (as rec'd, 35 deg TOA) Conductive (null)			AlN



Aluminium Nitride (etch crater) (FW=40.99)

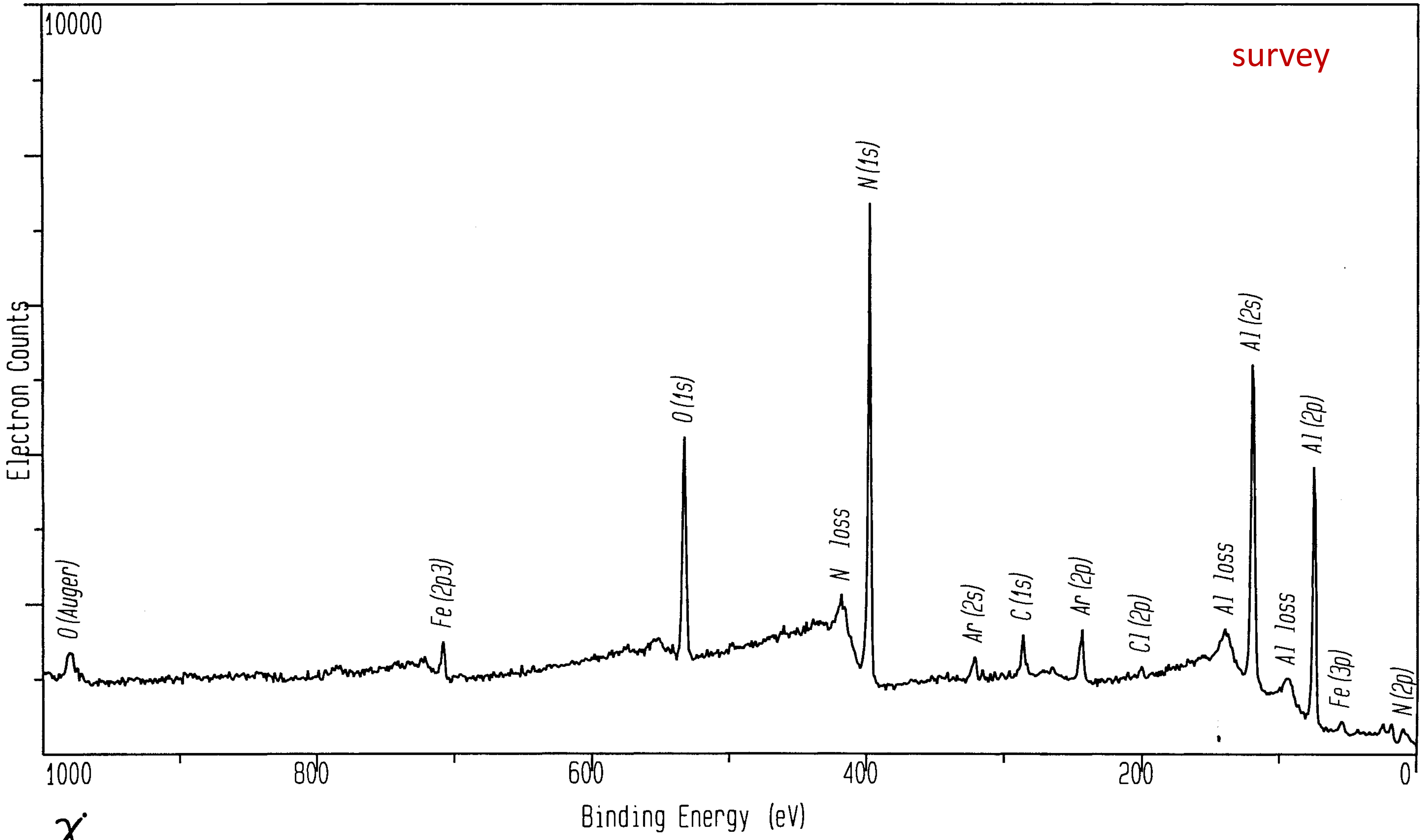
Detailed Surface Composition Table

File name: ALN_4.MRS
Region: 1
Description: Bottom of AlN coating (Ion Etch Crater: 200 Angstrom depth)

Operator: Vince Crist
Date: Tue Jun 11 14:19 1991

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	980.4	980.4	0.00	3957	0	
* Fe2p3	707.7	707.7	6.71	1836	274	0.64
* O 1s	532.5	532.5	2.27	12094	5322	12.35
N loss	417.9	417.9	0.00	7226	0	
* N 1s	397.3	397.3	1.62	20173	12490	29.00
Ar2s	320.7	320.7	1.91	1604	842	
* C 1s	285.8	285.8	1.00	2763	2766	6.42
* Ar2p	242.9	242.9	3.16	3281	1040	2.41
* Cl2p	200.4	200.4	2.46	477	194	0.45
Al loss	139.1	139.1	0.00	6227	0	
* Al2s	119.0	119.0	0.87	18217	20991	48.73
Al loss	93.8	93.8	0.00	4323	0	
Al2p	74.1	74.1	0.64	12323	19216	
Fe3p	53.6	53.6	2.03	881	435	
N 2p	9.0	9.0	0.00	1514	0	

File: ALN_4 Region: 1	Spot: 150x800 Resolution: 4	Flood Gun: Off Scans, Time: 4	Data Points: 1024 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	Bottom of Al_N coating Ion Etch Crater (200 ang depth) (null)			AlN



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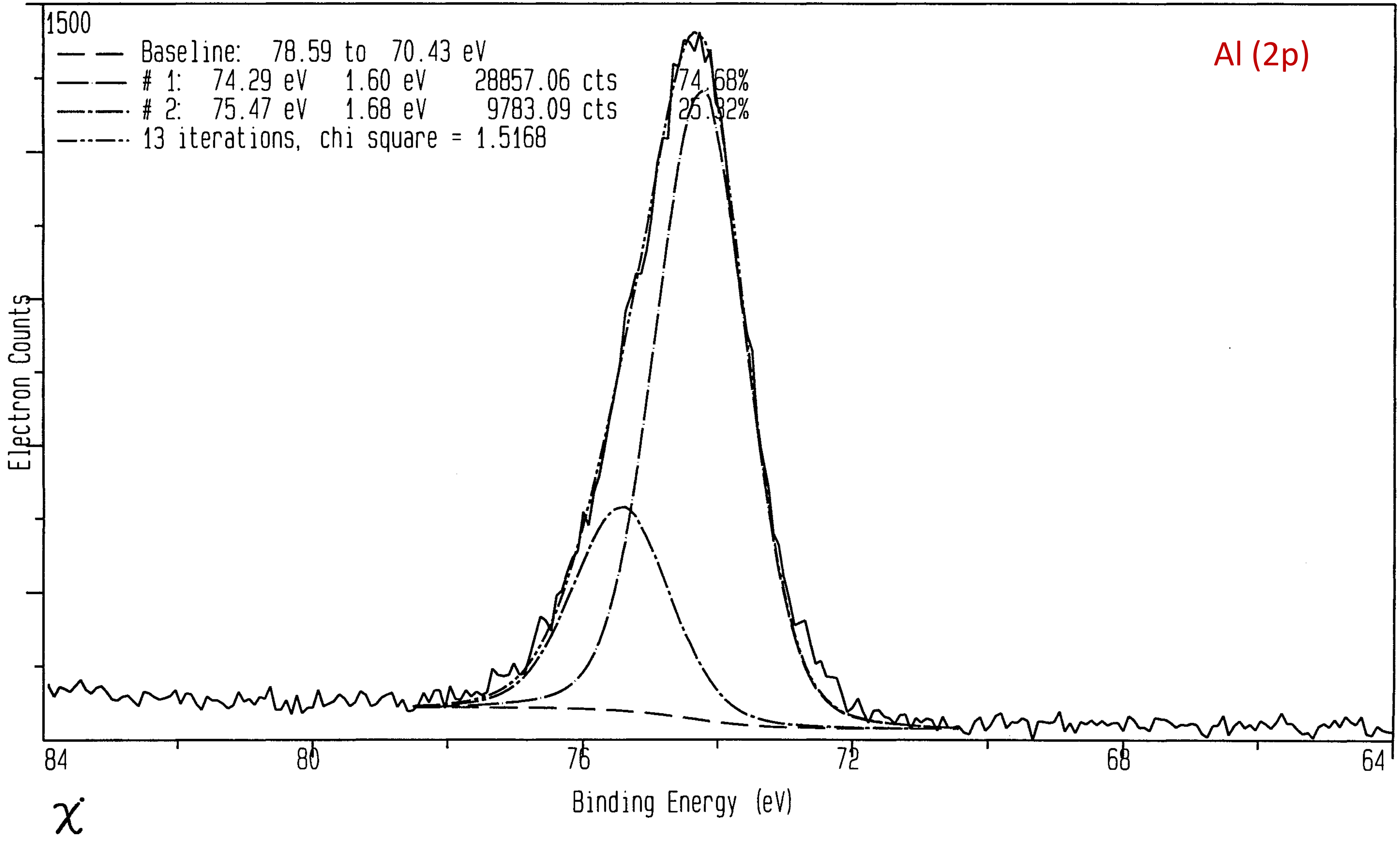
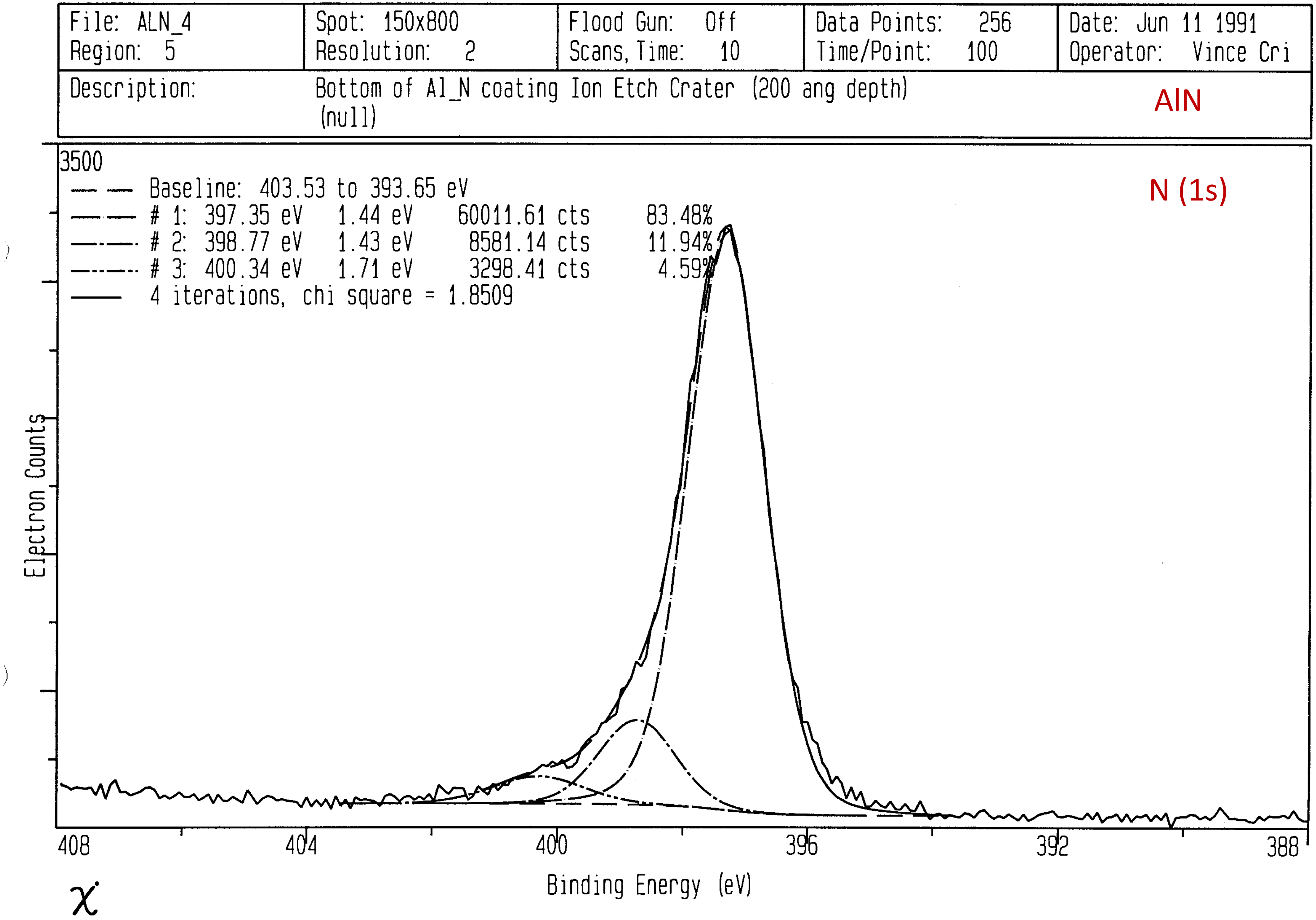
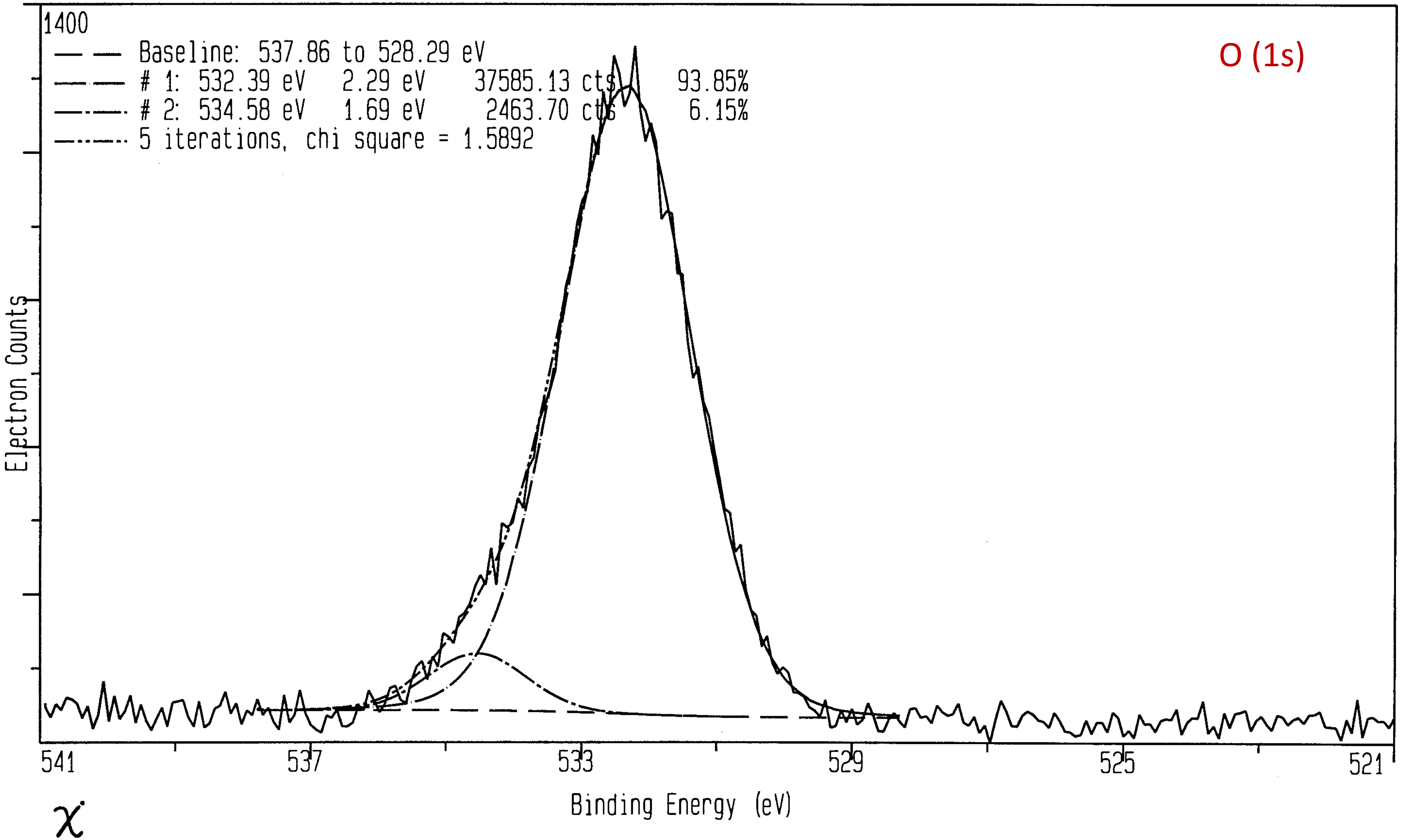
File: ALN_4	Spot: 150x800	Flood Gun: Off	Data Points: 256	Date: Jun 11 1991
Region: 4	Resolution: 2	Scans, Time: 10	Time/Point: 100	Operator: Vince Cri
Description:	Bottom of Al_N coating Ion Etch Crater (200 ang depth) (null)			AlN




File: ALN_4
Region: 5
Spot: 150x800
Resolution: 2
Flood Gun: Off
Scans, Time: 10
Data Points: 256
Time/Point: 100
Date: Jun 11 1991
Operator: Vince Cri
Description: Bottom of Al_N coating Ion Etch Crater (200 ang depth)
(null)
AlN
3500
Baseline: 403.53 to 393.65 eV
1: 397.35 eV 1.44 eV 60011.61 cts 83.48%
2: 398.77 eV 1.43 eV 8581.14 cts 11.94%
3: 400.34 eV 1.71 eV 3298.41 cts 4.59%
4 iterations, chi square = 1.8509
N (1s)
Electron Counts
408
404
400
396
392
388
Binding Energy (eV)

File: ALN_4 Region: 3	Spot: 150x800 Resolution: 2	Flood Gun: Off Scans, Time: 6	Data Points: 256 Time/Point: 100	Date: Jun 11 1991 Operator: Vince Cri
Description:	Bottom of Al_N coating Ion Etch Crater (200 ang depth) (null)			AlN



