

Acetates

Name of directory: Acetate
Proper name: Metal acetates
Purpose of spectra: To provide reference spectra for metal acetates.

Overview: Metal acetates offer a way to correlate metal oxides to carbonates and also hydroxides. For this reason we are planning to analyze many metal acetates, but they have a strong tendency to decompose into HOAc and a hydroxide species, and they tend to outgas HOAc.

Materials: BaOAc, RbOAc

Observations: none

Number of materials: 2
Number of spectra: 15
Form of sample: powder
Electrical behavior: insulator
Special treatment: pressed onto 3M double sided adhesive tape, excess removed
Charge compensation: yes, flood gun (ca. 4 eV) (mesh-screen not used)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments X-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Acetoacetates

Name of directory: Ac-Ac
Proper name: Metal acetoacetates
Purpose of spectra: To reveal the typical surface chemical composition of Metal acetoacetates.

Overview: Metal acetoacetates can be used as catalysts or as a way to make thin metal films or even metal lines. The metal acetoacetates in this data set are the generous gift of Prof. John Nelson at the University of Nevada in Reno. Prof. Nelson has synthesized some of these metal salts and has purified them by conventional means.

Materials: Al(acac)₃, Co(acac)₂, Co(acac)₃, Cr(acac)₃, Cu(acac), Cu(acac)₂, Fe(acac)₃, Hf(acac)₄, Li(acac), Mg(acac)₂, Mn(acac)₃, MoO₂(acac), Na(acac), Nd(acac)₃, Ni(acac)₂, Pb(acac)₃, Tl(acac), Zn(acac)₂, and Zr(acac)₄.

Observations: Some of the materials are not as pure as expected which makes it difficult to interpret the BE data. Many of the salts have very complicated C(1s) and O(1s) spectra, and there is a good chance that these samples were damaged by the X-ray source while being analyzed.

Number of materials: >19
Number of spectra: >150
Form of sample: powder
Type of material: Insulator
Class of material: Metallorganic salts
Special treatment: pressed into thin 3mm diameter disks.
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Alloys - section 1

Name of directory: Alloys_1
Proper name: Metal alloys section 1
Purpose of spectra: To provide reference spectra of alloys in their "as-received" state and after exposing the near surface bulk by scraping with a knife and mild ion etching.

Overview: We have analyzed many alloys "*as received*" from their makers and also "*after scraping*" the surface with a knife to reveal the sub-surface bulk. In many cases we have also collected data after a "*light ion etch*" so that we can minimize the effect of contamination on the quantitative results. The light ion etching was typically done at 1-2 KeV for 5-10 seconds, which should have been just enough to decrease the loosely bound contaminants. There should not have been any preferential sputtering under those mild conditions. The samples were obtained from various sources. One source, Metal Samples Co., in the USA provided a 54 alloy kit which we analyzed as received and after scraping away the surface region with a knife. The CuNi series was obtained from Mr. Hareyama while he was a student at Muroran University. The AuCu and CoNi series were obtained from Dr. K. Yoshihara at the National Research Institute for Metals in Tsukuba, Japan. Other alloys were obtained from Prof. Tanaka at the Nagoya Institute of Technology.

Materials: 20-CB-3 alloy, 29-4-2 alloy, Al-1100 alloy, Al-2024 alloy, Al-3003 alloy, Al-5086 alloy, Al-6061 alloy, Al-7075 alloy, AuCu 25:75 alloy, AuCu 50:50 alloy, AuCu 75:25 alloy, CDA-260 alloy, CDA-360 alloy, CDA-443 alloy, CDA-464 alloy, CDA-706 alloy, CDA-715 alloy, CoNi 75:25 alloy, CoNi 50:50 alloy, CoNi 45:55 alloy, CoNi 25:75 alloy, CrMo 1.25:0.5 alloy, CrMo 2.25:1.0 alloy, CrMo 5.0:0.5 alloy, CrMo 9.0:1.0 alloy, CuNi 10:90 alloy, CuNi 20:80 alloy, CuNi 30:70 alloy, CuNi 40:60 alloy, CuNi 50:50 alloy, CuNi 60:40 alloy, CuNi 70:30 alloy, CuNi 80:20 alloy, CuTi 30:70 alloy, CuTiSi 27:63:10 alloy, CuTiAl 24:56:20 alloy, CuZn 65:35 alloy, C-1010 alloy, C-1020 alloy

Observations: The Cu (2p₃) and Au (4f₇) signals exhibited a small but discernible energy shift as a function of the concentration of the two components. The atom % derived from the AuCu series were very close to the theoretical values. The CoNi and CuNi series did not show this behavior. The 54 samples in the alloy kit purchased from the Metal Samples Co. were all contaminated with various inorganic materials. We decided not to wash any of the samples with any kind of solvents so as to preserve their original state which might be due to the method of production or the method of cutting or some other procedure.

Number of materials: >44
Number of spectra: >500
Form of sample: thin sheets (0.2-2mm thick)
Electrical behavior: conductor
Class of material: metal
Special treatment: as received (dirty), and after scraping and ion etching
Charge compensation: no
Ion etching/cleaning: yes, lightly ion etched - tried to avoid preferential sputtering.
Tried to decrease carbon contamination.
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Alloys – section 2

Name of directory: Alloys_2
Proper name: Metal alloys – section 2
Purpose of spectra: To provide reference spectra of alloys in their "as-received" state and after exposing the near surface bulk by scraping with a knife and very mild ion etching.

Overview: We have analyzed many alloys "*as received*" from their makers and also "*after scraping*" the surface with a knife to reveal the sub-surface bulk. In most cases we have also collected data after a "*light ion etch*" so that we can minimize the effect of contamination on the quantitative results. The light ion etching was typically done at 1-2 KeV for 5-10 seconds, which should have been just enough to decrease the loosely bound contaminants. There should not have been any preferential sputtering under those mild conditions. The samples were obtained from various sources. One source, Metal Samples Co., in the USA provided a 54 alloy kit which we analyzed as received and after scraping away the surface region with a knife. The CuNi series was obtained from Mr. Hareyama while he was a student at Muroran University. The AuCu and CoNi series were obtained from Dr. K. Yoshihara at the National Research Institute for Metals in Tsukuba, Japan. Other alloys were obtained from Prof. Tanaka at the Nagoya Institute of Technology.

Materials: E-26-1 alloy, FeNiMoB 40:38:4:18 alloy, F-255 alloy, HA-25 alloy, HB-2 alloy, HC-276 alloy, HG-3 alloy, HgTe, HX alloy, I-600 alloy, I-625 alloy, I-750X alloy, I-800 alloy, I-825 alloy, CuNi (Monel) alloy, M-400 alloy, N-200 alloy, Pd:Fe 73.8:26.2 alloy, 304 SS alloy, 304L SS alloy, 310 SS alloy, 316L SS alloy, 347 SS alloy, 410 SS alloy, 4140 alloy, 430 SS alloy, 904L alloy, TiVAl alloy, Ti GR-02 alloy, Ti GR-07 alloy, Ti GR-12 alloy, and Wood's metal alloy.

Observations: The 54 samples in the alloy kit purchased from the Metal Samples Co. were all contaminated with various inorganic materials. We decided not to wash any of the samples with any kind of solvents so as to preserve their original state which might be due to the method of production or the method of cutting or some other procedure.

Number of materials: >33
Number of spectra: >350
Form of sample: thin sheets (0.2-2mm thick)
Electrical behavior: conductor
Class of material: metal
Special treatment: as received (dirty), and after scraping and ion etching
Charge compensation: no
Ion etching/cleaning: yes, lightly ion etched - tried to avoid preferential sputtering. Tried to decrease carbon contamination.
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Alumino-silicates

Name of directory: Alum-Sil
Proper name: Alumino-silicates (from natural minerals)
Purpose of spectra: To provide reference spectra for those materials.

Overview: These alumino-silicates are natural minerals.

Materials: Almandine ($\text{Fe}_3\text{Al}_2(\text{SiO}_4)_3$), Kunzite ($\text{LiAlSi}_2\text{O}_6$), Pyrope ($\text{Mg}_3\text{Al}_2(\text{SiO}_4)_3$)

Observations: none at this time.

Number of materials: 3
Number of spectra: >40
Form of sample: poly-morphic crystals
Electrical behavior: insulator
Special treatment: freshly fractured in air just prior to analysis
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.98 eV (+/-0.078)
Ref BE for Cu (2p3): 932.67 eV (+/-0.078)
Ref BE for Cu (3s): 122.45 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Angle-resolved XPS

Name of directory: Angl-Res
Proper name: Angle-resolved XPS (i.e. angle dependent XPS)
Purpose of spectra: To reveal changes in surface chemical composition as a function of depth where the depth is limited to the escape depth of photoemitted electrons, which is limited to a depth of 50 to 100 angstroms.

Overview: Angle resolved XPS studies of several materials are provided as examples which can be used as a guide to studying similar samples. The Ag and Au samples were ion etched to reveal changes in the peak shape and energy loss background of these two elements as a function of electron take-off-angle. The step sizes for changing angles was too large to reveal any Photo-electron Diffraction patterns.