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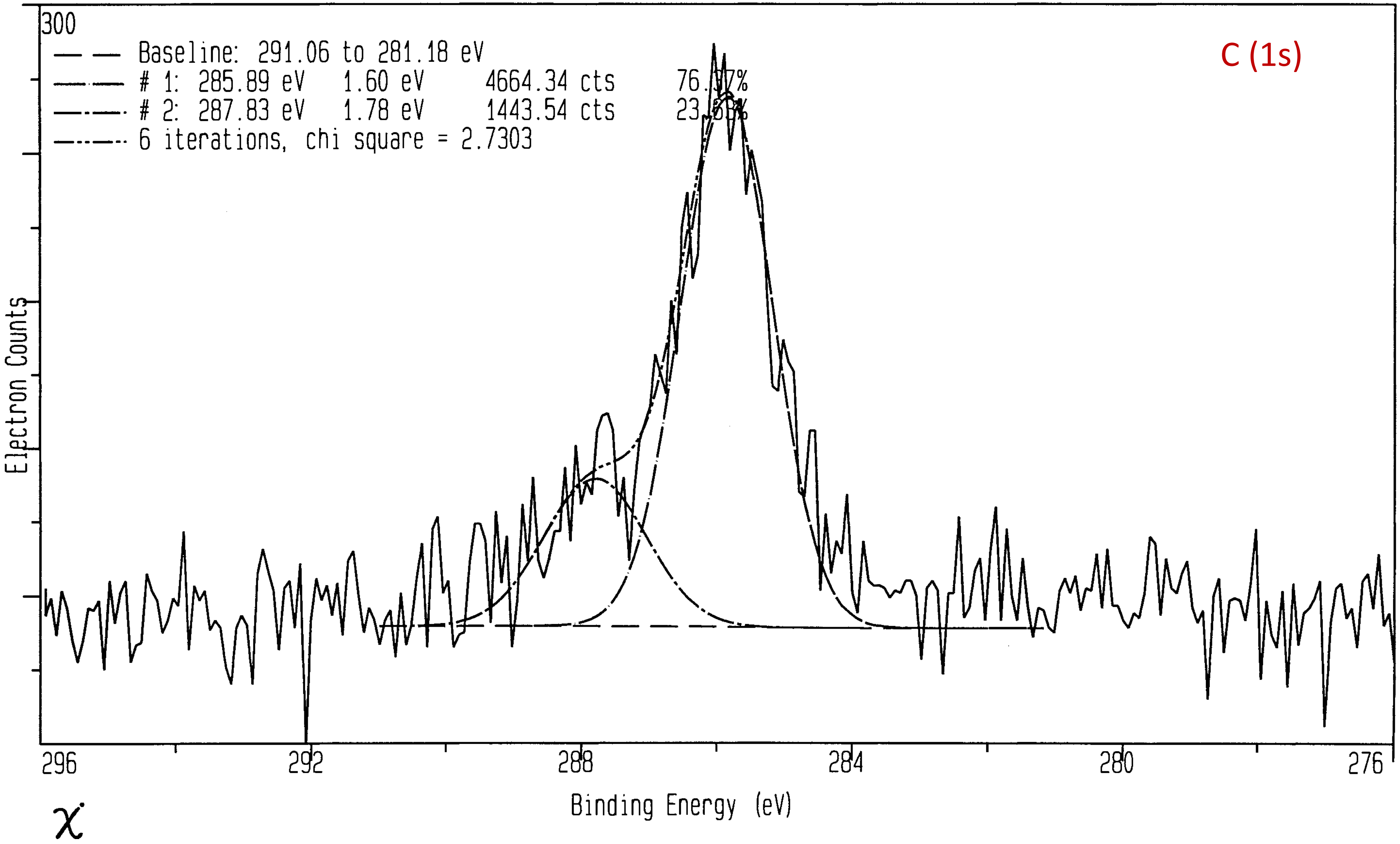
File: ALN_4 Region: 2	Spot: 150x800 Resolution: 2	Flood Gun: Off Scans, Time: 6	Data Points: 256 Time/Point: 100	Date: Jun 11 1991 Operator: Vince Cri
Description:	Bottom of Al_N coating Ion Etch Crater (200 ang depth) (null)			AlN



Beryllium Oxide (pressed pellet) (FW=25.01)

BeO

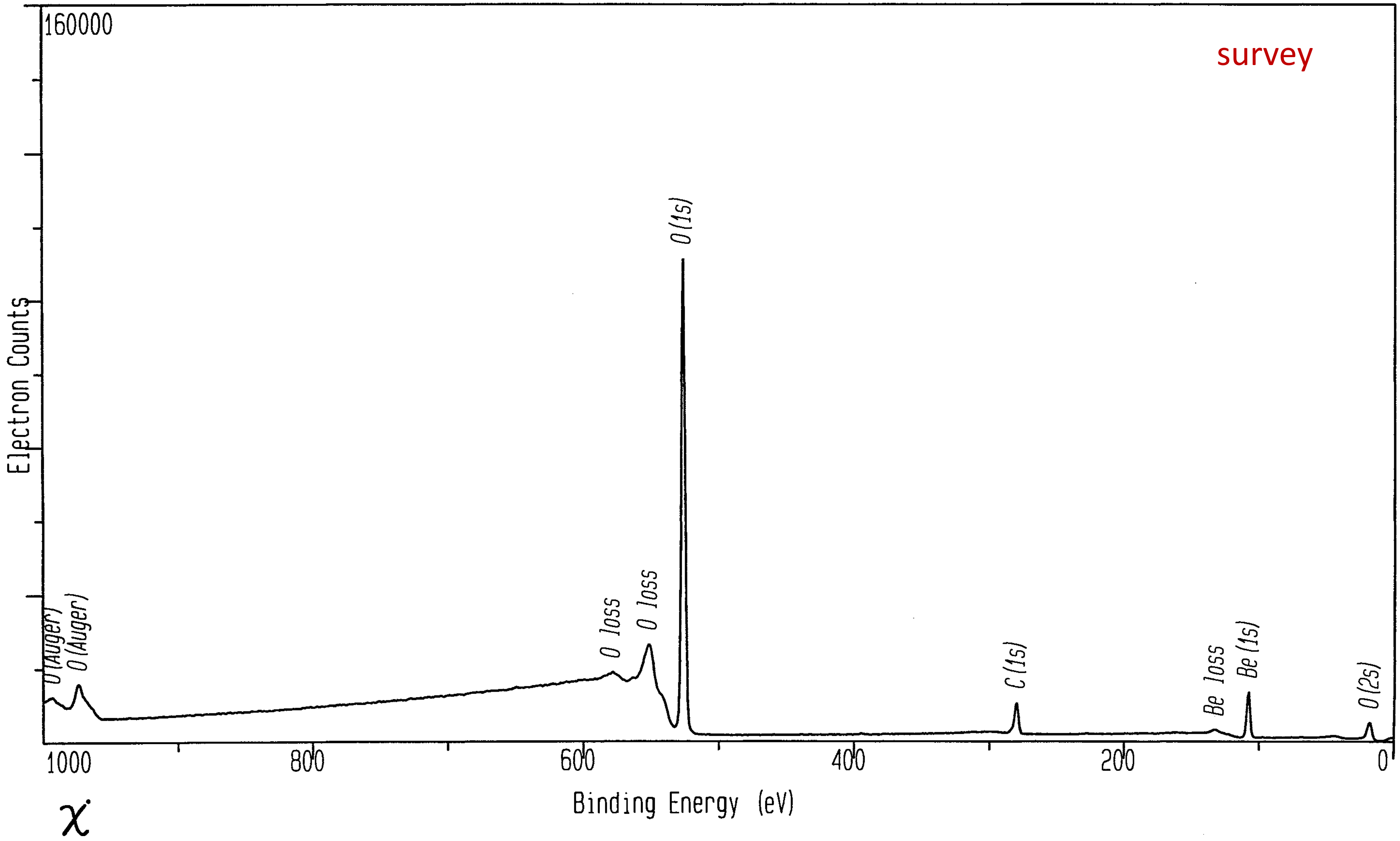
Detailed Surface Composition Table

File name: BEO_2.MRS
Region: 1
Description: BeO 99.99% Aldrich lot# 00213JX screen 90 TOA

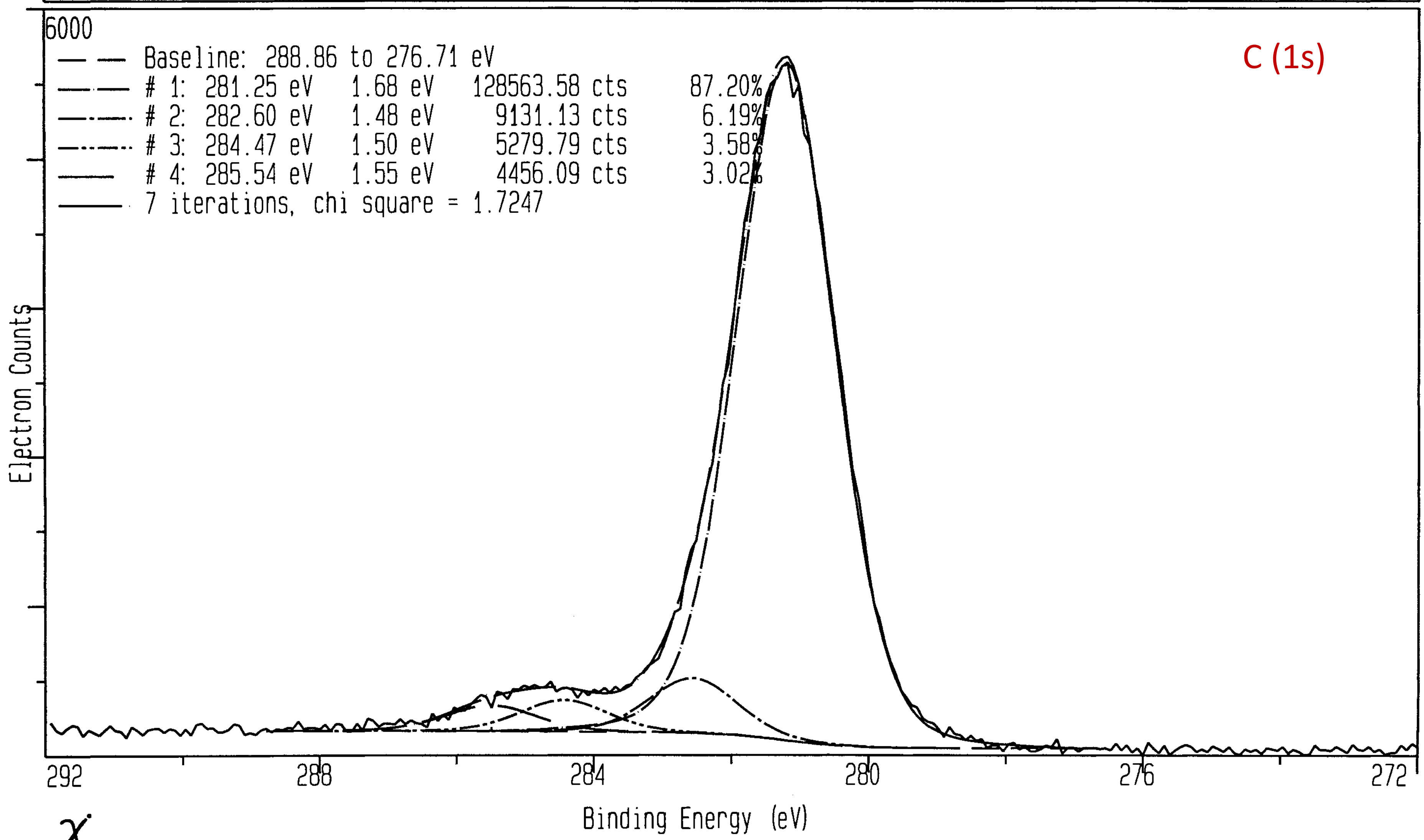
Operator: V. Crist
Date: Mon Jun 13 16:18 1994

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	999.1	993.2	0.00	5125	0	
O Auger	979.6	973.7	0.00	28565	0	
O loss	583.8	577.9	0.00	7143	0	
O loss	556.7	550.8	0.00	83254	0	
* O 1s	531.4	525.5	2.24	169273	75557	48.87
* C 1s	285.0	279.1	1.01	12455	12387	8.01
Be loss	137.3	131.4	0.00	6255	0	
* Be1s	112.9	107.0	0.23	15336	66655	43.11
O 2s	22.9	17.0	0.18	9292	52148	

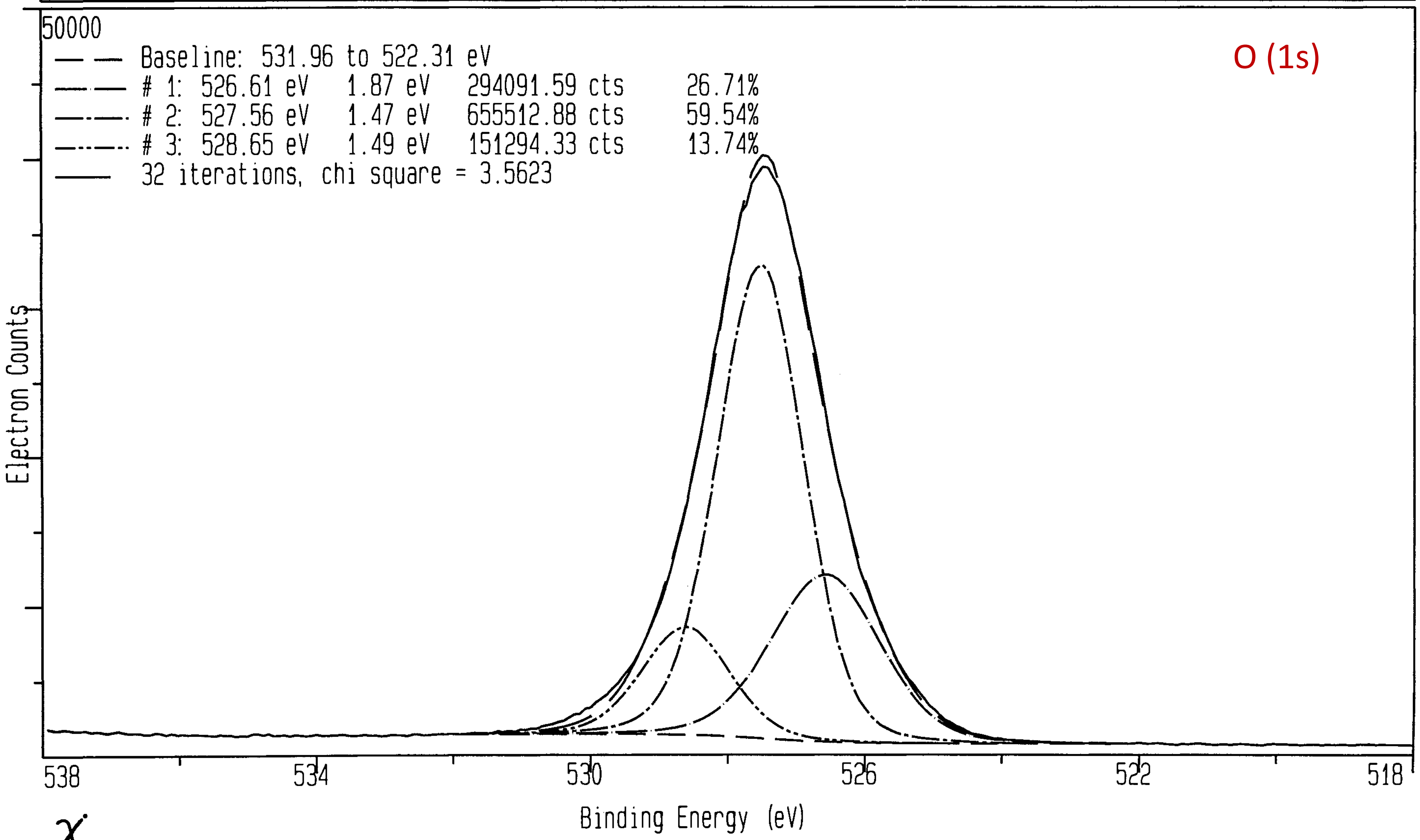
File: BEO_2 Region: 1	Spot: 250x1000 Resolution: 4	Flood Gun: 6.0 Scans, Time: 10	Data Points: 1024 Time/Point: 200	Date: Jun 13 1994 Operator: V. Crist
Description:	BeO 99.99% Aldr lot# 00213JX scrn 90 TOA			BeO



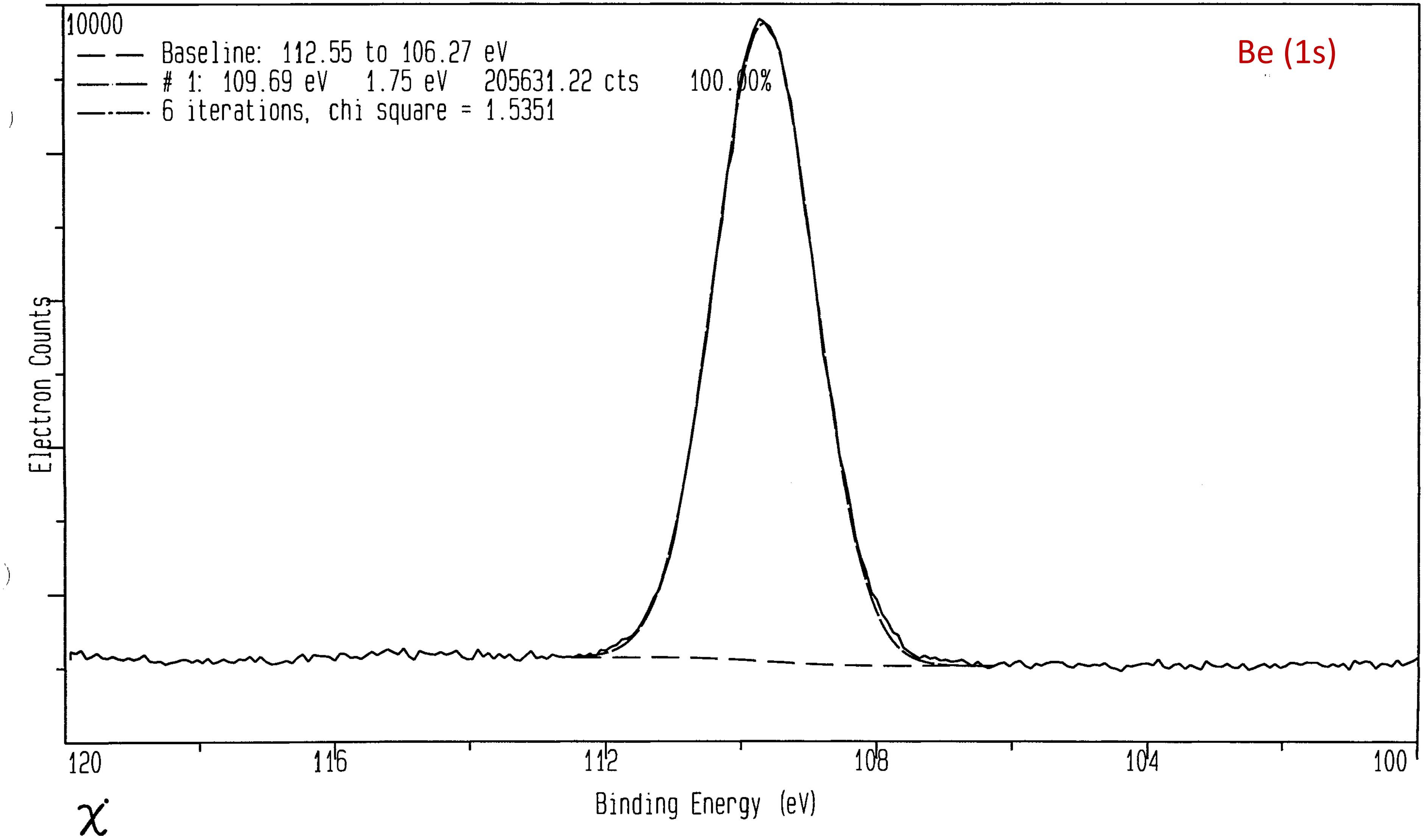
File: BEO_1 Region: 7	Spot: 250x1000 Resolution: 2	Flood Gun: 4.0 Scans, Time: 20	Data Points: 256 Time/Point: 200	Date: Jan 28 1992 Operator: V. Crist
Description:	BeO (99.99%) 3mm pellet, Aldrich lot# 00213JX, screen, 90 TOA (null)			BeO



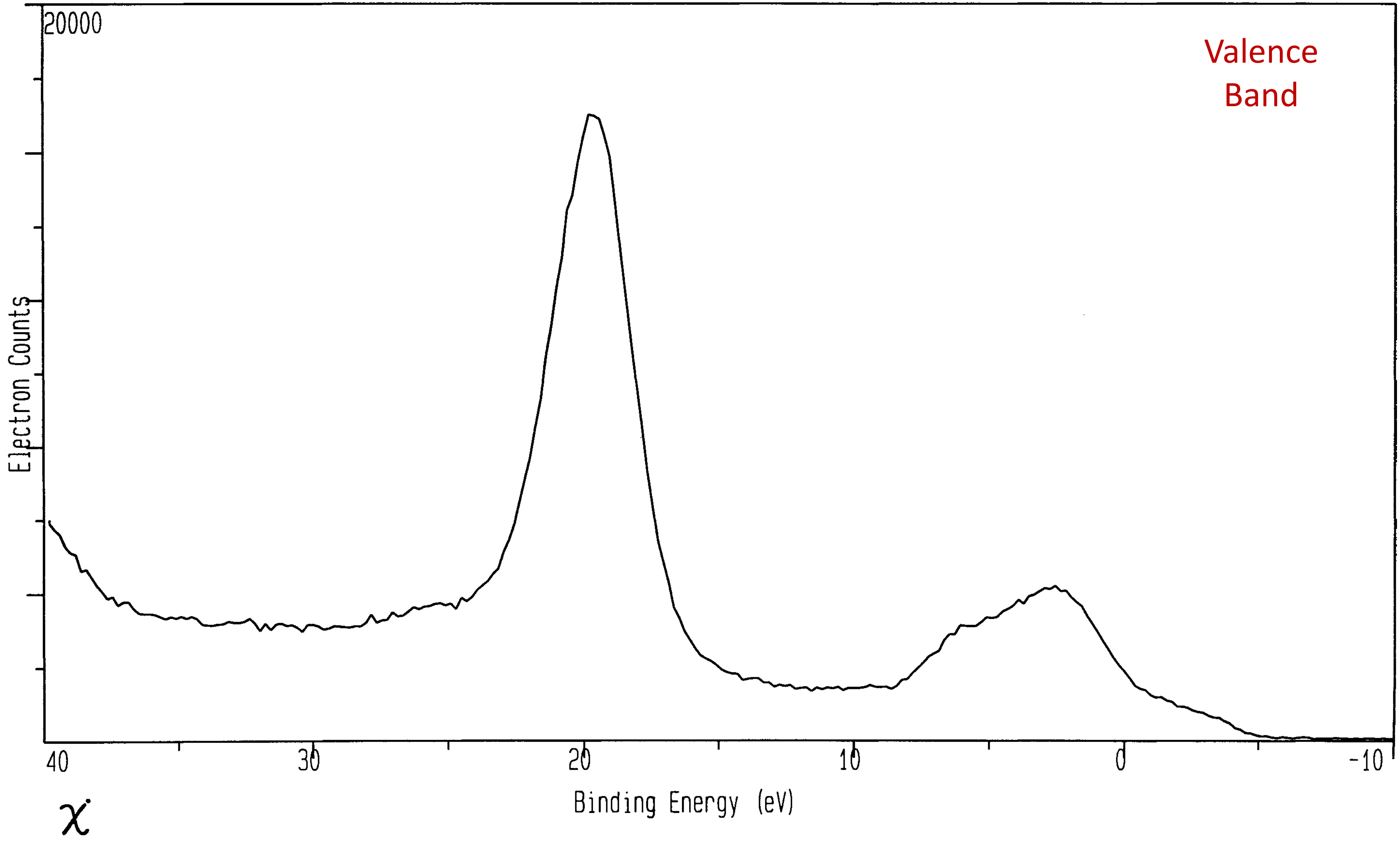
File: BEO_1	Spot: 250x1000	Flood Gun: 4.0	Data Points: 256	Date: Jan 28 1992
Region: 8	Resolution: 2	Scans, Time: 20	Time/Point: 200	Operator: V. Crist
Description:	BeO (99.99%) 3mm pellet, Aldrich lot# 00213JX, screen, 90 TOA (null)			BeO



File: BEO_1 Region: 5	Spot: 250x1000 Resolution: 2	Flood Gun: 4.0 Scans, Time: 60	Data Points: 256 Time/Point: 200	Date: Jan 28 1992 Operator: V. Crist
Description:	BeO (99.99%) 3mm pellet, Aldrich lot# 00213JX, screen, 90 TOA (null)			BeO



File: BEO_1 Region: 3	Spot: 250x1000 Resolution: 4	Flood Gun: 4.0 Scans, Time: 40	Data Points: 256 Time/Point: 200	Date: Jan 28 1992 Operator: V. Crist
Description:	BeO (99.99%) 3mm pellet, Aldrich lot# 00213JX, screen, 90 TOA (null)			BeO



Carbon (exposed bulk) (FW=12.01)

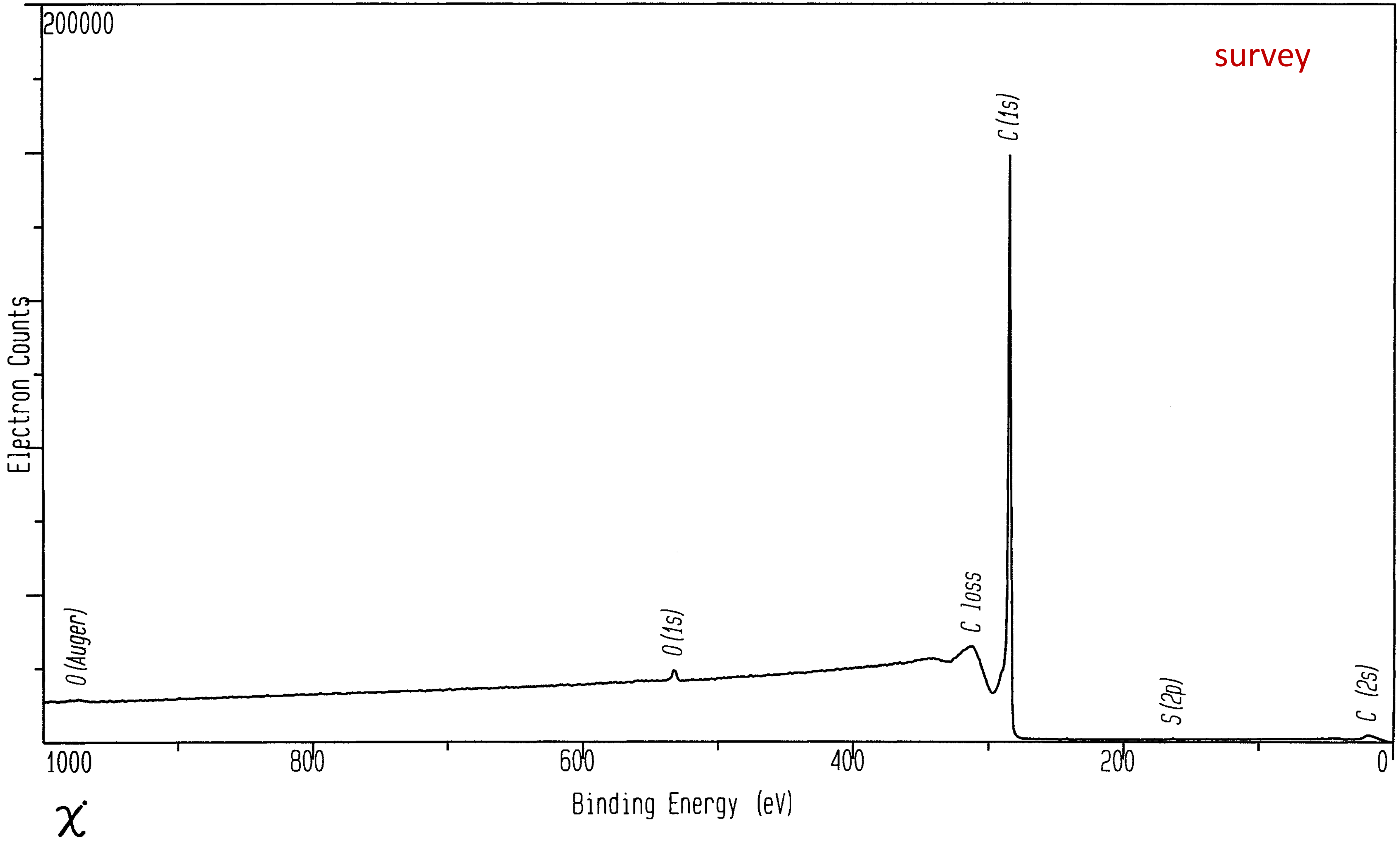
Detailed Surface Composition Table

File name: C_2.MRS
Region: 4
Description: CARBON (C) SHEET (90 DEG TOA, SCRAPED WITH RAZOR BLADE)

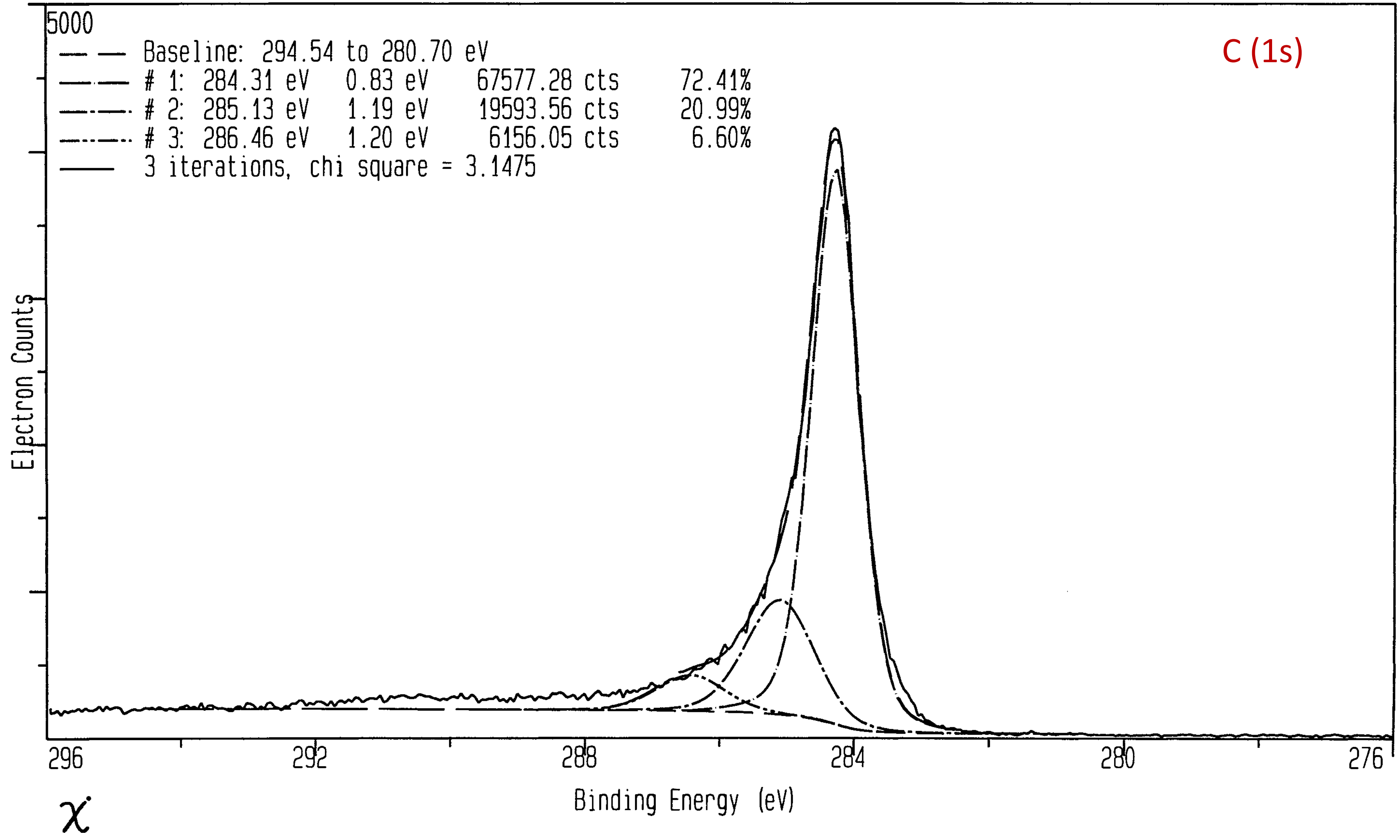
Operator: BVC
Date: Tue Jan 19 1988

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	975.6	974.5	0.00	1847	0	
* O 1s	533.7	532.5	2.22	6524	2938	1.35
C loss	312.8	311.6	0.00	30476	0	
* C 1s	285.0	283.8	1.00	214145	213981	98.65
S 2p	163.7	162.5	1.88	341	181	
C (2s)	18.7	17.5	0.00	8789	0	

File: C_2 Region: 4	Spot: 1000 Resolution: 4	Flood Gun: Off Scans, Time: 10	Data Points: 1024 Time/Point: 200	Date: 1/19/1988 Operator: BVC
Description:	CARBON (C) SHEET (GRAPHITE) (90 DEG TOA, SCRAPED WITH RAZOR BLADE) (null)			C



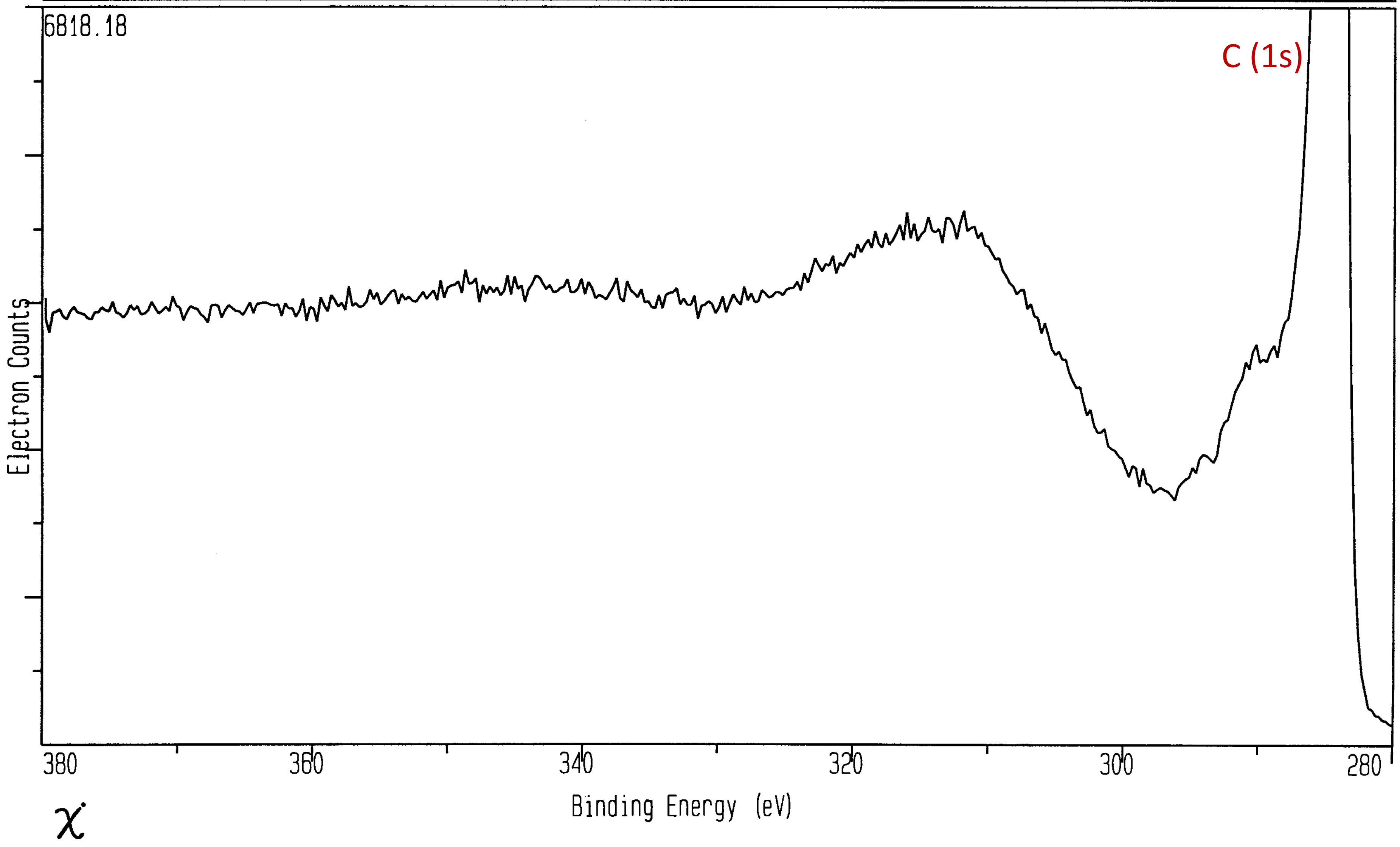
File: C_2	Spot: 150	Flood Gun: Off	Data Points: 384	Date: 1/19/1988
Region: 1	Resolution: 1	Scans, Time: 30	Time/Point: 200	Operator: BVC
Description:	CARBON (C) SHEET (GRAPHITE) (90 DEG TOA, SCRAPED WITH RAZOR BLADE) (null)			C