Materials: Ag, Au, CrSi, Fluoro-ether lubricant, GaAs, HOPG (Graphite), Si, Te, Ta₂O₅, and 200 Ang SiO₂/Si

Observations: Because the X-ray beam was always smaller than the electron lense field of view the changes in signal intensity directly reflect the true physics of photoemission. Many other XPS systems show a behavior that is directly dependent on the electron collection lense.

Number of materials: 10
Number of spectra: >200
Type of material: various
Form of sample: native oxide films, thin films, wafers, pressed powders
Special treatment: as received, unless otherwise specified in the datafile
Charge compensation: flood gun at 4 eV if needed
Ion etching/cleaning: refer to individual datafiles for specific details
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: varied from ca. zero (0) to 90 degrees (and beyond)
Instrument used: Surface Science Instruments X-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Anti-static materials

Name of directory: Antistat
Proper name: Anti-static materials
Purpose of spectra: Reveal the surface composition of bags used to store printed circuit boards and other electrical devices which might rub off of the bag and onto the surface of the item(s) stored in the bags. Reveal the chemical composition of anti-static sprays which are used to control static electric charge.

Overview: These materials are used to avoid static electrical damage that might occur by a static discharge.

Materials: Complex (plastic bags with special spray coatings or chemical agents that are mixed in with the plastic of the bag.)

Observations: It may be possible that these bags are a source of contamination to various electrical components that might eventually lead to electrical breakdown.

Number of materials: 6
Number of spectra: 40
Form of sample: plastic bags and spray solutions
Type of material: real world product made of several materials
Special treatment: none
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments X-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Bio-technology materials

Name of directory: Bio-Tech
Proper name: Bio-technological materials
Purpose of spectra: To look for any correlation between living tissues and differences in surface chemical composition.

Overview: At one time medical doctors thought that by analyzing the surface chemistry of human hair of Alzheimer patients that they might find a clue as to cause of Alzheimer.

Materials: Hair from patients who had Alzheimer disease. Freeze-dried P. Dengis (CIFA) yeast.

Observations: none

Number of materials: 9
Number of spectra: >50
Form of sample: Fibers and pressed powders
Class of material: Biological materials
Special treatment: pressed onto double sided adhesive tape
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments X-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.3393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Borides

Name of directory: Boride
Proper name: Metal borides
Purpose of spectra: To reveal the typical surface chemical composition of metal borides.

Overview: Metal borides are used as cathode filaments and as hard materials.

Materials: CrB, LaB₆, MoB, Ni₃B, Ni₃B with Carbon, and WB.

Observations: Metal boride powders are often heavily contaminated with surface oxides and are electrically conductive.

Number of materials: 6
Number of spectra: 36
Form of sample: powder
Electrical behavior: conductor
Class of material: inorganic salt
Special treatment: pressed into thin 3mm diameter disks.
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: ion etched to removed surface oxides as much as possible
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Calibration of energy scale

Name of directory: Calibrat

Proper name: Energy scale calibration

Purpose of spectra: To check and to adjust the energy scale of the SSI XPS systems. Calibration was checked every 2-3 weeks and pass energies were adjusted if the reference energies deviated from the allowed tolerances listed below.

Overview: Calibration was checked every 2-3 weeks for the 10 years used to collect all of the data in the database. Many of the spectra used to check calibration were saved, but not all of the calibration spectra were saved in the early years of the project.

Materials: 99+% Gold (Au) foil or 1 micron thick gold on a silicon wafer or PET (Mylar), and 99+% Copper (Cu) foil

Observations: To maintain proper calibration, the gold and copper samples had to be ion etched enough to reveal bulk material. Insufficient etching seemed to cause an error in determining the BE of the peaks used to check the reference energies. Based on our experience, the linearity of the SSI systems is constant for many months, perhaps years.

Number of materials: 2

Number of spectra: >300

Form of sample: metal foils

Type of material: conductors

Class of material: metals

Special treatment: none

Charge compensation: none

Ion etching/cleaning: gold (Au) was ion etched at >2KeV for ca. 20 sec
copper (Cu) was ion etched at >2KeV for >120 sec

Ref BE for Au (4f7): 83.96 eV (+/-0.078)

Ref BE for Cu (2p3): 932.47 eV (+/-0.078)

Ref BE for Cu (3s): 122.39 eV (+/-0.15)

Electron TOA: 35 degrees

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Capture of oxygen and carbon

Name of directory: Captur_1

Proper name: Capture of oxygen and carbon by ion etched metals

Purpose of spectra: To reveal the typical surface chemical composition of thin oxide films and carbides that form "naturally" in cryopumped UHV conditions.

Overview: Practical study of the behavior of pure elements that were ion etched clean and left in cryopumped UHV overnight for 12-14 hours during which the surface captures whatever gases are in the cryopumped UHV. (No additional ion etching.) Data was collected on a time-lapse basis without any additional ion etching. The argon gas flow was stopped and the ion gun was turned off after the ion cleaning.

Materials: Ag, Al, As, Au, Be, Bi, Cd, Co, Cr, Cu, Fe, Ge, Hf, In, Ir, Mg, Mn, Mo, Nb, Ni, Pb, Pd, Pt, Re, Rh, Sb, Sc, Si, Sn, Ta, Te, Ti, Tl, V, W, Y, Zn, Zr

Observations: Elements on the left side of the periodic table tended to form carbides and oxides. Elements on the right side of the periodic table tended to build up carbon contamination.

Number of materials: 42

Number of spectra: >1,800

Form of sample: chips and foils

Electrical Behavior: conductor

Class of material: pure elements

Special treatment: scraped in air and quickly inserted into prep-lock HV

Charge compensation: none

Ion etching/cleaning: ion etched at 3-5 KeV for 30-50 minutes

Ref BE for Au (4f7): 83.98 eV (+/-0.078)

Ref BE for Cu (2p3): 932.67 eV (+/-0.078)

Ref BE for Cu (3s): 122.45 eV (+/-0.15)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Capture study – End point

Name of directory: Captur_2
Proper name: Surface composition at end of Captur_1 studies.
Purpose of spectra: To reveal the typical surface chemical composition of elements ion etched and left in cryopumped UHV for >12 hours.

Overview: This group was meant to reveal the basic behavior of metals exposed to long term UHV after ion etching.

Materials: Ag, As, Co, Fe, Ge, Hf, Mo, Ni, Pb, Pd, Pt, Ru, Sb, Sn, Ta, Te, Tl

Observations: The amount of oxide or carbon species that form after long term exposure to cryopumped UHV is very small. The thickness of these overlayers is estimated to be between 5-15 angstroms in general. These overlayers probably represent the initial stages of oxidation or contamination and possible the formation of intermediate sub-oxide species or intermediate carbon species.

Number of materials: 17
Number of spectra: 23
Form of sample: metal foils or chips
Electrical behavior: conductor
Class of material: metal
Special treatment: scraped with knife in air to expose bulk
Charge compensation: no
Ion etching/cleaning: ion etched 30-40 minutes at 2-5 KeV.
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Carbides

Name of directory: Carbide
Proper name: Metal carbides
Purpose of spectra: To reveal the typical surface chemical composition of metal carbides.

Overview: Carbides develop oxide surface layers, but those layers are relatively thin because the carbide signal can still be observed for the carbides that are provided in this database.

Materials: NbC, TaC, VC

Observations: Ion etching seemed to produce a kind of hydrocarbon that could not be removed by further ion etching.

Number of materials: 3
Number of spectra: 40
Form of sample: powder
Electrical behavior: conductive
Class of material: inorganic compound
Special treatment: pressed into thin 3mm diameter disks
Charge compensation: none
Ion etching/cleaning: Yes, as needed
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Carbon

Name of directory: Carbon

Proper name: Different forms of carbon

Purpose of spectra: To reveal the typical surface chemical composition of carbon.

Overview: Carbon (C) comes in several different forms which have various uses.

Materials: natural graphite, HOPG, diamond, diamond-like-films, poly-ethylene, and wax paper.

Observations: Diamond has a characteristic peak in the valence band region not seen in many diamond-like carbon (DLC) films. Graphite has a $\pi \rightarrow \pi^*$ peak which is characteristic of the sp^2 nature of the carbon in some of its various forms (e.g. graphite, HOPG). Attempts to peak-fit the C (1s) of HOPG and graphite are often difficult because the physics of the material is more complicated than the physics behind the use of various asymmetric tail functions used for peak-fitting.

Number of materials: 13

Number of spectra: >120

Form of sample: crystalline and powder

Electrical behavior: conductor or insulator

Class of material: inorganic and organic

Special treatment: various

Charge compensation: flood gun (ca. 4 eV) and nickel mesh-screen (80% T) on insulators

Ion etching/cleaning: none

Ref BE for Au (4f7): 83.96 eV (+/-0.078)

Ref BE for Cu (2p3): 932.47 eV (+/-0.078)

Ref BE for Cu (3s): 122.39 eV (+/-0.15)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Carbon black materials

Name of directory: C_Black
Proper name: different carbon black materials
Purpose of spectra: To reveal the typical surface chemical composition of carbon black powders exposed to different treatments.

Overview: This set of spectra is part of a study done on the standard carbon black material.