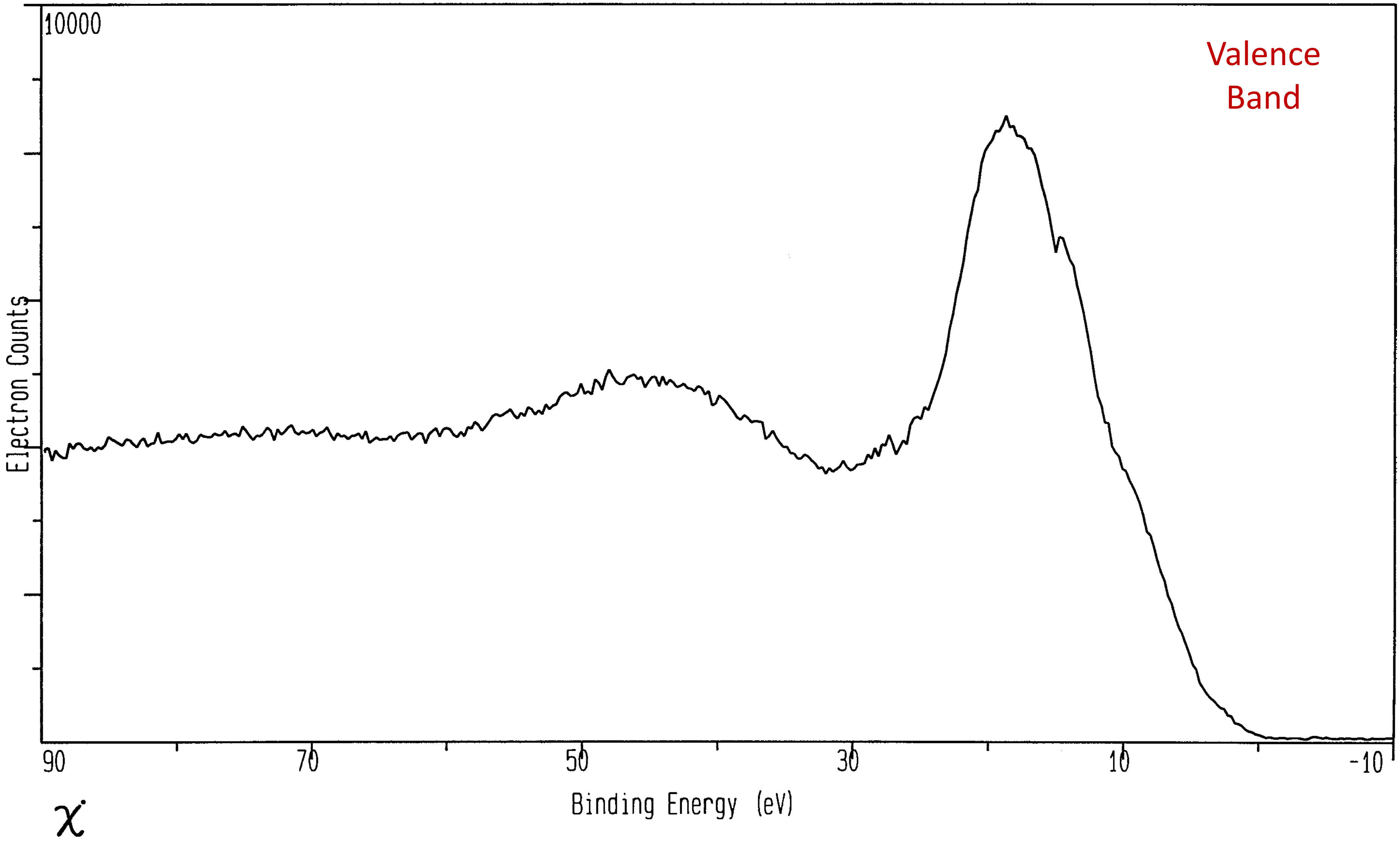
File: C_2 Region: 6	Spot: 1000 Resolution: 2	Flood Gun: Off Scans, Time: 12	Data Points: 384 Time/Point: 200	Date: 1/19/1988 Operator: BVC

Description: CARBON (C) SHEET (GRAPHITE) (90 DEG TOA, SCRAPED WITH RAZOR BLADE)
(null)

C



File: C_2B Region: 1	Spot: 1000 Resolution: 4	Flood Gun: Off Scans, Time: 40	Data Points: 384 Time/Point: 200	Date: 1/19/1988 Operator: BVC
Description:	CARBON (C) SHEET (GRAPHITE) (90 DEG TOA, SCRAPED WITH RAZOR BLADE) (null)			C



Cadmium Oxide (pressed pellet) (FW=128.40) CdO

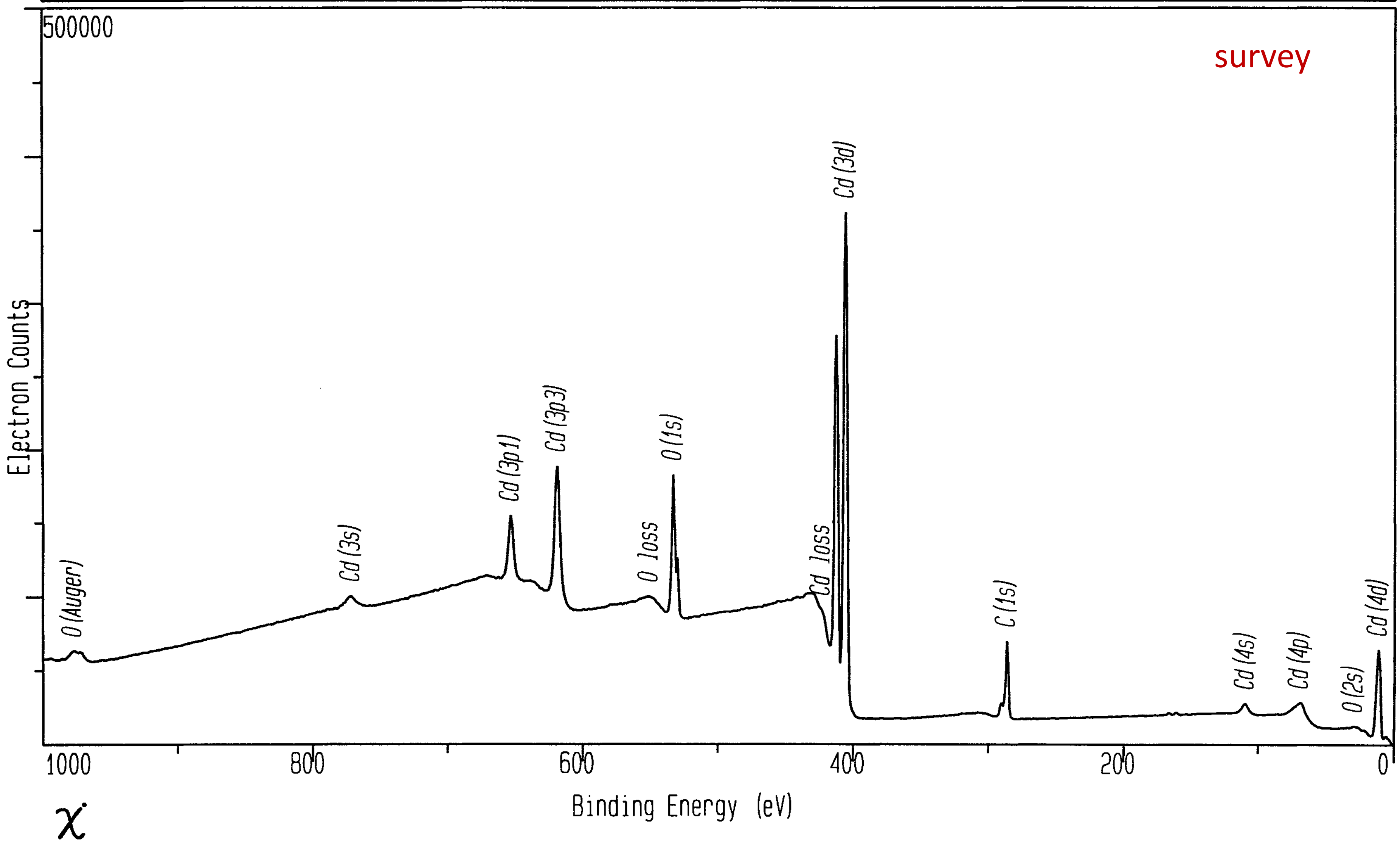
Detailed Surface Composition Table

File name: CDO_1.MRS
Region: 1
Description: CdO (99.99+%) Aldrich lot #01318EV, 3mm pellet, 35 TOA

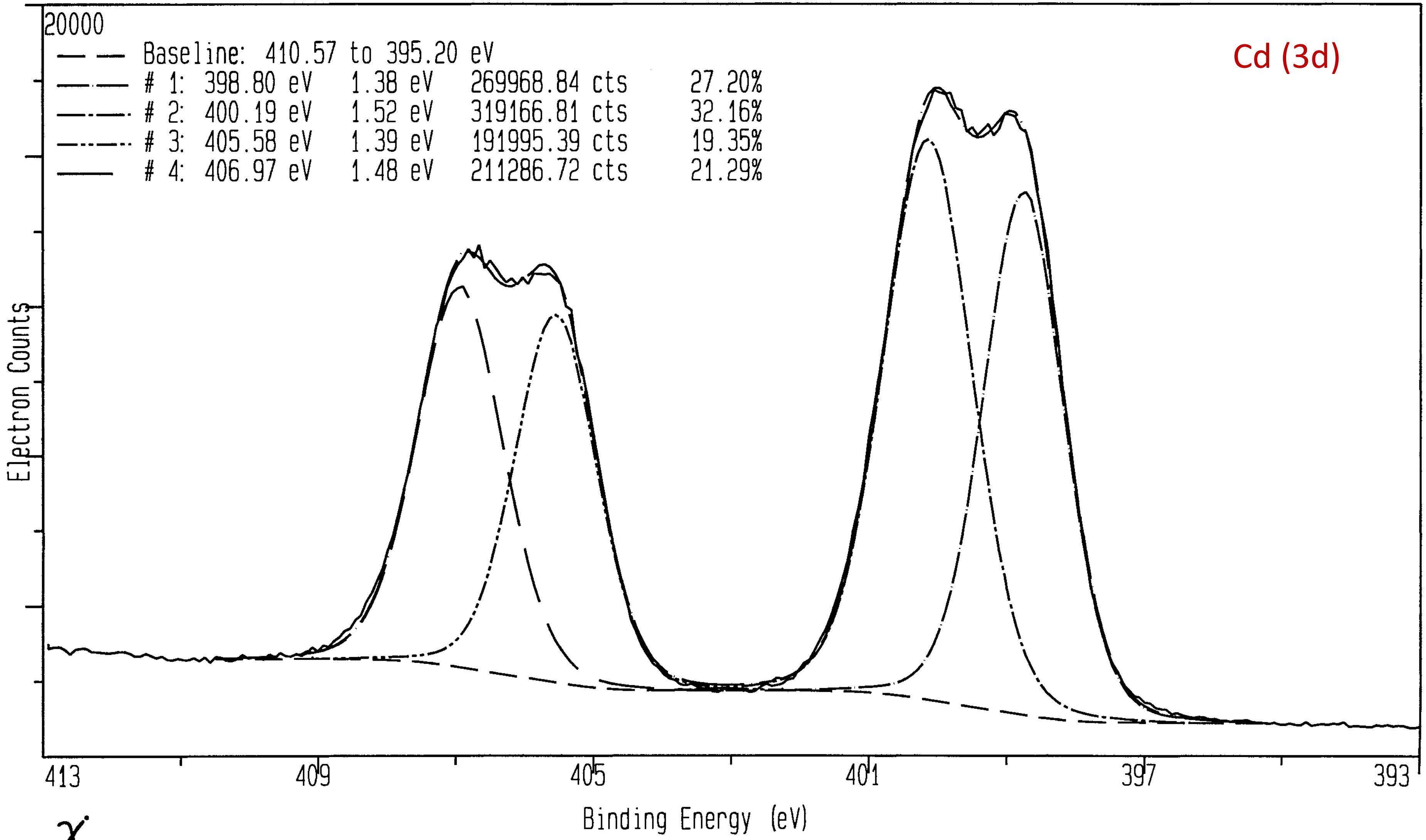
Operator: Vince Crist
Date: Tue Jun 11 19:17 1991

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	976.5	977.1	0.00	12898	0	
Cd3s	770.7	771.3	1.63	11751	7206	
Cd3p1	652.1	652.7	2.72	34692	12748	
* Cd3p3	617.9	618.5	5.76	75695	13152	20.34
O loss	549.4	550.0	0.00	11430	0	
* O 1s	531.7	532.3	2.22	55630	25044	38.74
Cd loss	422.2	422.8	0.00	34823	0	
Cd3d	404.6	405.2	17.81	299087	16796	
* C 1s	285.0	285.6	1.00	26427	26453	40.92
Cd4s	108.4	109.0	0.82	7725	9424	
Cd4p	67.5	68.1	2.75	26731	9726	
Cd loss	27.6	28.2	0.18	8067	44732	
Cd4d	10.2	10.8	2.42	37971	15705	

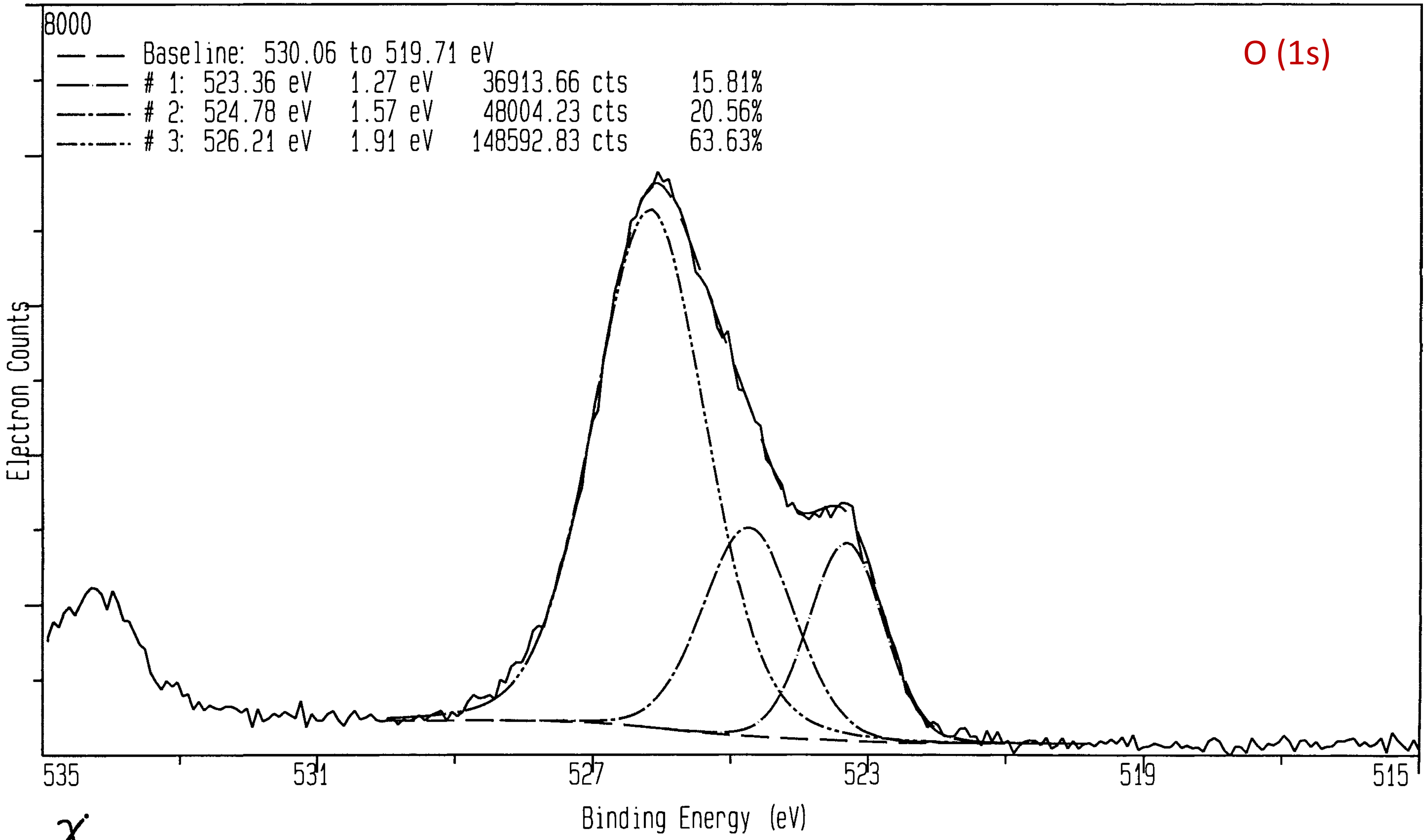
File: CDO_1 Region: 1	Spot: 250x1000 Resolution: 4	Flood Gun: 3.0 Scans, Time: 30	Data Points: 1024 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	CdO (99.99+%) Aldrich lot #01318EV, 3mm pellet, 35 TOA, screen (null)			CdO



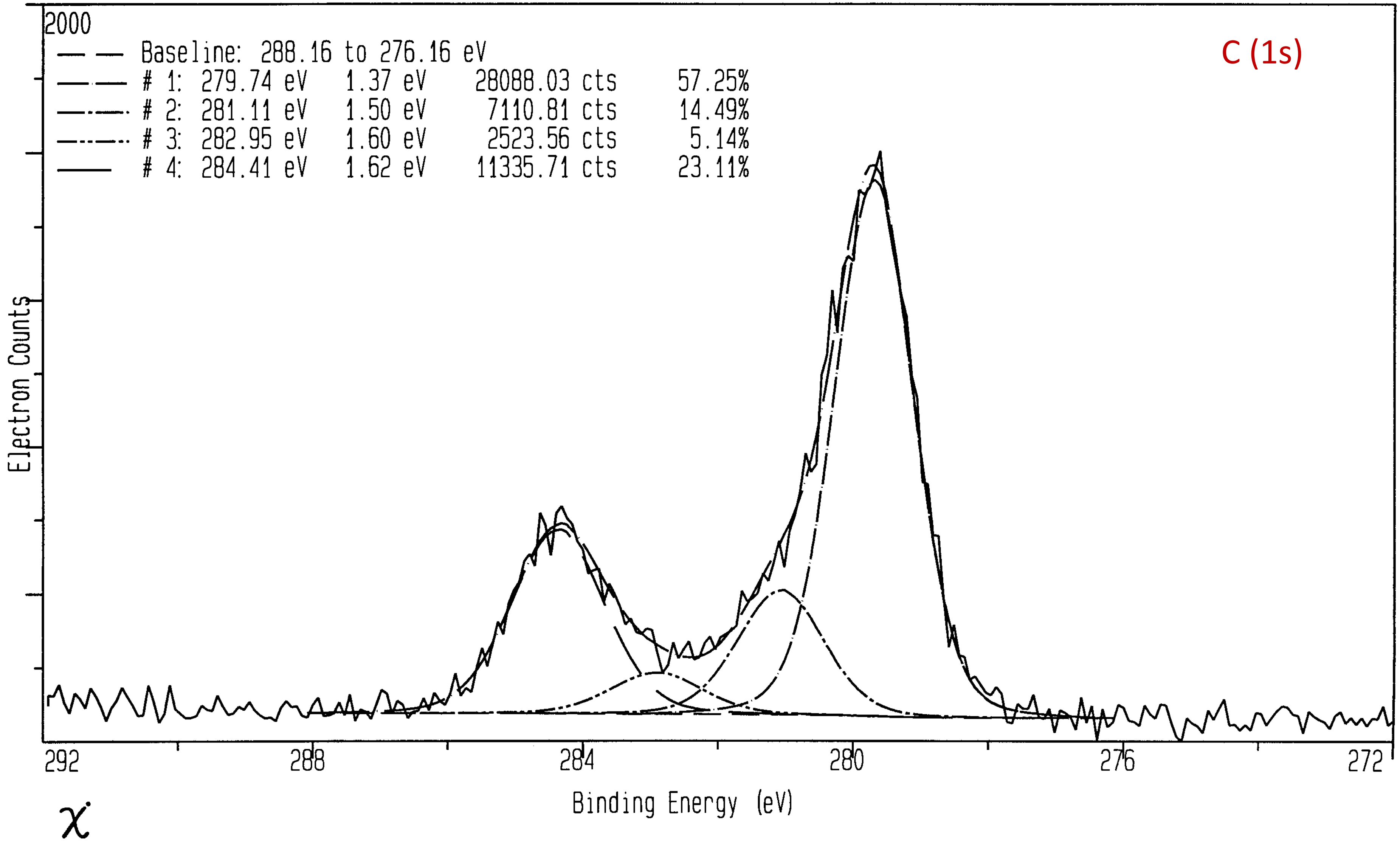
File: CDO_1 Region: 2	Spot: 150x800 Resolution: 2	Flood Gun: 3.0 Scans, Time: 10	Data Points: 296 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	CdO (99.99+%) Aldrich lot #01318EV, 3mm pellet, 35 TOA, screen (null)			CdO

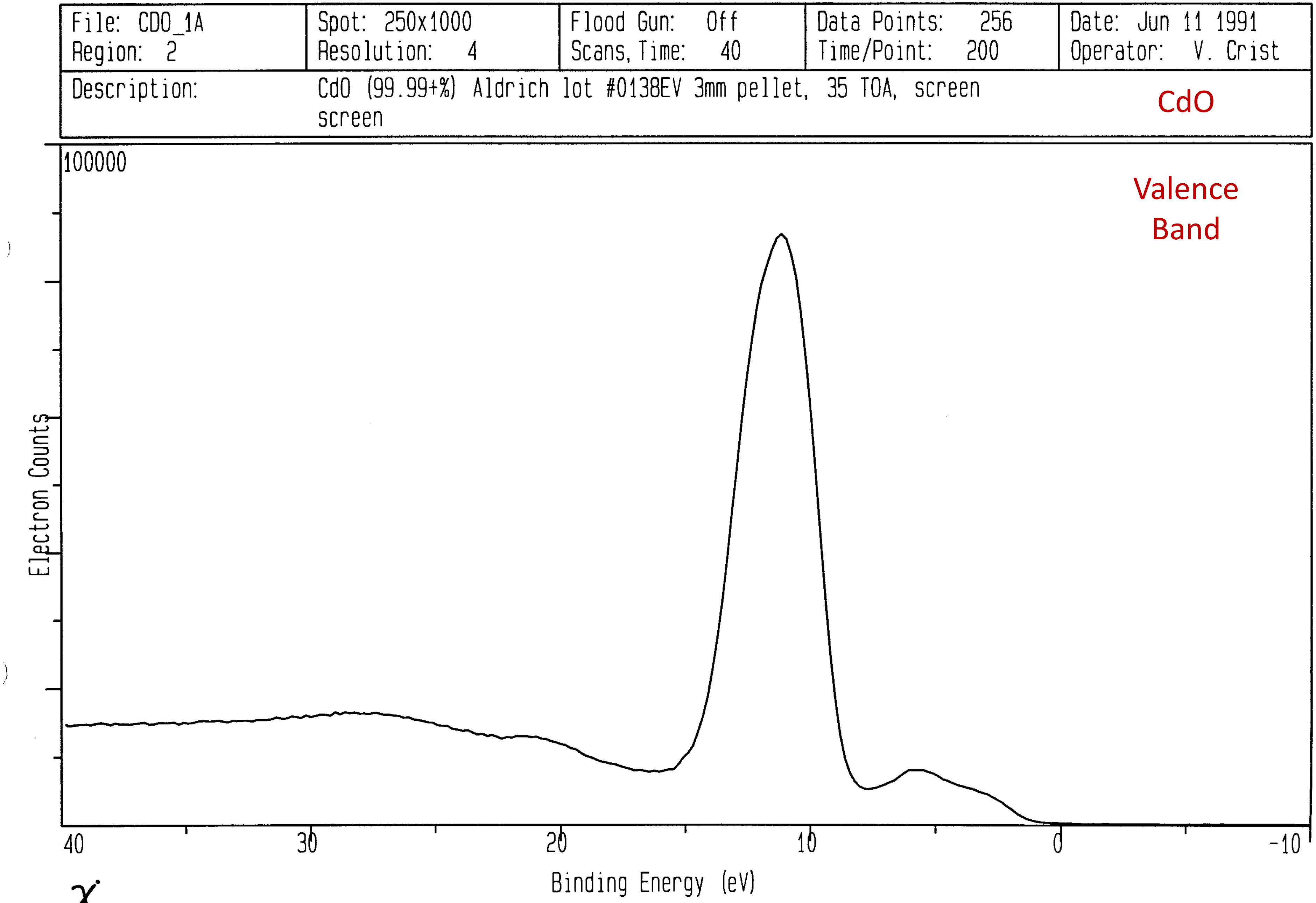


File: CDO_1 Region: 4	Spot: 150x800 Resolution: 2	Flood Gun: 3.0 Scans, Time: 10	Data Points: 258 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	CdO (99.99+%) Aldrich lot #01318EV, 3mm pellet, 35 TOA, screen (null)			CdO

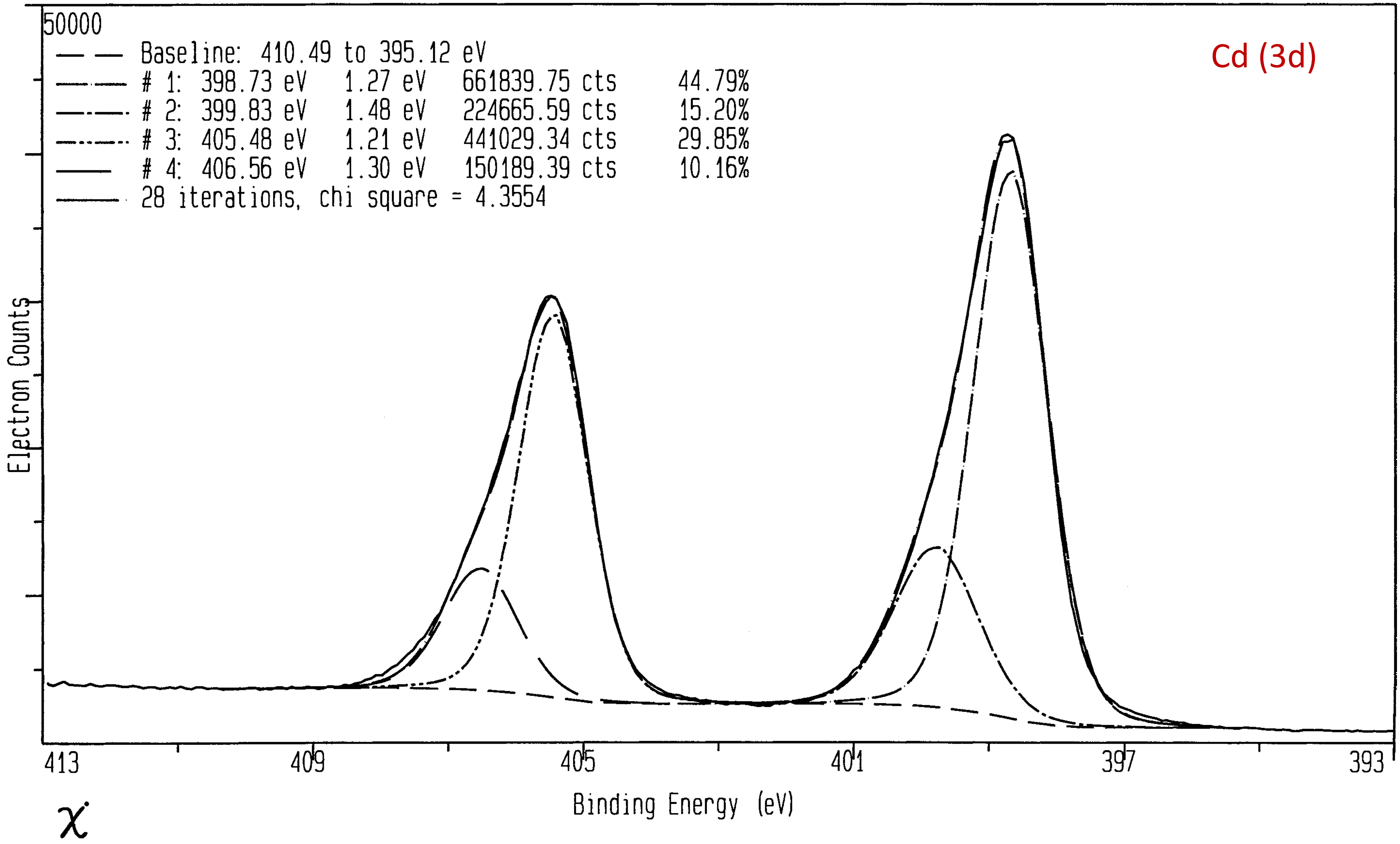


File: CDO_1 Region: 3	Spot: 150x800 Resolution: 2	Flood Gun: 3.0 Scans, Time: 10	Data Points: 256 Time/Point: 200	Date: Jun 11 1991 Operator: Vince Cri
Description:	CdO (99.99+%) Aldrich lot #01318EV, 3mm pellet, 35 TOA, screen (null)			CdO

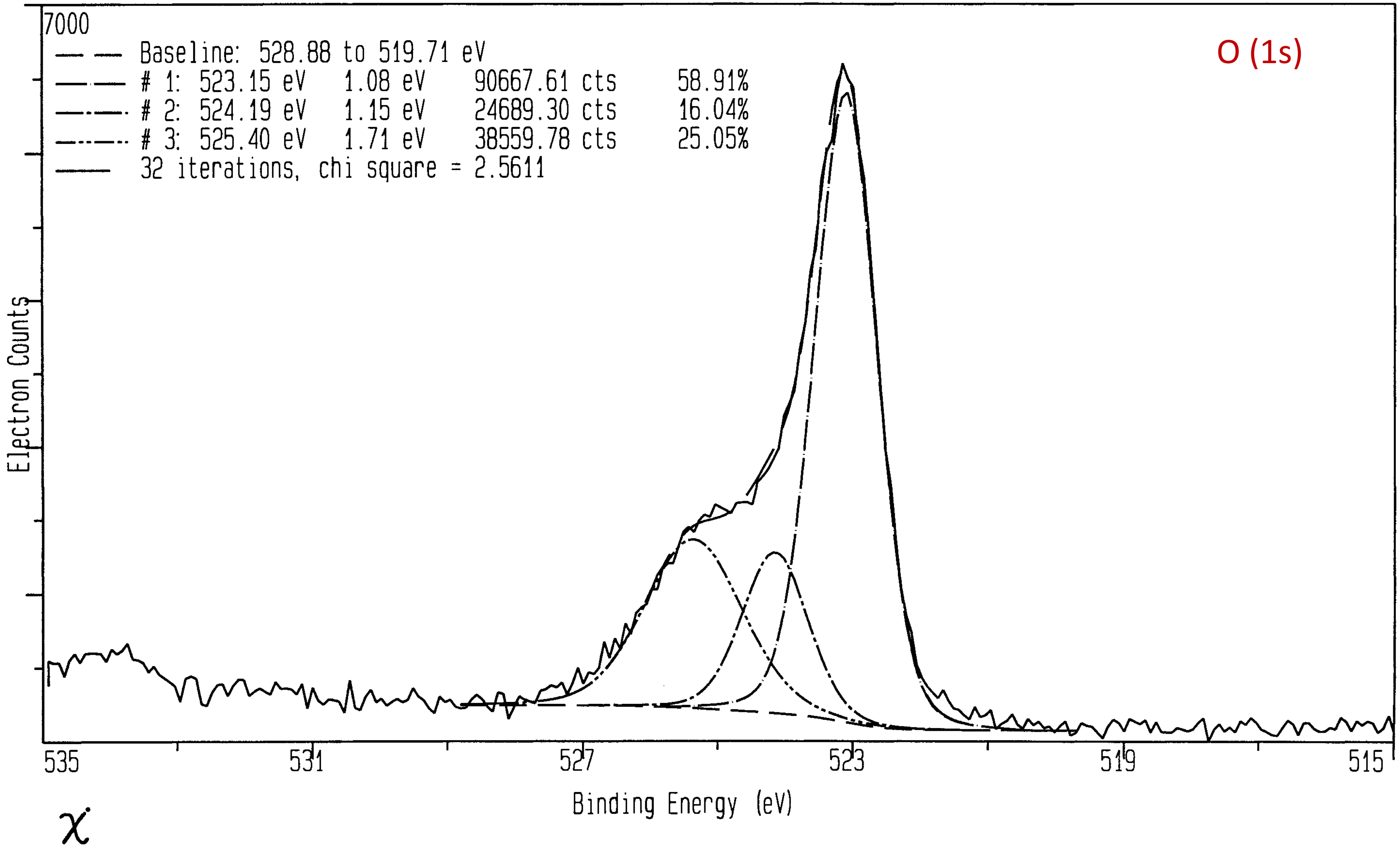



File: CDO_1A
Region: 2
Spot: 250x1000
Resolution: 4
Flood Gun: Off
Scans, Time: 40
Data Points: 256
Time/Point: 200
Date: Jun 11 1991
Operator: V. Crist
Description: CdO (99.99+%) Aldrich lot #0138EV 3mm pellet, 35 TOA, screen
screen
CdO
Valence
Band
100000
Electron Counts
40
30
20
10
0
-10
Binding Energy (eV)

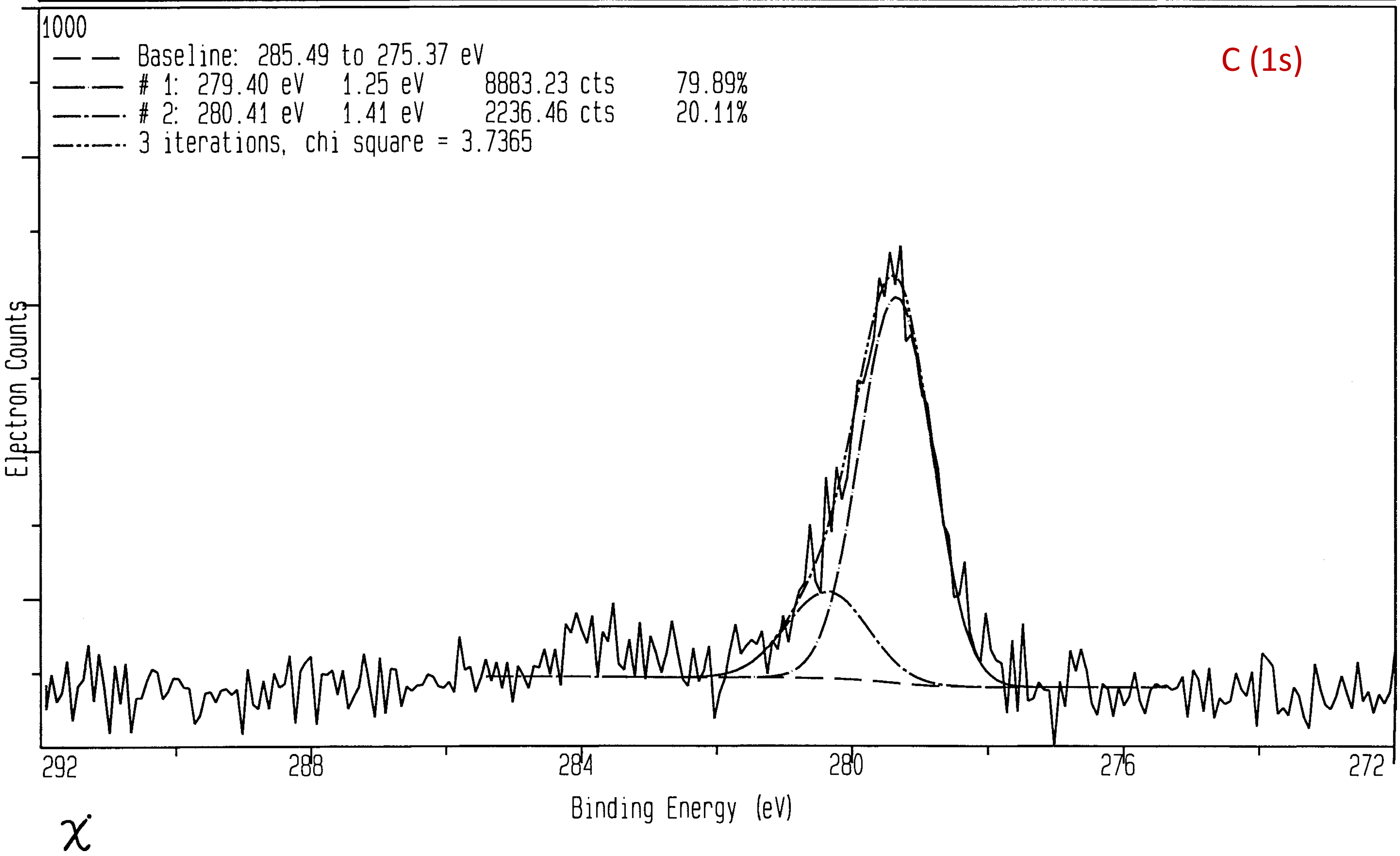
File: CDO_3 Region: 1	Spot: 150x800 Resolution: 2	Flood Gun: 3.0 Scans, Time: 10	Data Points: 256 Time/Point: 200	Date: Jun 12 1991 Operator: Vince Cri
Description:	CdO (CdO_01) pellet, scrn, after 30 sec 3KV, 10mA ion etch (null)			CdO



File: CDO_3 Region: 3	Spot: 150x800 Resolution: 2	Flood Gun: 3.0 Scans, Time: 10	Data Points: 256 Time/Point: 200	Date: Jun 12 1991 Operator: Vince Cri
Description:	CdO (CdO_01) pellet, scrn, after 30 sec 3KV, 10mA ion etch (null)			CdO



File: CD0_3 Region: 2	Spot: 150x800 Resolution: 2	Flood Gun: 3.0 Scans, Time: 10	Data Points: 256 Time/Point: 200	Date: Jun 12 1991 Operator: Vince Cri
Description:	CdO (CdO_01) pellet, scrn, after 30 sec 3KV, 10mA ion etch (null)			CdO



Cadmium Selenide (pressed pellet) (FW=191.36)