Materials: CB_01 (standard), CB_0150, CB_0300, CB_0450, CB_1000, CB_1200, CB_1400, CB_L

Observations: Carbon black powders contain small amounts of sulfur and chlorine which can be removed by high temperature treatment. The oxygen contamination of these powders can not be removed by high temperature treatment.

Number of materials: 8
Number of spectra: 30
Form of sample: powder
Electrical behavior: conductor
Class of material: inorganic
Special treatment: pressed onto indium metal foil
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Carbon fibers

Name of directory: C_fibers
Proper name: Carbon fibers
Purpose of spectra: To reveal the typical surface and bulk chemical composition of one kind of carbon fiber.

Overview: none

Materials: F-300 carbon fibers with sizing agent, and F-300 carbon fibers without sizing agent

Observations: Sizing agent contains a alcohol or ether type component which is not observed in the fiber without the sizing agent. The depth profile revealed the presence of barium (Ba) and nitrogen (N) in the fibers without the sizing agent.

Number of materials: 2
Number of spectra: 7 in normal mode (plus 360 in depth profile mode)
Form of sample: bundle of fibers
Electrical behavior: conductor (with sizing) and insulator (no sizing)
Class of material: fiber
Special treatment: none (except for depth profile analysis)
Charge compensation: flood gun used on insulating sample
Ion etching/cleaning: as done for depth profile
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: (round surface)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Carbonates

Name of directory: Carbonat
Proper name: Metal carbonates
Purpose of spectra: To reveal the typical surface chemical composition of metal carbonates.

Overview: Carbonates are an integral part of any study of oxides, hydroxides, and corrosion because they interchange with the oxides and hydroxides by various mechanisms.

Materials: Azurite, BaCO₃, BiCO₃, CaCO₃, Calcite (CaCO₃), CdCO₃, Cerrusite (PbCO₃), CuCO₃, LaYCO₃, LiCO₃, Magnesite (MgCO₃), MgCO₃, MnCO₃, SrCO₃, Y₂CO₃.

Observations: Carbonates are often overlooked as not being part of the carbon contamination. Carbonates are materials that form naturally from metal oxides or metal hydroxides by absorbing CO₂ from the air. Many naturally formed native oxides have a small amount of metal carbonate at the surface. Carbonates can be damaged or degraded by ion beam etching or heating. The heat of high powered mono X-ray sources or non-mono X-ray sources is sometimes enough to degrade the carbonate to the pure metal or a oxide of the metal.

Number of materials: 15
Number of spectra: >150
Form of sample: powder and natural mineral
Electrical behavior: insulator
Class of material: inorganic salt
Special treatment: pressed into thin 3mm diameter disks or freshly fractured in air
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Catalyst materials

Name of directory: Catalyst

Proper name: Catalyst materials (new and used)

Purpose of spectra: To reveal the typical surface chemical composition of catalyst materials.

Overview: Catalysts need to be studied before use and after use. Catalysts can be easily damaged by X-rays and even flood gun electrons.

Materials: Platinum on alumina, CrFx on alumina, CuNi alloys, Monel, NiW on Alumina, Pd and Ce and Ze on alumina, Vanadium based catalyst

Observations: Some catalysts, (Pt/Alumina) are readily damaged by exposed to mono X-rays within the time needed to analyze the material. Other catalysts that use MoO₃/alumina are readily damaged by flood gun electrons within a few seconds or minutes of exposure.

Number of materials: 15

Number of spectra: >150

Form of sample: pellets or metal foils

Electrical behavior: insulators or conductor

Class of material: multi-component

Special treatment: as received or freshly fractured or scraped or ion etched

Charge compensation: yes if needed (mesh-screen used as needed)

Ion etching/cleaning: alloys were lightly ion etched

Ref BE for Au (4f₇): 83.96 eV (+/-0.078)

Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)

Ref BE for Cu (3s): 122.39 eV (+/-0.15)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Cathode filaments

Name of directory: Cathode

Proper name: Cathode filaments

Purpose of spectra: To reveal the typical surface chemical composition of cathodes.

Overview: These data are provided as an example of the degraded effects on thoriated tungsten ribbons used as electron sources for producing argon ions.

Materials: Cathodes were taken from the ion gun source and the electron gun source which were thoriated tungsten ribbons.

Observations: none

Number of materials: 1

Number of spectra: 10

Form of sample: metal ribbon

Electrical behavior: conductor

Class of material: mixed material

Special treatment: none

Charge compensation: none

Ion etching/cleaning: none

Ref BE for Au (4f7): 83.96 eV (+/-0.078)

Ref BE for Cu (2p3): 932.47 eV (+/-0.078)

Ref BE for Cu (3s): 122.39 eV (+/-0.15)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Cadmium oxide BE research

Name of directory: CdOx_Res

Proper name: Research done on CdOx surfaces.

Purpose of spectra: To reveal the typical surface chemical composition of Cadmium oxides.

Overview: The BE of CdO is reported to be lower than metallic Cd. This study was carried out to try to understand if the reports were correct or wrong.

Materials: Cd (air exposed), Cd (exposed to H₂O₂), Cd (exposed to NH₄OH), CdSe, CdO, CdO/InP

Observations: Cd metal seems to form a mixture of oxide, hydroxide and carbonate overlayers when exposed to various solutions. More work is needed to understand if CdO does or does not have a BE lower than Cd metal.

Number of materials: 6

Number of spectra: >20

Form of sample: metal foil or powder

Electrical behavior: conductor

Class of material: mixed

Special treatment: CdSe was pressed into thin 3mm diameter disks. Cadmium metal was exposed to H₂O₂, NH₄OH to try to produce a thin layer of CdO.

Charge compensation: none

Ion etching/cleaning: none

Ref BE for Au (4f₇): 83.96 eV (+/-0.078)

Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)

Ref BE for Cu (3s): 122.39 eV (+/-0.15)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Chalcogenides

Name of directory: Chalcogn
Proper name: Chalcogenides (Chalconides)
Purpose of spectra: To reveal the typical surface chemical composition of chalcogenides.

Overview: Chalcogenides are materials that contain one of the elements: S, SE or Te as the cation of a compound.

Materials: CdSe, CdTe, GeSe, GeSe₂, HgCdTe, SbTe, Se, Te, ZnSe

Observations: none

Number of materials: 9
Number of spectra: >80
Form of sample: powders or crystalline chips
Electrical behavior: semi-conductors and conductors
Class of material: Chalcogenides
Special treatment: pressed into thin 3mm diameter disks (as needed)
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Charge-compensation research

Name of directory: Chrg_Res
Proper name: Charge-compensation research
Purpose of spectra: To research the charge-compensation behavior of insulators under various conditions.

Overview: To study the effect of using different methods to try to compensate for the charge-up of various materials. The user needs to carefully evaluate each set of files as individual research projects. The entire set of files are the result of various research studies aimed at understanding charge compensation.

Materials: Al₂O₃, MgO, SiO₂, NaCl, Ta₂O₅, Au/teflon, Ag₂O, Bi₂O₃, Ga₂O₃, GeO₂, MoO₃, Nb₂O₅, PdO, Ta₂O₅, TiO₂, V₂O₅, WO₃, Cu/teflon, HDPE, Al, Zn, Zr,

Observations: A variety of methods were used to study the charge up and charge compensation behavior of various insulators and conductors mounted on insulators which were expose to X-rays with or without the flood gun.

Number of materials: 33
Number of spectra: >400
Form of sample: crystals, fused glass, pressed powder, thin films
Electrical behavior: insulators and thin films which are pseudo-conductive
Class of material: various
Special treatment: various
Charge compensation: yes, with and without the mesh-screen system
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Charge-compensation using grazing X-rays

Name of directory: Chrg_Grz
Proper name: Charge-compensation assisted by using grazing X-rays
Purpose of spectra: To study the charge-up behavior of insulators that are exposed to X-rays that come in at a grazing angle relative to the sample surface.

Overview: To study the effect of using grazing X-rays to minimize the charge-up due to X-ray irradiation of insulating materials.

Materials: Al₂O₃, MgO, SiO₂, NaCl, Ta₂O₅

Observations: Grazing angle X-ray irradiation can produce excellent results because the power density is greatly decreased it seems. In some cases, the data was as good as the data (FWHM) obtained by using the mesh-screen system.

Number of materials: 5
Number of spectra: 120
Form of sample: crystals, fused glass, pressed powder
Electrical behavior: insulator
Class of material: binary metal oxides
Special treatment: as received
Charge compensation: yes by flood gun without mesh-screen advantage
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Charge-up of adventitious carbon

Name of directory: Chrg_C
Proper name: Charge-up of adventitious carbon
Purpose of spectra: To study the charge-up behavior of carbon because it is so often used to charge reference insulators, and we have some doubt that a constant BE value should be used.

Overview: To study the validity of using the C (1s) BE of hydrocarbons as a universal means to charge reference all insulators.

Materials: Carbon on all kinds of substrates. Especially interested in the hydrocarbon signal.

Observations: Very thin layers of hydrocarbon on different materials appears to have different BEs, which can vary by as much as 1 eV, e.g. from 284.4 eV to 286.5 eV. There appears to be some sort of surface physics that affects the photoemission processes in the hydrocarbon overlayers. The effect is most obvious for elements in columns 2 and 3 of the periodic table, and to some extent columns 12-14. The effects observed for elements in columns 12-14 are more complex. Native Oxides of these elements are especially interesting to study by using a flood gun set to different voltages (2-15 eV) with the samples grounded and floating.