Detailed Surface Composition Table

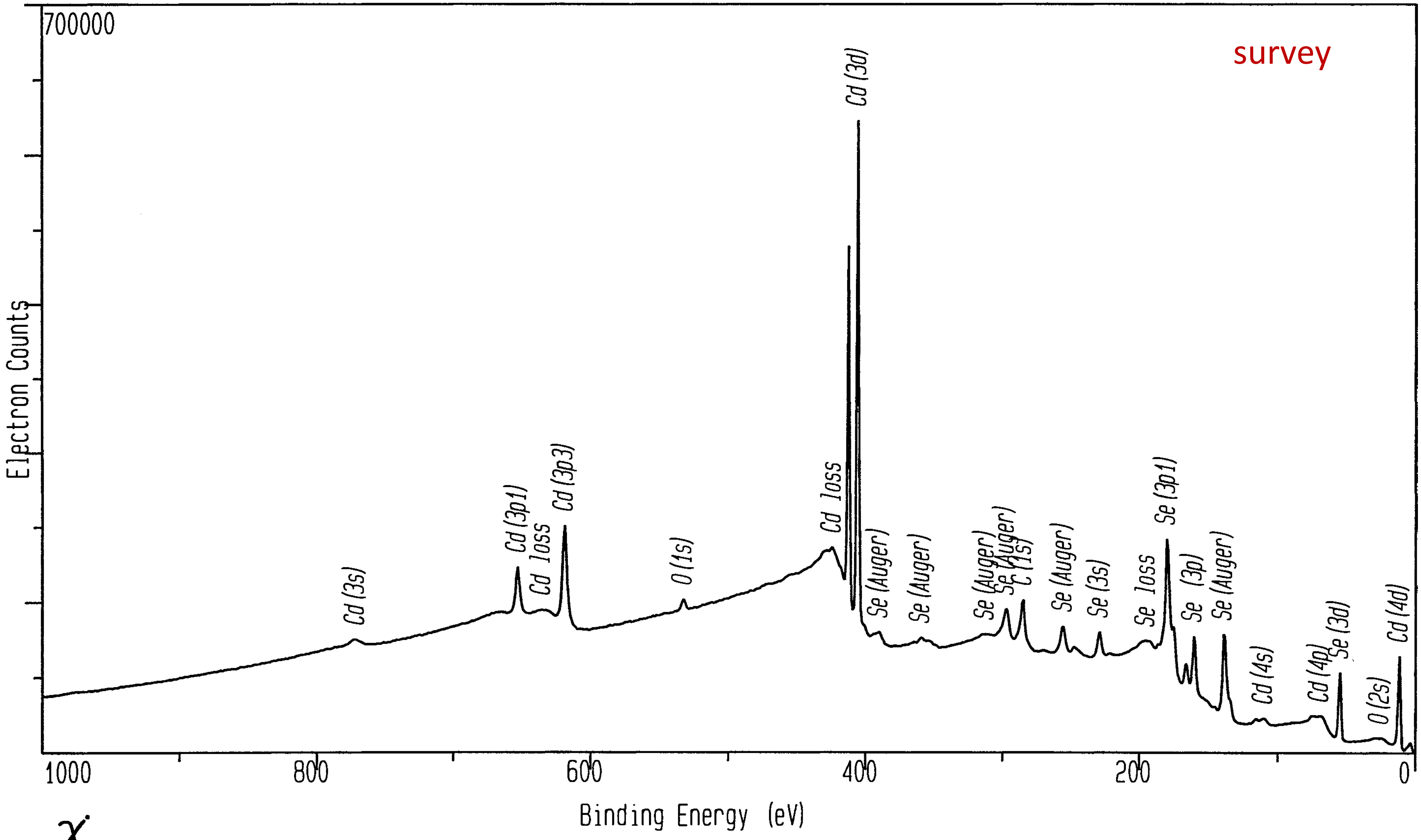
File name: CDSE_1.MRS
Region: 1
Description: CdSe (99.99%) Aldrich Chemical Co.,lot #00323JX, As received
Electronic Grade, 3 micron powder, pressed pellet
Operator: V. Crist
Date: Tue Jul 26 04:07 1994

	Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
	Cd3s	771.3	771.3	1.63	15843	9716	
	Cd3p1	652.7	652.7	2.72	41412	15219	
	Cd loss	635.0	635.1	0.00	10712	0	
*	Cd3p3	618.4	618.5	5.75	89795	15619	29.31
*	O 1s	532.3	532.4	2.22	10122	4557	8.55
	Cd loss	423.9	423.9	0.00	101951	0	
	Cd3d	405.2	405.2	17.81	344884	19366	
	SeAuger	389.8	389.9	0.19	11006	58506	
	SeAuger	359.0	359.1	0.19	20632	106087	
	SeAuger	311.9	312.0	0.20	8584	42022	
	SeAuger	296.9	297.0	0.00	33632	0	
*	C 1s	285.0	285.1	1.00	21113	21123	39.64
	SeAuger	255.6	255.7	0.00	42377	0	
	Se3s	228.9	229.0	1.51	19058	12624	
	Se loss	194.9	195.0	0.53	24485	46218	
	Se3p1	179.6	179.7	0.23	153371	660583	
	Se (3p)	160.2	160.3	4.90	55325	11291	
	SeAuger	138.4	138.5	0.00	76247	0	
	Cd4s	109.6	109.7	0.81	13217	16226	
	Cd4p	68.5	68.6	2.74	54154	19738	
*	Se3d	54.0	54.1	2.83	33948	11994	22.51
	Cd loss	24.0	24.1	0.18	16669	92765	
	Cd4d	10.8	10.9	2.42	45940	19003	

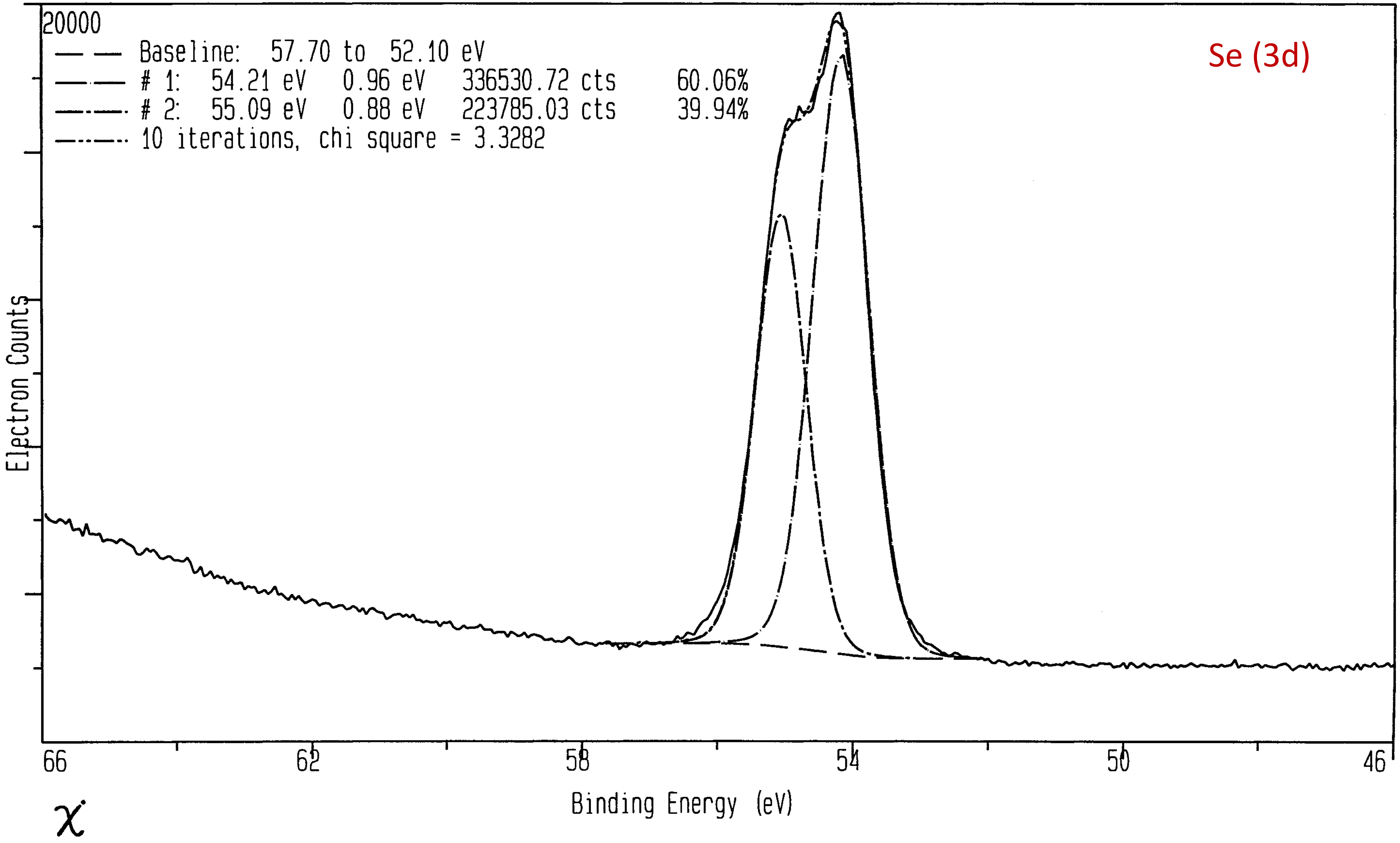
File: CDSE_1	Spot: 250x1000	Flood Gun: Off	Data Points: 1024	Date: Jul 26 1994
Region: 1	Resolution: 4	Scans, Time: 20	Time/Point: 200	Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			

CdSe

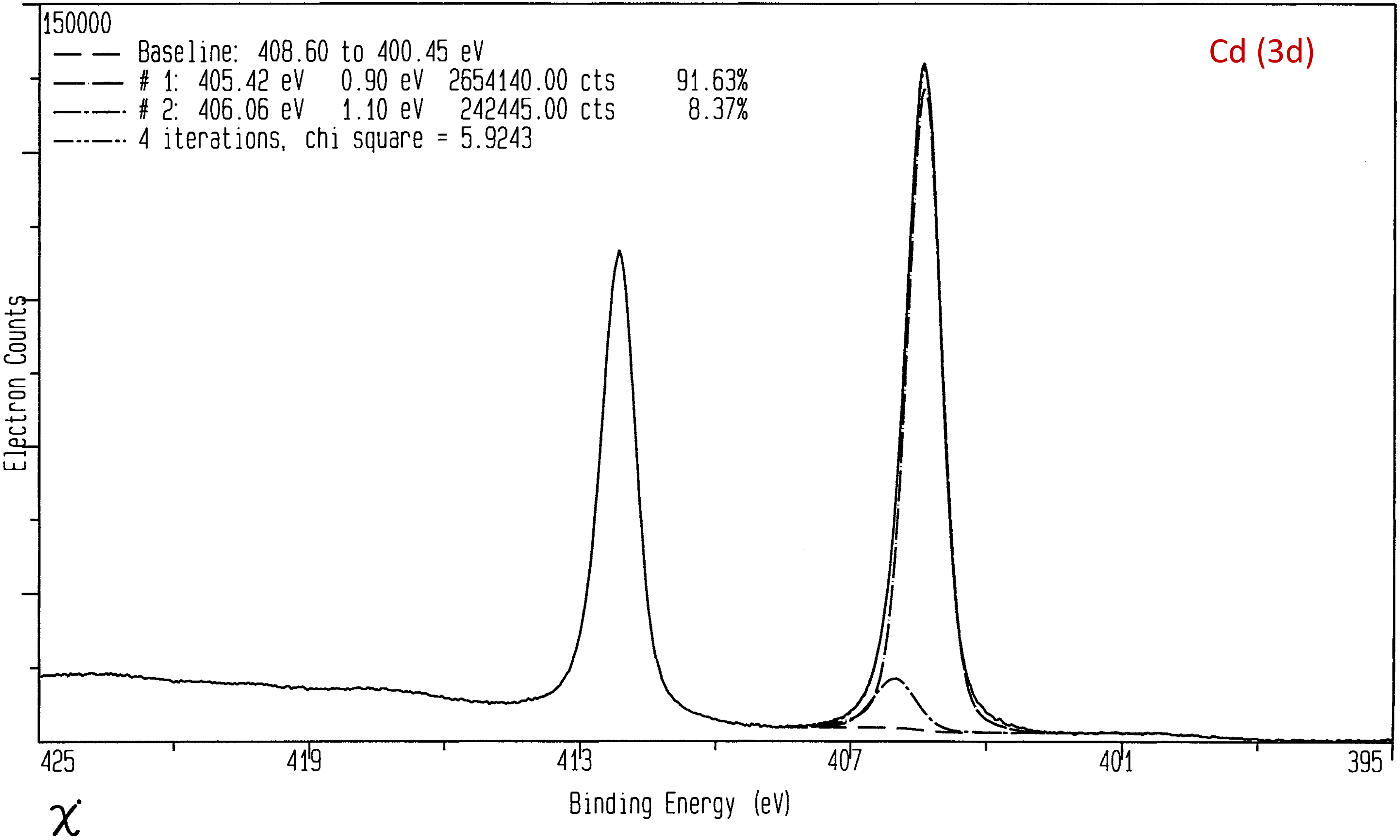
survey



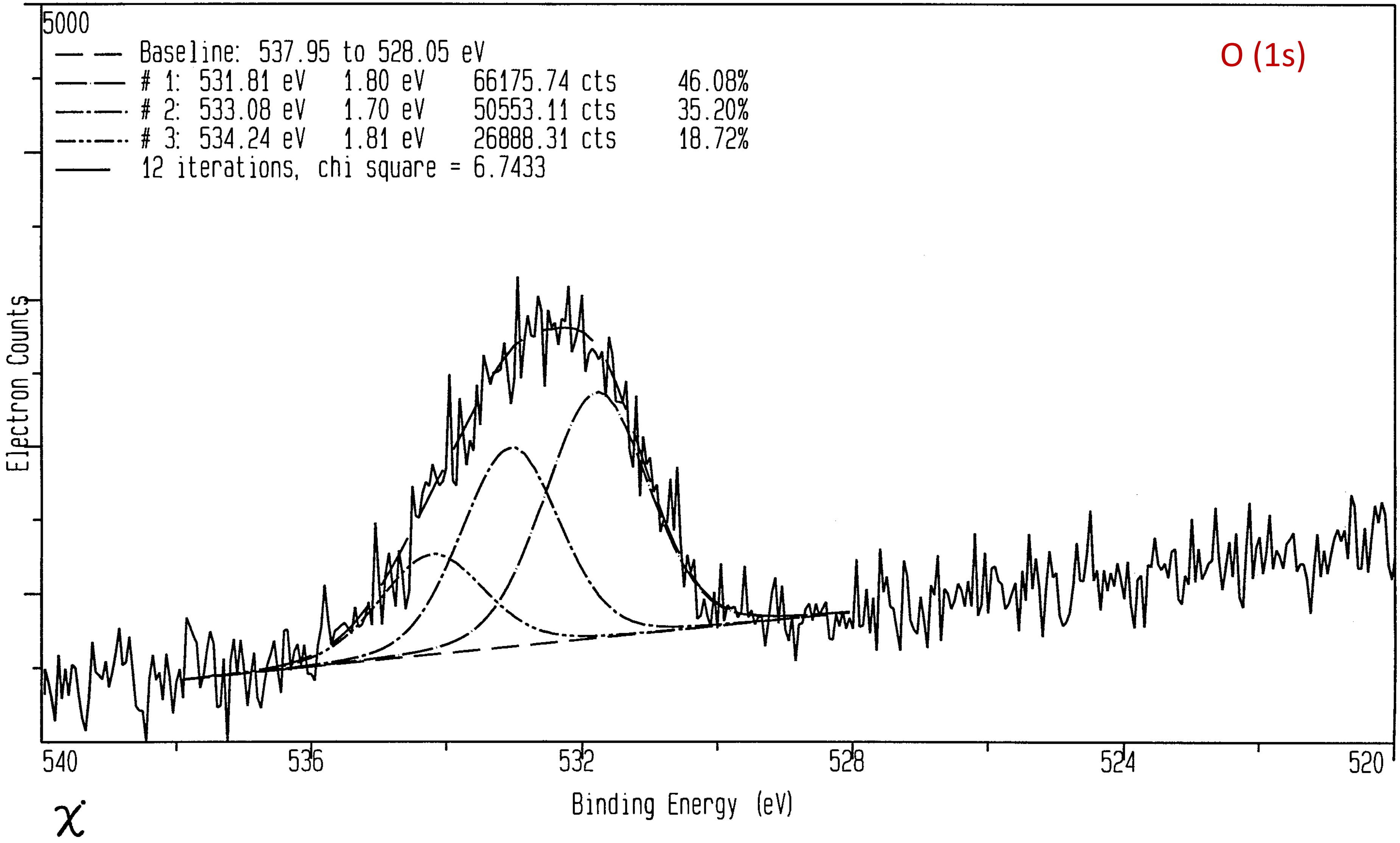
File: CDSE_1	Spot: 250x1000	Flood Gun: Off	Data Points: 401	Date: Jul 26 1994
Region: 7	Resolution: 2	Scans, Time: 20	Time/Point: 200	Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			CdSe