Number of materials: 15
Number of spectra: >200
Form of sample: variable
Electrical behavior: variable
Class of material: variable
Special treatment: as received normally
Charge compensation: yes as needed to study the effect of charging
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Charge-up of Al₂O₃

Name of directory: Chrg_AIO
Proper name: Charge up studies on aluminium oxide materials
Purpose of spectra: To study the charging behavior of thin and thick films of aluminum oxides under various experimental conditions.

Overview: The charging behavior of aluminium oxide thin films is complicated and presents a challenge to be able to properly assign the chemical species that form on native oxides and that exist as thick plates. Tests of charging behavior in the presence of the mesh-screen system was studied.

Materials: Native aluminium oxides on various substrates. Pure aluminium oxide forms.

Observations: Native oxide films were found to suffer differential charging which seems to be due to vertical stratification of the electrons supplied by a defocussed electron flood gun. The process was found to be reversible.

Number of materials: 10
Number of spectra: >150
Form of sample: thin films or thick plates
Electrical behavior: differential charging
Class of material: insulator
Special treatment: as received, or scratched to produce rough area
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Chromatographic materials

Name of directory: Chromato
Proper name: Chromatographic materials
Purpose of spectra: To reveal the typical surface chemical composition of chromatographic materials.

Overview: The surface of chromatographic materials is critical to the retention of chemicals as they pass over the material

Materials: Ion exchange beads, plasma treated polystyrene beads

Observations: xx

Number of materials: 5
Number of spectra: 20
Form of sample: beads or powders
Electrical behavior: insulator
Class of material: mixed
Special treatment: as received
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Contamination from gloves

Name of directory: Glove
Proper name: Contamination caused by gloves
Purpose of spectra: To reveal the typical surface chemical composition of contamination caused by touching materials with plastic gloves.

Overview: Study of contamination that occurs when a gloved hand touches any material. Gloves contain various organic chemicals and have coatings made of organic or inorganic materials which are designed to make the glove soft or to keep the users' hand dry.

Materials: Aluminium foil contaminated by contact with plastic gloves, pieces of gloves, finger cots, and a spray used as a mold release agent.

Observations: Silicone oil and various "plasticizer" chemicals is a major component in soft pliable gloves which is easily transferred to a material touched by the glove. CaO and other similar drying agents (CaSO₄, Na₂SO₄) are also used to keep the users' hand dry. Silicone oil, various long chain organic acids and amides are used as mold release agents so that the gloves are easily removed from the mold used to make the gloves.

For comparison the user should compare any spectrum to that obtained from the Al_control sample (Al_contr.mrs) and the finger sample (Finger_1.mrs) to see what is normally on the surface of aluminium foil before it is touched by anything and also after it has been touched by an unprotected human finger.

Number of materials: 22
Number of spectra: >50
Form of sample: Deliberately contaminated aluminium foil
Electrical behavior: conductor
Class of material: mixed
Special treatment: gloved hand touched to aluminium foil
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Damage from argon ions

Name of directory: Dmg_Ion
Proper name: Damage from argon ion beams
Purpose of spectra: To reveal the typical changes that occur to various materials that are exposed to argon ion beams. The changes range from removal of surface contamination to degradation of chemical composition of the bulk material.

Overview: Argon ion beam etching of various materials produces various effects. Some materials suffer chemical degradation, while other materials are simply cleaned by argon ion beam etching. The reasons for the various behaviors are not yet fully defined.

Materials: C, CdO, CuO, MoO₃, MoS₂, Si, Si₃N₄, SnO₂, TiO₂, WO₃, Y₂O₃, ZrO₂

Observations: Ion beam etching clearly causes some materials to lose one or more elemental components. The result appears as a reduction process. In some cases the XPS signals become broader which indicates the presence of different species. In the case of silicon, it appears that the peak broadening is due to the production of regions with different electron densities which are most likely due to the production of different amorphous structures.

Number of materials: 12
Number of spectra: >90
Form of sample: pressed powders, crystals, paper, wafers
Electrical behavior: various
Class of material: inorganic and semiconductor
Special treatment: powders were pressed into thin 3mm diameter disks
Charge compensation: yes, flood gun (ca. 4 eV) as needed
Ion etching/cleaning: yes, beam voltage varied from 2-5 KeV
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Damage from flood gun electrons

Name of directory: Dmg_Elec
Proper name: Damage from flood gun electrons
Purpose of spectra: To study the damage caused by low voltage electrons that are emitted by the flood gun used to compensate charging.

Overview: Low voltage (1-20 eV) electrons which originate from a flood gun have been clearly found to damage a few materials, which are mainly organic polymers. There is some evidence that flood gun electrons also damage a Molybdenum based catalyst, but that data is not documented in this data set. Low voltage electrons have the potential to break a wide variety of chemical bonds, but the damage is either minimal or localized to the very top layer. There seems to be a much greater chance for insulating materials to act as capacitors and to hold a potential that might or might not lead to breakdown of the sample surface chemistry.

Materials: Na₂S₂O₃ (hydrated), poly(acrylic acid) on aluminum foil, high density poly(ethylene) pellet, poly(ethylene terephthalate) pellet, poly(styrene) pellet, and poly(tetrafluoroethylene)

Observations: By comparison to work done by K. Siegbahn on Na₂S₂O₃ our results show a dramatic decrease in damage. The reason for this has not been studied. Our work on Na₂S₂O₃ focussed the advantage of using the mesh-screen to decrease or the amount of damage to Na₂S₂O₃. The mesh-screen was found to decrease the rate of damage by at least a factor of 6X. Poly(acrylic acid) on aluminium foil which was analyzed in two separate experiments with the flood gun turned OFF and ON. Poly(acrylic acid) was found to be damaged by the use of the flood gun. Long term exposure of Polystyrene to flood gun does not appear to cause any observable damage. Long term exposure of HDPE, PET, and Teflon to X-rays and flood guns produced damage which is attributed to the X-ray beam, but it is also possible that some of the damage was caused by the user of the flood gun, but it is doubtful that the flood gun caused any significant amount of damage.

Number of materials: 5
Number of spectra: >100
Form of sample: polymorphic crystal or thin films on aluminum or pellets
Electrical behavior: insulator (thin films on aluminum were conductive)
Class of material: inorganic and organic polymers
Special treatment: as received, deposited as thin film, or exposed bulk
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Damage from monochromatic X-rays

Name of directory: Dmg_Xray
Proper name: Damage from monochromatic X-rays
Purpose of spectra: To reveal the changes that occur to organic polymers and inorganic compounds as a function of exposure to monochromatic X-rays (and to some extent flood gun electrons).

Overview: Damage is perhaps better described as "change". This study was done to reveal the changes that occur due to long term (10-14 hr) exposure to monochromatic X-rays. Based on a reference book on polymer degradation (W. Schnabel) we learned that changes can be synergistically due to heat, electrons, X-rays, and Bremmstrahlung from non-mono sources. The Schnabel book also explained that hydrocarbon polymers can lose hydrogen, and that polymers with benzene rings are more stable to X-rays.

Materials: The polymers are described by their monomeric names: Acetal, Acrylic acid, Amide, Butene, Carbonate, HDPE (Ethylene), Iso-hexene, Kapton, Nitrocellulose based filter paper, Nylon 6, Acrylonitrile (PAN), Ethylene Oxide (PEO), Ethylene terephthalate (PET, Mylar), Methyl methacrylate (PMMA), Phenylene sulfide (PPS), Propylene (industrial grade), Vinyl acetate (PVA), Vinyl chloride (PVC), Vinylidene di-fluoride (PVDF), Styrene, Sulphone, Tetrafluoroethylene (Teflon). Two inorganic salts were also studied, i.e. CuSO₄ and K₂CrO₄.

Observations: The changes that occurred fell into two basic groups. Group 1 is described as the loss of one or more elements or a chemical species group. Group 2 is described as a rearrangement of the chemical bonds with or without the loss on one or more elements. We observed that HDPE and other pure hydrocarbons lost hydrogen and that there was a shift in BE peak max to lower BE indicating the formation of sp² (double bond) type carbons. We also observed that polymers with benzene rings and the cyano group (CN) were relatively stable to long term exposure. The X-ray energy is somehow absorbed by the benzene ring and CN group and dissipated in a "harmless" manner.

The two inorganic salts are known to be damaged fairly quickly by non-mono sources. Our work showed that these two inorganic salts suffered very little damage during a 12 hour exposure. Only the CuSO₄ sample showed a small bit of "reduction" as observed by a small shoulder at lower BE. The K₂CrO₄ sample did not experience any noted change.

Number of materials: 24
Number of spectra: >500
Form of sample: pellet
Electrical behavior: insulator
Class of material: organic polymers and 2 inorganic salts
Special treatment: polymer pellets were cut to expose fresh clean bulk
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Depth profile examples

Name of directory: Dpth-Pro
Proper name: Depth Profile Examples
Purpose of spectra: To give examples of depth profiles done which might help users to understand thin films or to decide what experimental conditions to use when performing a depth profile or to know what problems (damage) might occur.

Overview: Depth profiles examples are provided as a guide to doing depth profiles on other similar materials.

Materials: 304-SS, 316-SS, 430-SS, Ag/Cr, Al/acrylate, Al/AlGaP, Al/AlGaAs, Al/GaP, Al/GaSb, Al/TiSb, BiSrCaCuOx, C/CoNi, Cr/PET, Co/NbN, SiO₂/Si, GaAs, TiO₂/SiO₂/TiO₂ (laser mirror), magnetic tape, C/Cu, CrOx/Cr, SiOx/Si, Oil/steel, IC Bond Pad, Plasma treated Carbon, plasma treated polyester, SiCN/Si, SiOx/TiSi, TiN/Si

Observations: Damage depends on argon ion beam voltage and the angle of incidence. We have tried Xenon gas a few times, but did not notice any real difference. Based on our preliminary results, grazing angle of incidence may be a technique that deserves more study. Depth profiles on organic polymers mainly produce some sort of amorphotized carbon or graphite which etchs very slowly. Under certain conditions it is possible to get some limited chemical state information from organic polymers that contain esters or plasma treated layers. It seems best to float any thin film that contains a mixture of conductive and non-conductive layers which will minimize differential charging at the interfaces.

Number of materials: 43
Number of spectra: >5,000
Form of sample: multi-layered thin films
Electrical behavior: variable
Class of material: thin films
Special treatment: depth profiled, some samples were wrapped with Aluminum foil with a small hole to minimize charging. Some samples which had conductive and insulating layers were deliberately floated to avoid differential charging at the interfaces
Charge compensation: yes, flood gun (ca. 4 eV) as needed
Ion etching/cleaning: depth profile sequential etch/analyze mode was used
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe & S-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Diamond

Name of directory: Diamond
Proper name: Diamond
Purpose of spectra: To reveal the typical surface chemical composition of diamond and related types of carbon.

Overview: Diamond was analyzed before and after ion etching to observe the effects of mild ion beam etching. Various diamond-like-films (DLF) were studied to see if they resembled pure diamond which can be discerned by observing a sharp peak in the valence band region, which should not be confused with the Ar 3p signal produced by ion etching. Highly oriented pyrolytic graphite (HOPG) is an alternate form of carbon which is often the result of trying to produce diamond like films. The HOPG samples were freshly delaminated to expose a clean bulk surface.

Materials: Industrial grade diamond, diamond-like-films, and HOPG

Observations: Mild ion etching of freshly fractured industrial diamond produced an increase in the low BE C (1s) signal. Cleaning with solvents had no effect to simplify the complicated C (1s) spectrum of industrial diamond.

Number of materials: 9
Number of spectra: 50
Form of sample: crystalline and thin films
Electrical behavior: insulator or conductor
Class of material: inorganic
Special treatment: fractured in air or as received
Charge compensation: flood gun (ca. 4 eV) and mesh-screen used on diamond
Ion etching/cleaning: light etching done to observe damage effects
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Elements: Al - Lu

Name of directory: Elem_A-L

Proper name: Elements: Aluminium (Al) - Lutetium (Lu)

Purpose of spectra: To provide basic spectra and basic physics of the elements.

Overview: Spectra from pure elements provide the basis for understanding the physics of chemical compounds and they provide a reference point for chemical state identification. Most of these spectra were obtained when the author was still learning how to make reliable spectra. As a result this set of spectra are sometimes contaminated with carbon and oxygen which yielded valuable information, but may mask some of the physics of the pure elements. The error in the BEs of a few elements is as large as +/-0.15 eV due to mis-calibration of the energy scale. Please refer to our Ref_BE_1 directory for high quality, reliable spectra from pure elements which can be used as research grade spectra.

Valence band spectra are available for all materials. Auger signal spectra are often provided. High energy range spectra (1,000 to 1,400 eV) are normally provided. In many data sets the user will find energy loss regions to help study the energy loss process. There are always C (1s) and O (1s) spectra which helped us to learn the approximate BEs of carbides and initial state oxides or suboxides.

Materials: Ag, Al, Ar/C, Ar/B, As, Au, B, BN, BaCO₃, Be, Bi, Br (KBr), C, Ca, CaF₂, Cd, CeO₂, Cl (NaCl), Co, Cr, Cs (CsCl), Cu, Dy, Er, F (LiF), F (CaF₂), Fe, Ga, Gd, Ge, Hf, Hg, Ho, I (KI), In, Ir, K (KBr), KI, Kr/C, La₂O₃, Li, LiF, LiOH, Lu

Observations: Elements can be cleaned and left in cryopumped UHV for many hours in the 10(-9) torr range, but they will form various contaminants which appear to be carbides, hydrocarbons, carbonyls, oxides, and hydroxides that seem to form from long term exposure to the various gases in the cryopumped UHV. The freshly ion etched surface of many metals seems to be reactive enough to breakdown the gases (CO, H₂O, H₂, CO₂, etc.) in the UHV chamber.

Number of materials:	48
Number of spectra:	>450
Form of sample:	foils, chips, blocks
Electrical behavior:	conductor unless element is presented as a compound
Class of material:	metals, compounds
Special treatment:	scraped clean or fractured in air to expose bulk
Charge compensation:	if needed for compounds that are insulators
Ion etching/cleaning:	as needed to clean surface, except for compounds
Ref BE for Au (4f₇):	83.96 eV (+/-0.078)
Ref BE for Cu (2p₃):	932.47 eV (+/-0.078)
Ref BE for Cu (3s):	122.39 eV (+/-0.15)
Electron TOA:	90 degrees (maximum sampling depth)
Instrument used:	Surface Science Instruments X-Probe
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Elements: Mg - Zr

Name of directory: Elem_M-Z

Proper name: Elements: Magnesium (Mg) - Zirconium (Zr)

Purpose of spectra: To provide basic spectra and basic physics of the elements.

Overview: Spectra from pure elements provide the basis for understanding the physics of chemical compounds and they provide a reference point for chemical state identification. Most of these spectra were obtained when the author was still learning how to make reliable spectra. As a result this set of spectra are sometimes contaminated with carbon and oxygen which yielded valuable information, but may mask some of the physics of the pure elements. The error in the BEs of a few elements is as large as +/-0.15 eV due to mis-calibration of the energy scale. Please refer to our Ref_BE_1 directory for high quality, reliable spectra from pure elements which can be used as research grade spectra.

Valence band spectra are available for all materials. Auger signal spectra are often provided. High energy range spectra (1,000 to 1,400 eV) are normally provided. In many data sets the user will find energy loss regions to help study the energy loss process. There are always C (1s) and O (1s) spectra which helped us to learn the approximate BEs of carbides and initial state oxides or suboxides.

Materials: Mg, Mn, Mo, N (BN), Na (NaCl), Nb, Nd, Ni, O (K₂CrO₄), O (LiOH), P, Pb, Pd, Pr, Pt, Rb (RbOAc), Re, Rh, Ru, S, Sb, Sc, Se, Si, Sm, Sm (Sm₂O₃), Sn, Sr (SrCO₃), Ta, Tb, Te, Ti, Tl, Tm, V, W, Y, Yb, Zn, Zr.

Observations: Elements can be cleaned and left in cryopumped UHV for many hours in the 10(-9) torr range, but they will form various contaminants which appear to be carbides, hydrocarbons, carbonyls, oxides, and hydroxides that seem to form from long term exposure to the various gases in the cryopumped UHV. The freshly ion etched surface of many metals seems to be reactive enough to breakdown the gases (CO, H₂O, H₂, CO₂, etc.) in the UHV chamber.

Number of materials:	39
Number of spectra:	>350
Form of sample:	foils, chips, blocks
Electrical behavior:	conductor unless element is presented as a compound
Class of material:	metals, compounds
Special treatment:	scraped clean or fractured in air to expose bulk
Charge compensation:	if needed for compounds that are insulators
Ion etching/cleaning:	as needed to clean surface, except for compounds
Ref BE for Au (4f₇):	83.96 eV (+/-0.078)
Ref BE for Cu (2p₃):	932.47 eV (+/-0.078)
Ref BE for Cu (3s):	122.39 eV (+/-0.15)
Electron TOA:	90 degrees (maximum sampling depth)
Instrument used:	Surface Science Instruments X-Probe
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Etch rate calibration

Name of directory: EtchRate
Proper name: Etch rate calibration
Purpose of spectra: To check the etching rate of the ion gun which allowed us to estimate a relative etch rate for other materials.

Overview: Etch rate estimation based on the depth profile of thermally grown 1,000 Angstrom thick SiO₂/silicon wafer.

Materials: 1,000 Angstroms of SiO₂/Si wafer (thermally grown)

Observations: This material gave reliable etch rate results in general, but revealed various unexplained physics when ion etched. The sample did not appear to need a flood gun to control charging until the sample had been ion etched for the first time. The initial etch cycle produced a noticeable shift in all XPS signals which indicated some sort of charge buildup. At the SiO₂/Si interface this layered material often showed irregular shifting of the XPS signals which have been attributed to various island like effects. Studies by Hoffman and Zalar which used sample rotation while etching might reveal the truth.