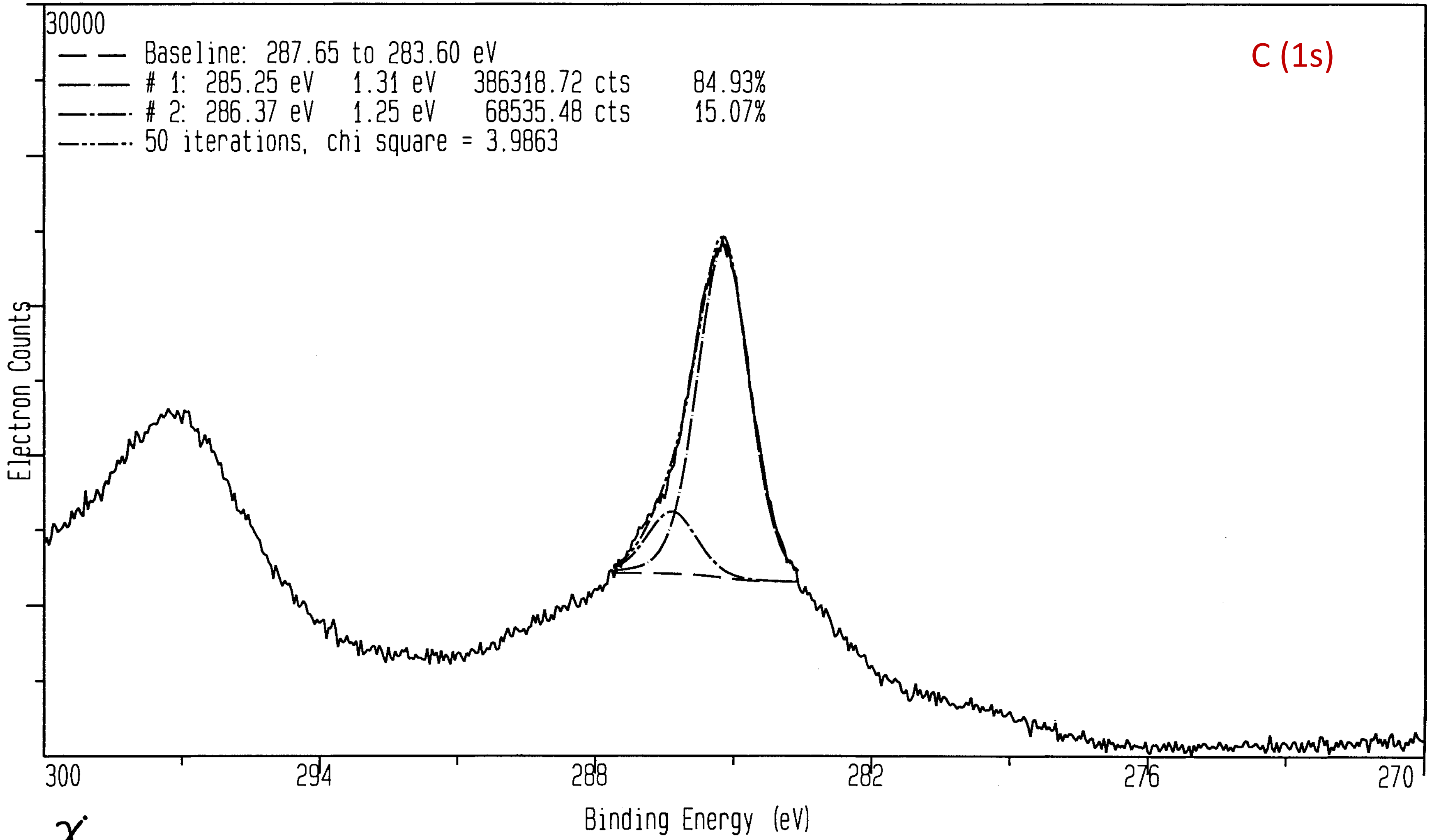
File: CDSE_1 Region: 6	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 15	Data Points: 601 Time/Point: 200	Date: Jul 26 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			CdSe



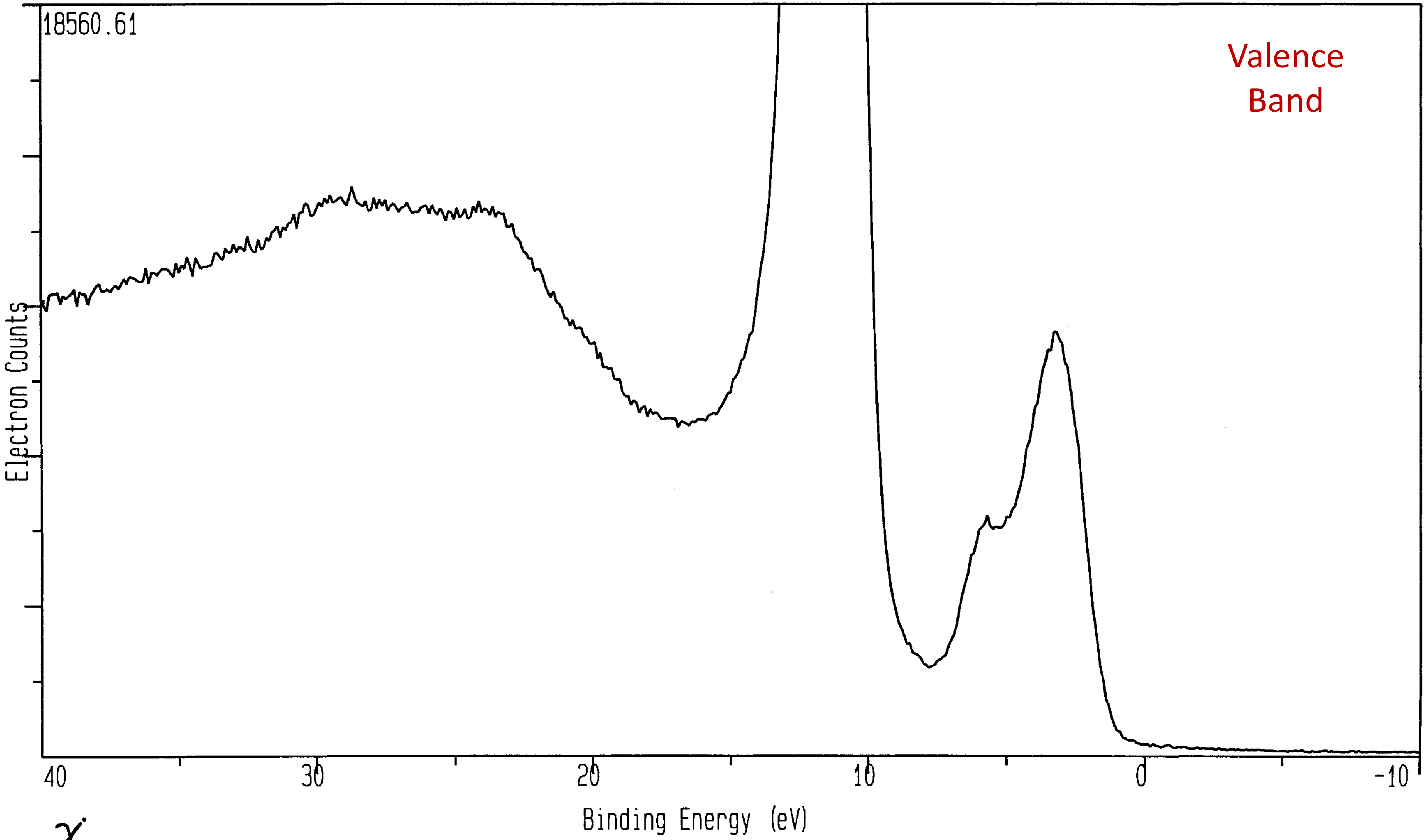
File: CDSE_1 Region: 4	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 20	Data Points: 401 Time/Point: 200	Date: Jul 26 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			CdSe



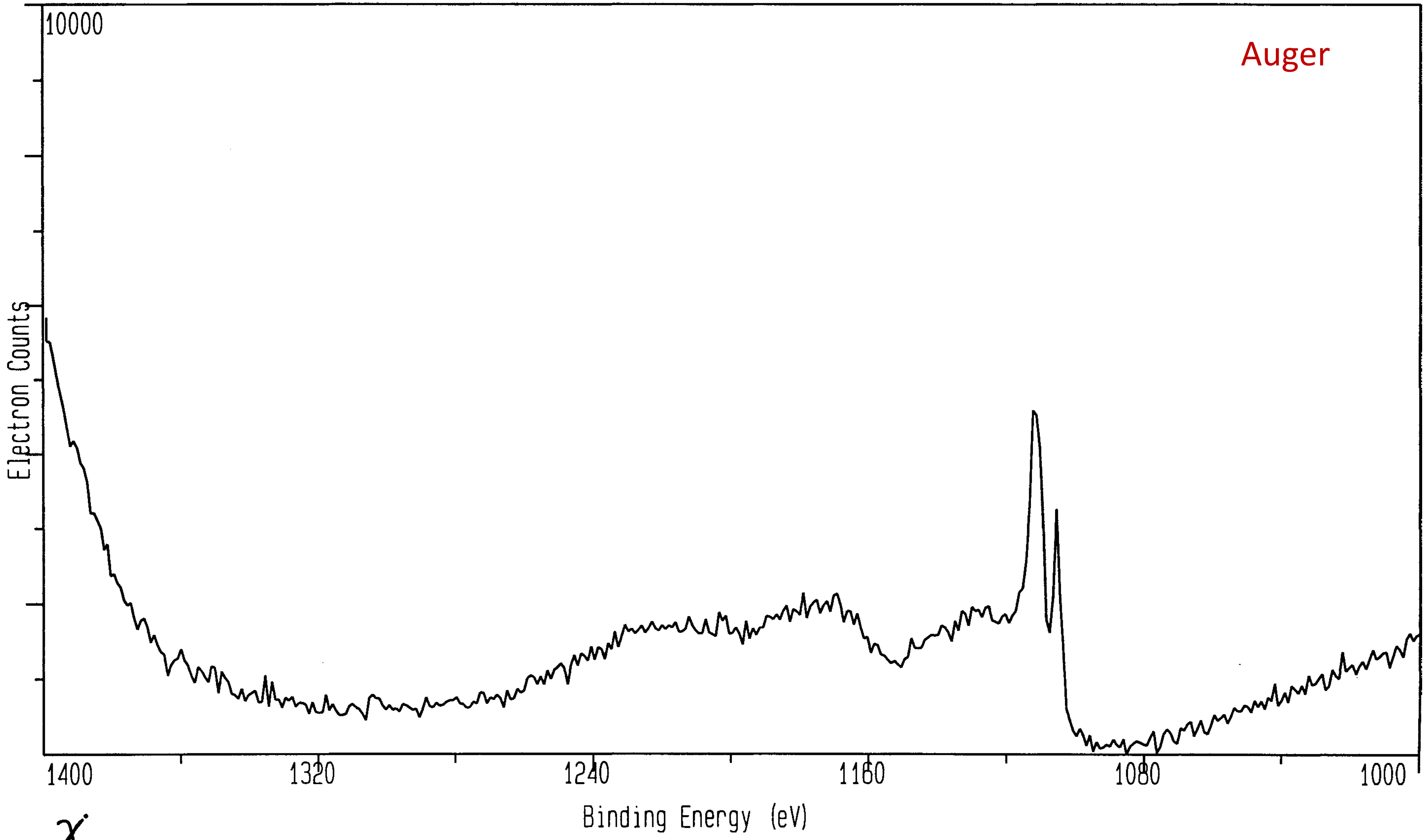
File: CDSE_1 Region: 5	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 30	Data Points: 601 Time/Point: 200	Date: Jul 26 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			CdSe



File: CDSE_1 Region: 3	Spot: 250x1000 Resolution: 4	Flood Gun: Off Scans, Time: 20	Data Points: 501 Time/Point: 200	Date: Jul 26 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			CdSe



File: CDSE_1 Region: 2	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 410 Time/Point: 200	Date: Jul 26 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr.Chem.Co., lot#00323JX As rec'd Electronic Grade, 3 micron powder, pressed pellet			CdSe



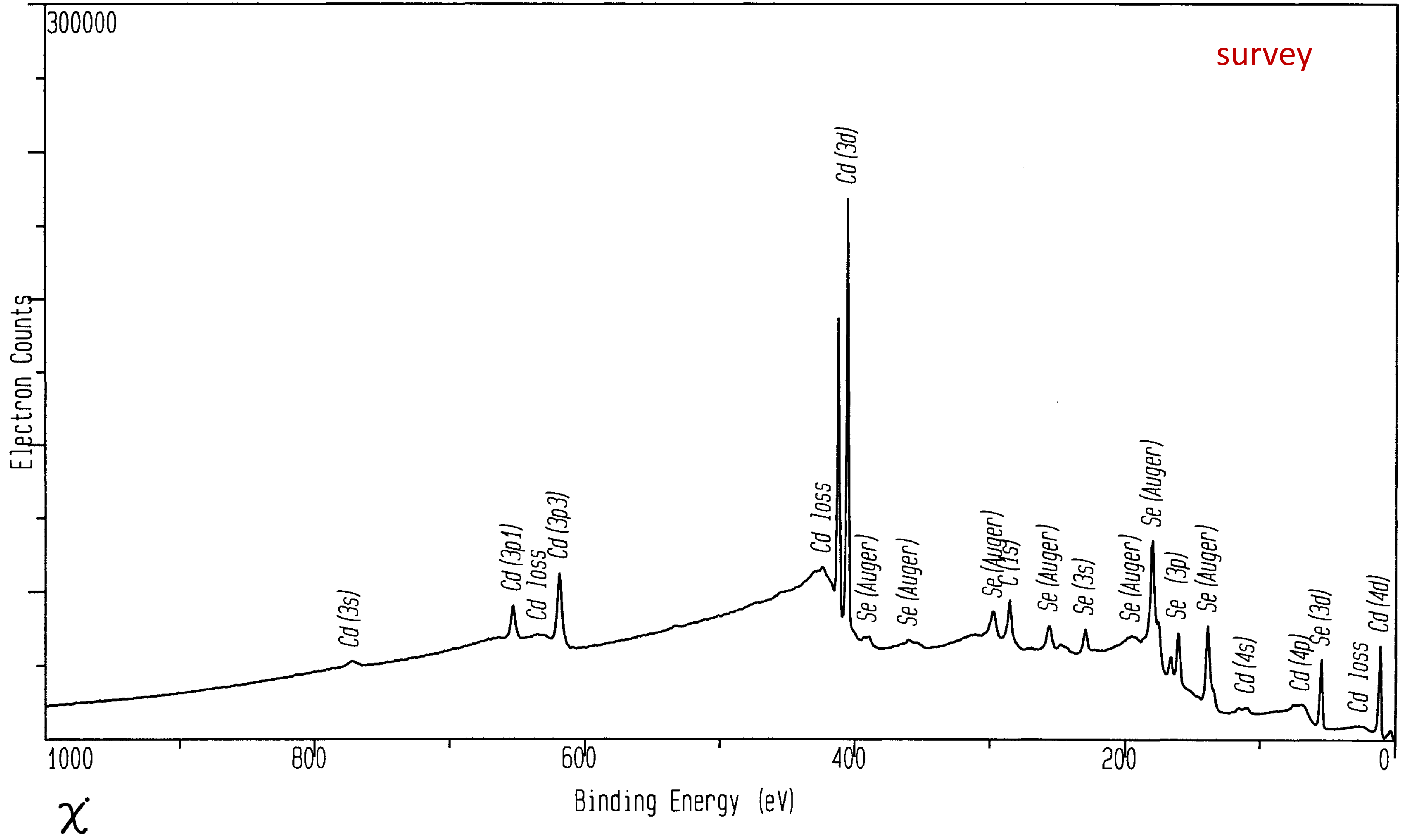
Cadmium Selenide (ion etched) (FW=191.36)

Detailed Surface Composition Table

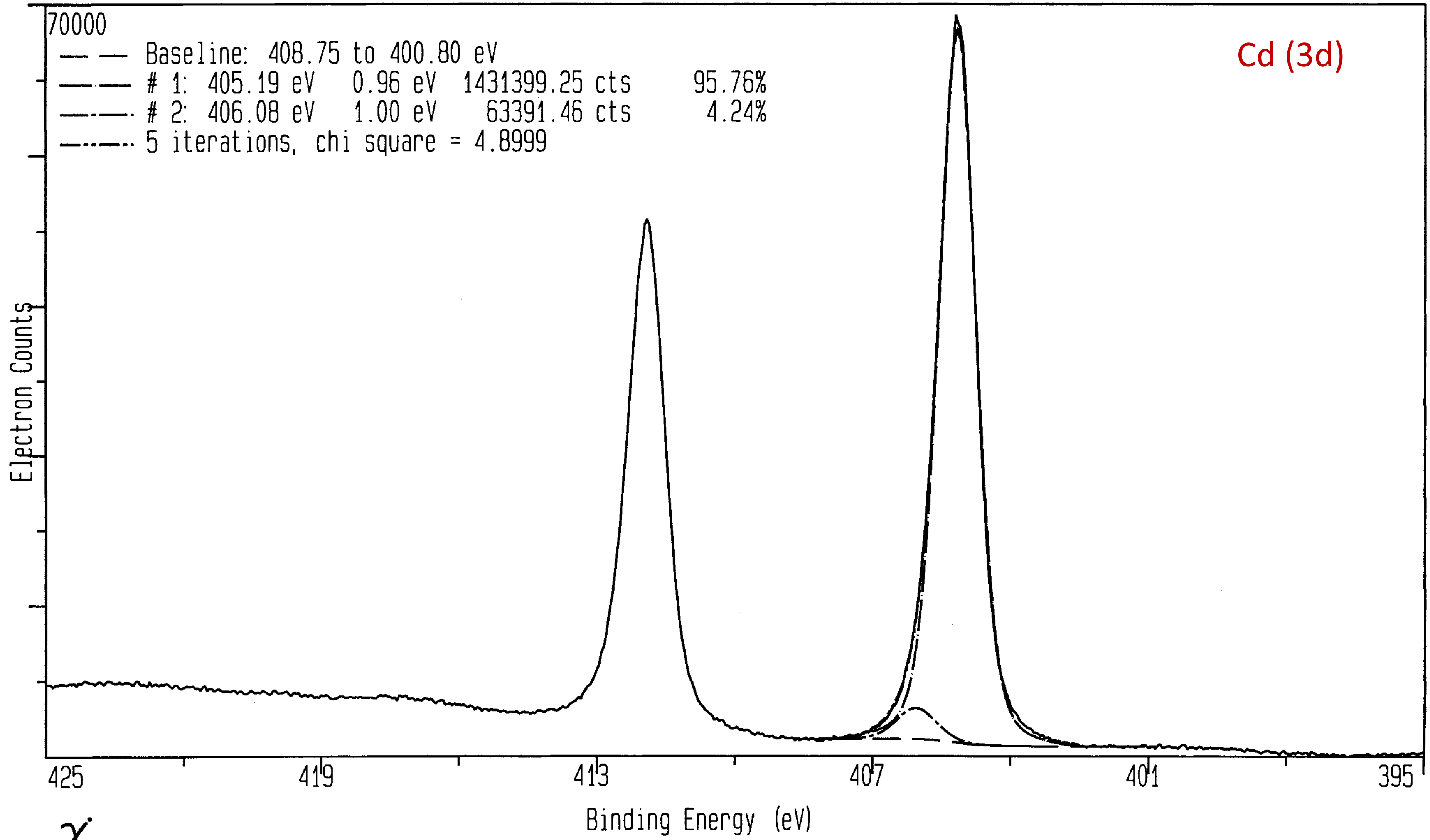
File name: CDSE_2_E.MRS
Region: 1
Description: CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched
Electronic grade 3 micron powder pressed pellet
Operator: V. Crist
Date: Thu Jul 28 08:39 1994

	Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
	Cd3s	772.9	772.8	1.63	7374	4533	
	Cd3p1	652.8	652.6	2.72	26144	9607	
	Cd loss	634.6	634.4	0.00	6481	0	
*	Cd3p3	618.5	618.4	5.75	58460	10165	27.54
	Cd loss	423.8	423.6	0.00	63802	0	
	Cd3d	405.3	405.1	17.81	253831	14249	
	SeAuger	389.7	389.5	0.19	7803	41462	
	SeAuger	359.6	359.4	0.19	14632	75263	
	SeAuger	297.1	297.0	0.00	27454	0	
*	C 1s	285.0	284.8	1.00	16253	16257	44.05
	SeAuger	255.7	255.5	0.00	36745	0	
	Se3s	229.1	228.9	1.51	17779	11775	
	SeAuger	194.9	194.7	0.23	15977	69445	
	SeAuger	179.6	179.4	0.00	128181	0	
	Se (3p)	160.3	160.1	4.95	44314	8950	
	SeAuger	138.4	138.2	0.00	63886	0	
	Cd4s	109.5	109.3	0.81	10843	13308	
	Cd4p	68.7	68.5	2.74	44191	16106	
*	Se3d	54.1	53.9	2.83	29682	10486	28.41
	Cd loss	25.9	25.7	0.00	6334	0	
	Cd4d	11.0	10.8	2.42	38885	16083	