Number of materials: 1
Number of spectra: 200
Form of sample: thin film
Electrical behavior: insulator layer (but still semi-conductive)
Class of material: thin film
Special treatment: none
Charge compensation: yes, flood gun (ca. 6-8 eV)
Ion etching/cleaning: yes, 2-4 KeV with argon ions
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X- & S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Etching of elements – long term

Name of directory: ElemEtch
Proper name: Pure elements exposed to repeated long term ion etching
Purpose of spectra: To reveal any artifacts that might occur from repeated long term ion etching of pure element. To generate high quality reliable wide scan, narrow scan, and valence band spectra for pure elements by repeated ion etching and measurement of the freshly cleaned surfaces.

Overview: Repeated long term ion etching was performed on pure elements to reveal any artifacts caused by the etching. This data set was also a practical way to obtain multiple spectra from clean elements which could be added together to give BE values that are based on repeated measurements which would make them more statistically valid. The reference energies of copper and/or gold were checked under various energy resolution conditions just prior to and just after each of these depth profile runs so as to maximize the reliability and accuracy of the BEs derived from the pure elements.

Materials: Ag, Al, As, Au, B, Be, Bi, C, Cd, Co, Cr, Cu, Dy, Er, Fe, Gd, Ge, Hf, Ho, In, Ir, Lu, Mg, Mn, Mo, Nb, Ni, Pb, Pd, Pt, Re, Rh, Ru, Sb, Sc, Se, Si, Sn, Ta, Tb, Te, Ti, Tl, Tm, V, W, Y, Yb, Zn, Zr

Observations: Repeated ion etching of some metals caused a very small energy shift (0.03 to 0.06 eV) towards lower BE when the first etch cycle data was compared to the last etch cycle data. For example: Copper (2p₃) was at 932.68 eV after the first etch cycle but appeared at 932.64 eV after the last etch cycle. This effect indicates that the surface of some metals has become more disordered and thus it is easier for the photoelectrons to escape the surface. This shift toward lower BE as etching was continued is most notable when comparing initial etch cycles with later etch cycles. The shift did not seem to be a progressive shift with more etching.

The Captur_1 directory contains data that, in effect, represent the opposite behavior. Some of the pure element signals exhibited a very small shift toward higher BE as the sample rested in UHV with no disturbance except for the accidental reaction with the gases in the cryopumped chamber. The Captur_1 data are indicative of a room temperature surface relaxation effect that is normally associated with high temperature heating of materials.

Number of materials: 50
Number of spectra: >3,000
Form of sample: metal foils or chips
Electrical behavior: conductor
Class of material: metals
Special treatment: scraped in air to remove native oxides
Charge compensation: none
Ion etching/cleaning: repeated ion etching just as in normal depth profiling
Ref BE for Au (4f₇): 83.98 eV (+/-0.05)
Ref BE for Cu (2p₃): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Flood gun effects on native oxides - part I

Name of directory: NtvOxFG1

Proper name: Study of flood gun effects on native oxides (part I)

Purpose of spectra: To study the effect of using a flood gun while analyzing native oxides that are grounded or floating.

Overview: Native Oxides offer XPS scientists a unique chance to try to determine reliable BEs for various metal oxides by allowing them to transfer the "traceability" of the BE of the pure metals to the BEs of the various native oxides that are present as very thin (10-70 Angstrom) layers on those pure metals. This is possible because the native oxides are either conductors or are thin enough that they might behave as though they are conductors even though they are actually insulators. This means that the electrons from the metal substrate should be able to move freely across these thin native oxide layers because the physics seem to support the free and easy transport of those electrons across those layers. This study was done to test that theory. Based on this study, it appears that we can assign reliable BEs to many native oxides after we are certain of the chemical composition of those native oxides. The problem is that we do not yet know if the main oxide signals are or are not due to the thermodynamically most stable oxides which is the basic assumption used in assigning chemical structures to native oxide films. If we can indeed safely assume that the major oxide component in a native oxide film is indeed the thermodynamically most stable oxide, then we can assign BEs to the oxide signals that are reliable and transferable to infinitely thick samples of those same oxides.

We have analyzed 45 naturally formed native oxides without any cleaning by simply mounting the samples and then collecting data. The data was collected by first analyzing the samples with the flood gun turned off. The next data set was collected by setting the flood gun to approximately 2 eV with a minimum current setting (ca. 0.5 microAmps). The next data set was collected by setting the flood gun to approximately 15 eV with almost maximum current setting (ca. 4.0 microAmps). The next two data sets were collected by mounting the native oxide on a thick insulator that was smaller in size than the metal sample. The floated sample was then exposed to 2 eV and ca. 0.5 microAmps current. The final data set on the floated samples was collected by setting the flood gun to 15 eV and ca. 4.0 microAmps.

Materials: Naturally formed "native oxides" of Ag, Al, As, Au, B, Be, Bi, C, Cd, Co, Cr, Cu, Fe, Ga, Ge, Hf, In, Ir, Lu, Mg, Mn, Mo, Nb, Ni

Observations: When the flood gun was applied to "grounded" native oxides, we observed several effects.

For native oxides of many transition metals, the flood gun had no effect on the oxide signals.

For native oxides of elements in the 2nd and 3rd columns of the periodic table we observed progressive shifting of the oxide signals towards lower BE as the flood gun was increased. This means that we observed a shift to lower BE for the "Beryllium Oxide" Be(1s) signal, the O (1s) and the C (1s) signals observed from XPS of the native oxide of beryllium. (As expected because it is a grounded true conductor, the beryllium metal Be (1s) signal did not shift.)

For native oxides of elements in columns 12-14 we observed a similar shift toward lower BEs as the flood gun was increased. Again, as expected, the pure metal signals did not shift.

The native oxides of certain elements showed various strange behaviors.

The native oxide of aluminum showed a strange sort of reversible, differential charging that appears to be due to "vertical" stratification of the electric potential. As the flood gun was increased the peak associated with the aluminum oxide not only moved to lower BE but it also became progressively broader (larger FWHM). When the flood gun voltage was set to 15 eV it was obvious that some of the aluminium oxide signal was at a BE lower than the BE of the pure metal.

The native oxides of hafnium and zirconium showed a different sort of unusual charging behavior. These elements showed a strange reversal in shifting as the flood gun was increased. When the flood gun was set to 2 eV the native oxide signals shifted toward lower BE just as observed for all other elements, but, when the flood gun was set to 15 eV, the XPS signals due to the native oxides shifted toward higher BE!

With more careful study of the data we observed that the C (1s) signal sometimes shifted slightly more than the O (1s) signal or the metal signal of the native oxides when the flood gun voltage was increased. This effect supports the previously mentioned vertical stratification of the electric potential of the flood gun electrons that strike (or are held by) the native oxide.

The study of the native oxides insulated by using teflon or glass substrates showed a simple linear response that was obvious and easy to understand. This implies that physics of the native oxides is complicated only when they are grounded.

Number of materials:	24
Number of spectra:	>300
Form of sample:	thin films on metal foils or chips
Electrical behavior:	conductor or semiconductor, except when the samples were deliberately insulated with teflon or glass
Class of material:	metals and metal oxides
Special treatment:	none
Charge compensation:	yes, flood gun (2-15 eV, min-max current settings) and nickel mesh-screen (80% T)
Ion etching/cleaning:	none
Ref BE for Au (4f7):	83.98 eV (+/-0.078)
Ref BE for Cu (2p3):	932.67 eV (+/-0.078)
Ref BE for Cu (3s):	122.45 eV (+/-0.15)
Electron TOA:	35 degrees
Instrument used:	Surface Science Instruments S-Probe (model 2703)
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Flood gun effects on native oxides - part 2

Name of directory: NtvOxFG2

Proper name: Study of flood gun effects on native oxides (part 2)

Purpose of spectra: To study the effect of using a flood gun while analyzing native oxides that are grounded or floating.

Overview: Native Oxides offer XPS scientists a unique chance to try to determine reliable BEs for various metal oxides by allowing them to transfer the "traceability" of the BE of the pure metals to the BEs of the various native oxides that are present as very thin (10-70 Angstrom) layers on those pure metals. This is possible because the native oxides are either conductors or are thin enough that they might behave as though they are conductors even though they are actually insulators. This means that the electrons from the metal substrate should be able to move freely across these thin native oxide layers because the physics seem to support the free and easy transport of those electrons across those layers. This study was done to test that theory. Based on this study, it appears that we can assign reliable BEs to many native oxides after we are certain of the chemical composition of those native oxides. The problem is that we do not yet know if the main oxide signals are or are not due to the thermodynamically most stable oxides which is the basic assumption used in assigning chemical structures to native oxide films. If we can indeed safely assume that the major oxide component in a native oxide film is indeed the thermodynamically most stable oxide, then we can assign BEs to the oxide signals that are reliable and transferable to infinitely thick samples of those same oxides.

We have analyzed 45 naturally formed native oxides without any cleaning by simply mounting the samples and then collecting data. The data was collected by first analyzing the samples with the flood gun turned off. The next data set was collected by setting the flood gun to approximately 2 eV with a minimum current setting (ca. 0.5 microAmps). The next data set was collected by setting the flood gun to approximately 15 eV with almost maximum current setting (ca. 4.0 microAmps). The next two data sets were collected by mounting the native oxide on a thick insulator that was smaller in size than the metal sample. The floated sample was then exposed to 2 eV and ca. 0.5 microAmps current. The final data set on the floated samples was collected by setting the flood gun to 15 eV and ca. 4.0 microAmps.