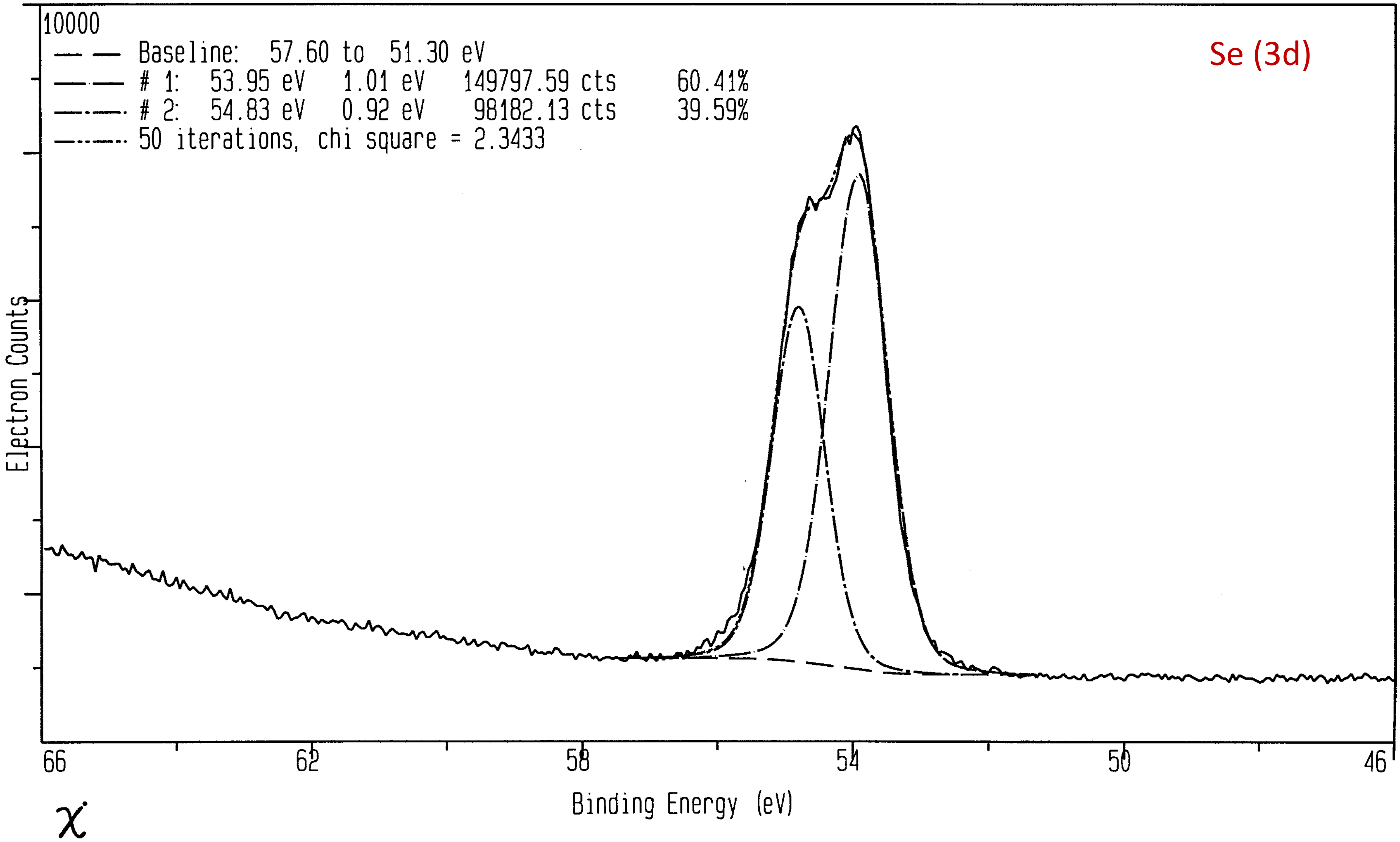
File: CDSE_2_E Region: 1	Spot: 250x1000 Resolution: 4	Flood Gun: Off Scans, Time: 10	Data Points: 1024 Time/Point: 200	Date: Jul 28 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched Electronic grade 3 micron powder pressed pellet			CdSe



File: CDSE_2_E Region: 6	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 601 Time/Point: 200	Date: Jul 28 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched Electronic grade 3 micron powder pressed pellet			CdSe



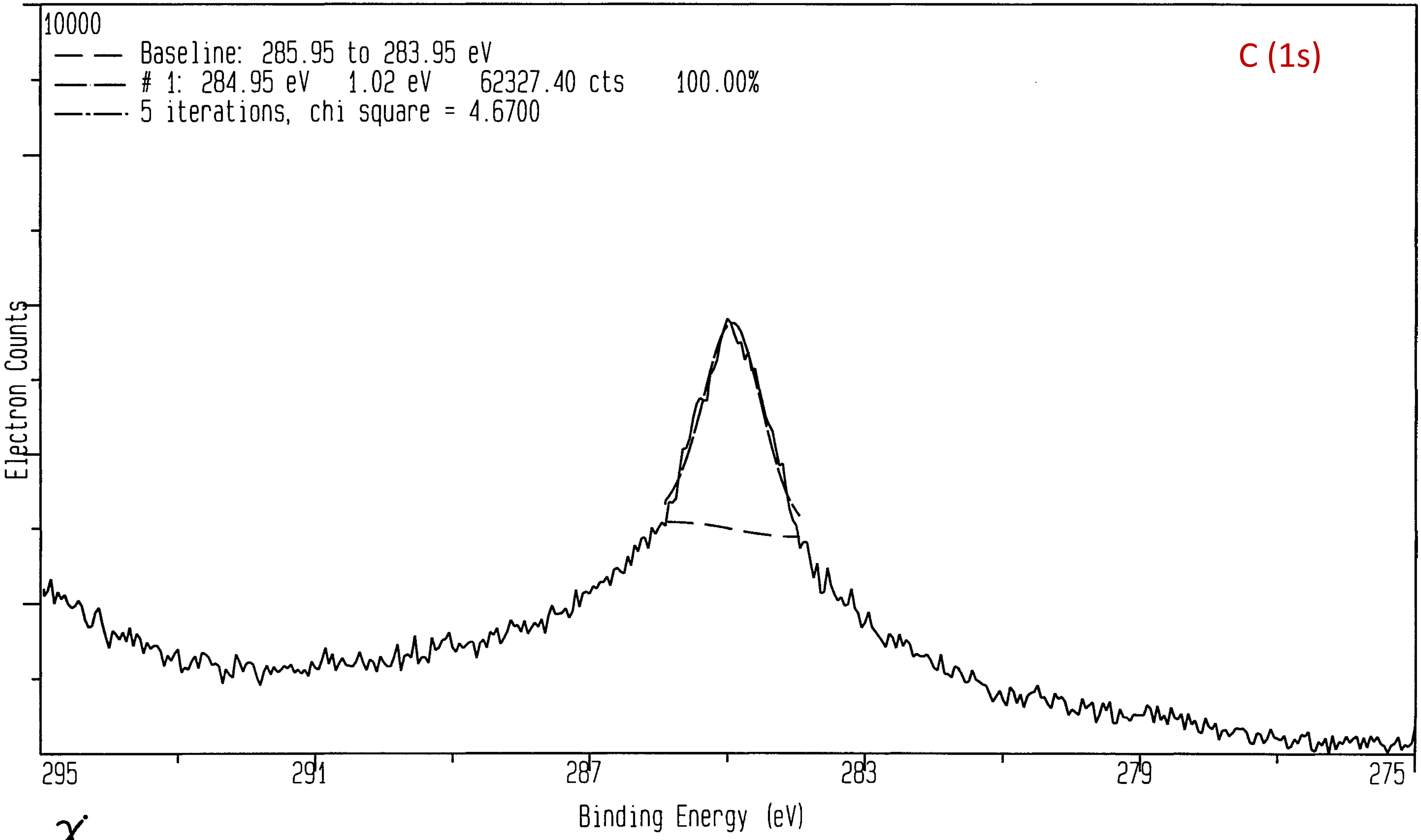
File: CDSE_2_E Region: 7	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 401 Time/Point: 200	Date: Jul 28 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched Electronic grade 3 micron powder pressed pellet			CdSe



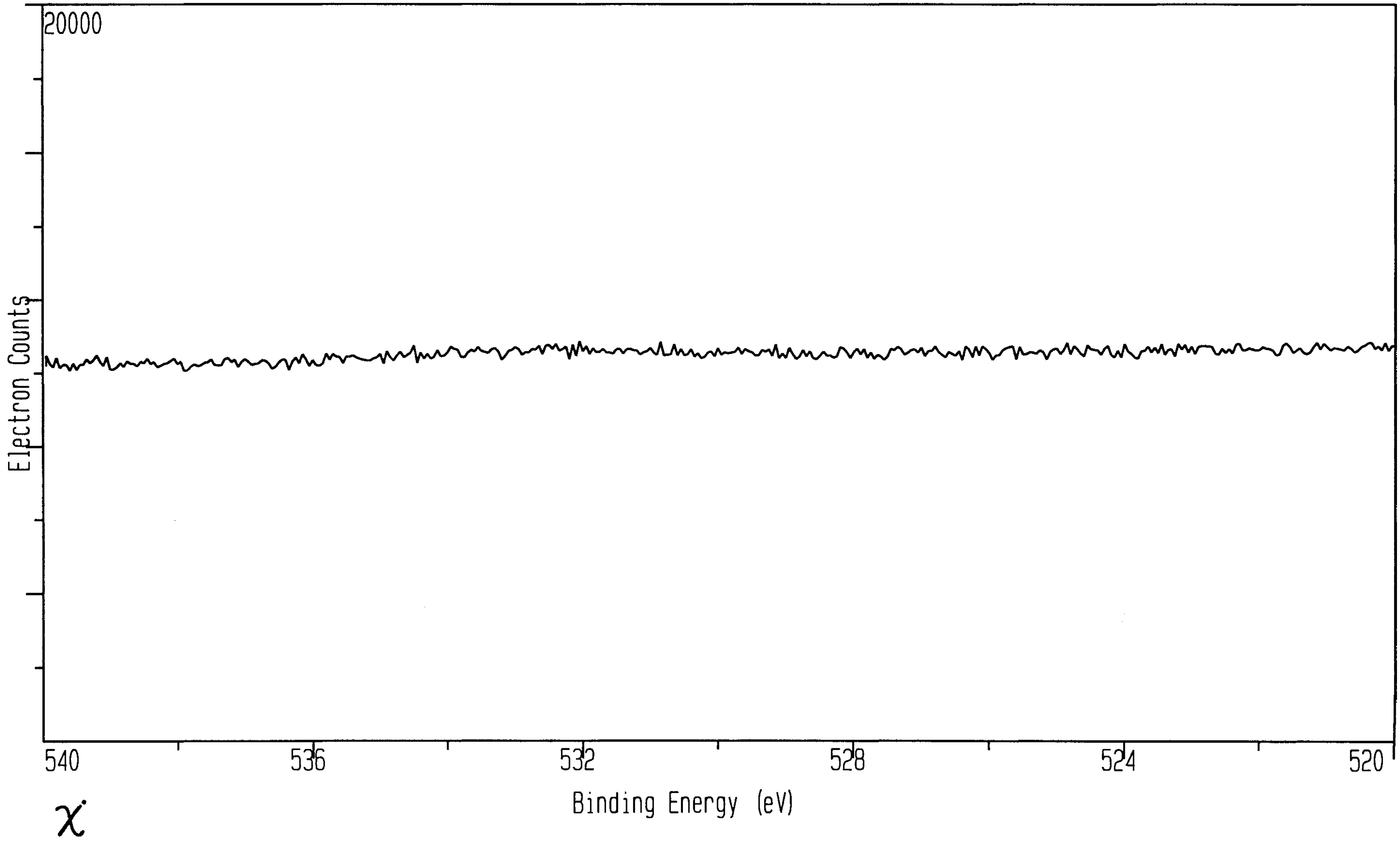
File: CDSE_2_E Region: 5	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 401 Time/Point: 200	Date: Jul 28 1994 Operator: V. Crist

Description: CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched
Electronic grade 3 micron powder pressed pellet

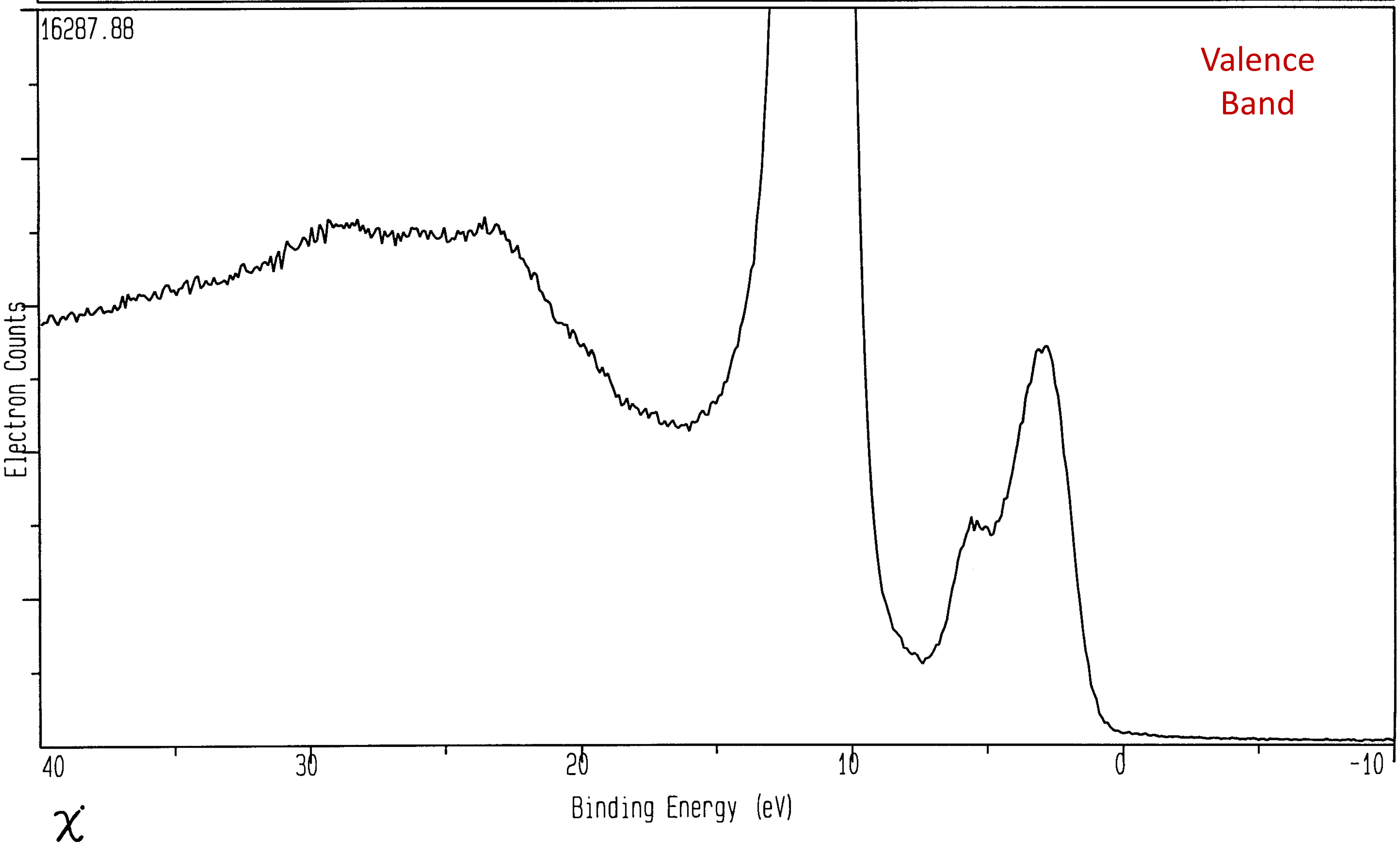
CdSe



File: CDSE_2_E Region: 4	Spot: 250x1000 Resolution: 2	Flood Gun: Off Scans, Time: 10	Data Points: 401 Time/Point: 200	Date: Jul 28 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched Electronic grade 3 micron powder pressed pellet			CdSe



File: CDSE_2_E Region: 3	Spot: 250x1000 Resolution: 4	Flood Gun: Off Scans, Time: 20	Data Points: 501 Time/Point: 200	Date: Jul 28 1994 Operator: V. Crist
Description:	CdSe (99.99%) Aldr Chem Co. lot#00323JX ion etched Electronic grade 3 micron powder pressed pellet			CdSe



Cadmium Telluride (as received) (FW=240.00)

Detailed Surface Composition Table

File name: CDTE_1.MRS
Region: 1
Description: Cadmium Telluride(CdTe) 99.99% Aldrich lot#03225CV, as received

Operator: V. Crist
Date: Thu Jul 28 22:29 1994

Signal	Corrected BE	Exper. BE	Sens Factor	Norm Area	Relative Area	Atom %
O Auger	973.2	973.0	0.00	3547	0	
Te3p1	871.0	870.8	2.21	11867	5381	
Te3p3	820.4	820.2	5.03	26776	5322	
Cd3s	772.0	771.8	1.63	6913	4243	
Cd3p1	652.8	652.5	2.72	20201	7421	
Cd loss	631.2	631.0	0.00	3311	0	
Cd3p3	618.5	618.3	5.75	44590	7750	
Te loss	595.6	595.3	0.00	8531	0	
Te3d3	583.8	583.6	8.88	81872	9217	
Te3d5	573.1	572.8	12.99	110261	8485	
O loss	546.5	546.3	0.00	2487	0	
* O 1s	530.7	530.4	2.23	22248	9992	23.48
Cd loss	423.6	423.3	5.49	73463	13377	
* Cd3d	405.3	405.1	17.81	188812	10600	24.91
* C 1s	285.0	284.7	1.00	11482	11483	26.99
Cl2p	198.3	198.0	2.48	1083	436	
Te4s	168.9	168.6	1.01	5180	5136	
Te+Cd	110.3	110.1	0.81	11981	14778	
Te loss	68.3	68.0	0.58	18187	31320	
* Te4d	40.5	40.2	4.53	47467	10475	24.62
Cd loss	22.8	22.6	0.18	5695	31654	
Cd4d	11.0	10.7	2.42	26603	11003	

APPENDIX "A"

ALPHABETICAL INDEX OF XPS SPECTRA IN VOLUME THREE SEMICONDUCTORS

LIST OF XPS SPECTRA IN VOLUME THREE

SEMICONDUCTORS

SEMICONDUCTORS (continued)

SEMICONDUCTORS (continued)