Materials: Naturally formed "native oxides" of P, Pb, Pd, Pt, Re, Rh, Ru, Sb, Sc, Se, Si, Sn, Ta, Te, Tl, V, W, Y, Zn, Zr

Observations: When the flood gun was applied to "grounded" native oxides, we observed several effects.

For native oxides of many transition metals, the flood gun had no effect on the oxide signals.

For native oxides of elements in the 2nd and 3rd columns of the periodic table we observed progressive shifting of the oxide signals towards lower BE as the flood gun was increased. This means that we observed a shift to lower BE for the "Beryllium Oxide" Be(1s) signal, the O (1s) and the C (1s) signals observed from XPS of the native oxide of beryllium. (As expected because it is a grounded true conductor, the beryllium metal Be (1s) signal did not shift.)

For native oxides of elements in columns 12-14 we observed a similar shift toward lower BEs as the flood gun was increased. Again, as expected, the pure metal signals did not shift.

The native oxides of certain elements showed various strange behaviors.

The native oxide of aluminum showed a strange sort of reversible, differential charging that appears to be due to "vertical" stratification of the electric potential. As the flood gun was increased the peak associated with the aluminum oxide not only moved to lower BE but it also became progressively broader (larger FWHM). When the flood gun voltage was set to 15 eV it was obvious that some of the aluminium oxide signal was at a BE lower than the BE of the pure metal.

The native oxides of hafnium and zirconium showed a different sort of unusual charging behavior. These elements showed a strange reversal in shifting as the flood gun was increased. When the flood gun was set to 2 eV the native oxide signals shifted toward lower BE just as observed for all other elements, but, when the flood gun was set to 15 eV, the XPS signals due to the native oxides shifted toward higher BE!

With more careful study of the data we observed that the C (1s) signal sometimes shifted slightly more than the O (1s) signal or the metal signal of the native oxides when the flood gun voltage was increased. This effect supports the previously mentioned vertical stratification of the electric potential of the flood gun electrons that strike (or are held by) the native oxide.

The study of the native oxides insulated by using teflon or glass substrates showed a simple linear response that was obvious and easy to understand. This implies that physics of the native oxides is complicated only when they are grounded.

Number of materials:	21
Number of spectra:	>250
Form of sample:	thin films on metal foils or chips
Electrical behavior:	conductor or semiconductor, except when the samples were deliberately insulated with teflon or glass
Class of material:	metals and metal oxides
Special treatment:	none
Charge compensation:	yes, flood gun (2-15 eV, min-max current settings) and nickel mesh-screen (80% T)
Ion etching/cleaning:	none
Ref BE for Au (4f7):	83.98 eV (+/-0.078)
Ref BE for Cu (2p3):	932.67 eV (+/-0.078)
Ref BE for Cu (3s):	122.45 eV (+/-0.15)
Electron TOA:	35 degrees
Instrument used:	Surface Science Instruments S-Probe (model 2703)
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Gas sensor device

Name of directory: Gas-Snsr
Proper name: Gas sensor devices for carbon monoxide
Purpose of spectra: To study the chemical composition of a gas sensor used to sense carbon monoxide which is produced by fires.

Overview: This study was done to help the inventor to study the surface chemical composition of the gas sensor which needed platinum at the surface to be effective.

Materials: alumina, PdFe wire, Pt coating

Observations: Based on the XPS results the inventor learned that he had to improve his method of depositing the platinum.

Number of materials: 7
Number of spectra: 36
Form of sample: mixed ceramic on a coil
Electrical behavior: insulator, except for coil
Class of material: inorganic
Special treatment: none
Charge compensation: yes, as needed with mesh-screen
Ion etching/cleaning: as needed to probe structure
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: typically 90 deg due to curved surface
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Name of directory: Glass
Proper name: Man-made glasses
Purpose of spectra: To reveal the typical surface chemical composition of various glasses and to reveal trends in a series of man-made glasses.

Overview: Most of these glasses are from a study by various students at Okayama University who attempted to synthesize new forms of glasses. These series provide some insight into the changes that occur when a series of oxides are mixed and heated in an attempt to produce a new kind of glass. The professors at Okayama University have written numerous papers on their efforts to produce glasses and have used XPS to assist their understanding of the synthetic materials they have produced.

Materials: Al₂O₃ (fused), Borosilicate glass, X:Y:Z series of CaF₂:P₂O₅:Al₂O₃, X:Y series of Cs₂O:SiO₂, X:Y:Z series of Na₂O:Cs₂O:SiO₂, X:Y:Z series of PbO:GeO₂:PbF₂, X:Y series of K₂O:SiO₂, X:Y series of Li₂O:SiO₂, X:Y series of Li₂O:TeO₂, X:Y series of Na₂O:SiO₂, X:Y series of Na₂O:TeO₂, X:Y:Z series of TeO₂:PbO:PbF₂, Normal Leaded (PbO) glass, Pyrex glass, SiO₂, Soda-lime glass, and Zirconia

Observations: Some of the glasses were ion etched after being analyzed to study preferential sputtering of the material. Some of the samples were too far from the mesh-screen which resulted in some differential charging.

Number of materials: 40
Number of spectra: >300
Form of sample: glass chips, fragments
Electrical behavior: insulating (unless otherwise noted)
Class of material: inorganic
Special treatment: fractured to expose fresh bulk
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Grazing X-rays effect

Name of directory: GrazingX
Proper name: Enhanced count-rate obtained by using grazing X-rays
Purpose of spectra: To reveal the enhanced count-rate available in some XPS systems which use mono X-rays.

Overview: This data set demonstrates that it is possible to increase the count-rate of some XPS systems which use focused mono X-ray beams by a factor as great as 500% (5X).

Materials: Ag/PET, NaCl crystal, Ta₂O₅

Observations: Depending on surface roughness the count-rate can be increased by 2-5X for many smooth surfaced materials which are positioned so that the X-ray beam grazes the surface. The reason for the increase is the increased probability of a X-ray photo striking a atom while still in the filed of view of the analyzer. The increase does not depend on material as far as we have seen. It mainly depends on surface roughness.

Number of materials: 3
Number of spectra: 90
Form of sample: thin film and crystal
Electrical behavior: conductor and insulator
Class of material: metal and inorganic salt
Special treatment: Ag surface was ion etched clean
Charge compensation: yes, flood gun (ca. 4 eV) for insulator only
Ion etching/cleaning: yes
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Halides

Name of directory: Halide
Proper name: Binary inorganic halides
Purpose of spectra: To reveal the typical surface chemical composition of binary organic halides.

Overview: none

Materials: CaF₂, CsBr, CuCl, KBr, KCl, KI, LiF, NaCl, TbF₃

Observations: Halides have complex valence band structures that might contain various exciton related information.

Number of materials: 10
Number of spectra: >100
Form of sample: single crystals, polymorphic crystals, and powders
Electrical behavior: insulator (except for CuCl)
Class of material: inorganic
Special treatment: freshly fractured in air or pressed into thin 3mm diameter disks
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Hard disk lubrication studies – part 1

Name of directory: HD_Lube1
Proper name: Line profiles of lubrication on hard disk surface
Purpose of spectra: To check for the uniform distribution of the fluoro-ether lubricant that is used on hard disk surfaces.

Overview: The uniform distribution of lubricant over a hard disk surface is critical to the lifetime of the hard disk. ESCA (XPS) used to be used as a QC method to check that distribution, but it has been replaced by FT-IR which is much faster but still depends on XPS for its initial calibration. Useful lubricant thickness is estimated to be between 10 and 30 angstroms of lubricant.

Materials: hard disk plates coated with fluoro-ether lubricant

Observations: The samples studied here were fairly uniform and represent well made disks.

Number of materials: 14
Number of spectra: 70
Form of sample: thin film
Electrical behavior: conductor
Class of material: mixed
Special treatment: none
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Hard disk lubrication studies – part 2

Name of directory: HD_Lube2
Proper name: Line profiles of lubrication on hard disk surface
Purpose of spectra: To check for the uniform distribution of the fluoro-ether lubricant that is used on hard disk surfaces.

Overview: The uniform distribution of lubricant over a hard disk surface is critical to the lifetime of the hard disk. ESCA (XPS) used to be used as a QC method to check that distribution, but it has been replaced by FT-IR which is much faster but still depends on XPS for its initial calibration. Useful lubricant thickness is estimated to be between 10 and 30 angstroms of lubricant.

Materials: hard disk plates coated with fluoro-ether lubricant

Observations: The samples studied here were fairly uniform and represent well made disks.

Number of materials: 42
Number of spectra: 84
Form of sample: thin film
Electrical behavior: conductor
Class of material: mixed
Special treatment: none
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Heat effects on materials

Name of directory: Heat_Eff

Proper name: Effect of heat on materials

Purpose of spectra: To study surface chemistry of materials that are heated.

Overview: Fresh bulk surface was exposed for these studies.

Materials: high purity (99.999%) aluminium pellet and a copper foil

Observations: Within a few minutes of heating at 100 C the aluminum sample suffered a modest increase in Al₂O₃ formation which led to differential charging and some charge-up. The copper foil changed color just slightly but then changed to black within a few minutes time with heat at about 600 C.

Number of materials: 2

Number of spectra: 20

Form of sample: pellet or foil

Electrical behavior: conductor (heating in air can form thick insulator)

Class of material: metal

Special treatment: heating to 100 C for various times

Charge compensation: none

Ion etching/cleaning: none

Ref BE for Au (4f₇): 83.96 eV (+/-0.078)

Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)

Ref BE for Cu (3s): 122.39 eV (+/-0.15)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Hydroxides

Name of directory: Hydroxid
Proper name: binary metal hydroxides
Purpose of spectra: To reveal the typical surface chemical composition of binary metal hydroxides.

Overview: Hydroxides are sometimes end products or intermediates in the oxidation of elements. They sometimes form carbonates by reacting with CO₂ in the air. They are most commonly formed by water reacting with pure elements. The number of commercially available hydroxides is limited so the number of hydroxides in this data set is thereby limited.

Materials: Al(OH)₃, Cd(OH)_x, Co(OH)₂, Cu(OH)₂, FeOOH, LiOH, Mg(OH)₂, and Ni (OH)₂

Observations: The BEs of hydroxides seem to be larger than oxides, but may be the same or similar to carbonates. Adsorbed water, which is a kind of hydroxide, seems to appear at 535-537 eV, but it is difficult to confirm this.

Number of materials: 8
Number of spectra: 60
Form of sample: powder or thin film in solution
Electrical behavior: insulator
Class of material: inorganic
Special treatment: pressed into thin 3mm diameter disks as needed
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Ion implanted materials

Name of directory: Ion_Impl
Proper name: Ion implanted materials
Purpose of spectra: To reveal the effects and depth distribution of implanting ions into various substrates.

Overview: Materials implanted with various ions undergo different chemical changes depending on the level of implanting and the chemical nature of the implanted ion. Ionic forms of oxygen, zirconium and zinc were implanted into the substrates listed in the materials category.

Materials: Oxygen, zirconium or zinc ions were implanted into Cr, Hf, Nb, W, Zr, Si, Fe, FeCr

Observations: Thermally stable oxides seem to form when the oxide implant layer moves to the surface region.

Number of materials: 12
Number of spectra: >300
Form of sample: implanted foil
Electrical behavior: conductor
Class of material: metal
Special treatment: ion implanted by Riken Institute at >20 KeV
Charge compensation: none
Ion etching/cleaning: depth profiling
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Laser-XPS research

Name of directory: LaserXPS
Proper name: Laser-XPS research
Purpose of spectra: To study the effects of CW laser on various materials in either a dynamic (simultaneous) mode or a static (sequential) mode.

Overview: We invented and patented a new technique which was intended to help reveal the presence or absence of species chemical groups that were susceptible to selected excitation by the different wavelengths provided by the CW dye and argon lasers. We did not observe the desired effect, but we did observe several phenomena that are potentially useful.

Materials: Au, BaO, CeO₂, Co, Cr, Cr₂O₃, Cu₂O, CuO, Fe, Fe₂O₃, GaAs, GaP, Ge, Graphite, InP, KBr, KCl, Mg, Mn, NiO, Poly(chlorostyrene), PET (Mylar), Poly(styrene), Poly(vinyl methyl ketone), Poly(vinyl naphthalene), S, Si, Si₃N₄, SiO₂, Sm₂O₃, TiO₂, YbaCuOx, ZnO

Observations: The UV lines of the Ar laser had enough energy to cause the Poly(vinyl naphthalene) to phosphoresce with a blue-white light. The dye laser could be used to improve charge control of KCl. The dye laser could clean the surfaces of dark colored materials by removing the hydrocarbon and/or the adsorbed water. The dye laser could promote valence electrons into the conduction band of semiconductors and cause the peaks to shift by 1-2 eV. The dye laser could cause reduction to metal states from oxides states for NiO and Cu₂O. The lasers was not observed to affect native oxides or white colored materials.

Number of materials: 44
Number of spectra: >650
Form of sample: wafers, pressed pellets, chips, foils
Electrical behavior: conductor, semi-conductor, and insulator
Class of material: metals, polymers, inorganics, semiconductors
Special treatment: fresh fracture, pressed into thin 3mm diameter disks as received
Charge compensation: flood gun (ca. 4 eV) as needed
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Lubricants

Name of directory: Lubricnt
Proper name: Lubricants
Purpose of spectra: To reveal the typical surface chemical composition of materials used as lubricants.

Overview: Lubricants are widely used to minimize friction. One popular lubricant is called silicone oil. It contaminants many materials and causes various problems, but is very useful as a lubricant.

Materials: MoS₂, WD-40 (a commercial spray lubricant), silicone oil

Observations: none

Number of materials: 3
Number of spectra: 9
Form of sample: chip and spray coating on gold coated plate
Electrical behavior: (conductor) due to thinness
Class of material: inorganic
Special treatment: freshly exposed bulk or sprayed on coating
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Magnetic recording materials

Name of directory: Mag_Mem
Proper name: Magnetic materials used magnetic recordings
Purpose of spectra: To study the surface chemical composition of materials used to produce magnetic recordings.

Overview: This collection of data reveals R&D efforts to improve magnetic recordings and their components. In one case there is a study of diamond coated sliders on a recording head. In other work there are tests done to see the effects of heating the aluminum substrate.

Materials: lubricated hard disks, aluminite disks, recording head (mainly CaTiO₃ or SrTiO₃), ferrite based tapes

Observations: XPS can be very useful to optimize the surface chemistry of materials used to produce magnetic recordings.

Number of materials: 16
Number of spectra: 80
Form of sample: thin films, disks, coated disks, recording heads, tapes
Electrical behavior: conductor
Class of material: mixed
Special treatment: none
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Natural minerals

Name of directory: Mineral

Proper name: Natural minerals (polymorphic crystals)

Purpose of spectra: To reveal the typical surface chemical composition of natural minerals. To look for BEs from pure binary oxides produced in nature. To obtain BEs from binary oxides with a minimum of charging effects which are available from smooth surfaces provided by freshly fracturing crystals.

Overview: We have been collecting natural minerals that should contain only 2-3 elements which represent materials that are often analyzed by XPS or used as natural sources of materials used by industry. Many of these minerals have contaminants that appear in various grades of the chemicals used in the chemical industry or semiconductor industry. Some of these natural mineral samples are actually very high quality, high purity crystals which would cost a lot of money to purchase, but are bought for very little money.

Materials: Almandine ($\text{Fe}_3\text{Al}_2(\text{SiO}_4)_3$), Anatase (TiO_2), Argentite (Ag_2S), Azurite ($\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$), Brookite (TiO_2), Calcite (CaCO_3), Cassiterite (SnO_2), Chrysoberyl (BeAl_2O_4), Cinnabar (HgS), Corundum ($\alpha\text{-Al}_2\text{O}_3$), Covellite (CuS), Cuprite (Cu_2O), Diaspore (AlOOH), Galena (PbS), Halite (NaCl), Hausmannite (Mn_3O_4), Hematite ($\alpha\text{-Fe}_2\text{O}_3$), Kunzite ($\text{LiAlSi}_2\text{O}_6$), Magnesite (MgCO_3), Opal ($\text{SiO}_2\text{-nH}_2\text{O}$), Orpiment (As_2S_3), Perovskite (CaTiO_3), Pyrite (FeS_2), Pyrope ($\text{Mg}_3\text{Al}_2(\text{SiO}_4)_3$), Realgar (As_2S_2), Rhodochrosite (MnCO_3), Rutiled-Quartz (SiO_2 with TiO_2), Rutile (TiO_2), Sapphire (Al_2O_3), Scheelite (CaWO_4), Spinel (MgAl_2O_4), Tantalite (Ta_2O_5), Xenotime (YPO_4), Zircon (ZrSiO_4).

Observations: Natural cuprite is the best source of Cu_2O . All other sources are contaminated with CuO or stabilizers such as SnO_2 or PbO_2 . Many inexpensive samples of natural minerals have various forms of Fe, Mg or Na contaminants.

Number of materials: 36

Number of spectra: >400

Form of sample: polymorphic crystals

Electrical behavior: insulators and conductors

Class of material: inorganic

Special treatment: freshly fractured in air just prior to analysis

Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)

Ion etching/cleaning: none

Ref BE for Au (4f7): 83.98 eV (+/-0.05)

Ref BE for Cu (2p3): 932.67 eV (+/-0.05)

Ref BE for Cu (3s): 122.45 eV (+/-0.1)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Nitrides

Name of directory: Nitride
Proper name: Metal nitrides
Purpose of spectra: To reveal the typical surface chemical composition of metal nitrides which are often used in the semiconductor industry.

Overview: Metal nitrides are widely used in the semi-conductor industry but suffer various problems such as auto-oxidation which changes their insulating powers.

Materials: AlN, BN, CrN, Si₃N₄, TiN

Observations: Si₃N₄ is readily oxidized and is difficult to analyze because the user normally wants an atom % ratio which can change if ion etching is used to remove the surface oxide. The same is true for the other nitrides as well. A study needs to be done on the man-made oxynitrides so that we can properly analyze the surface contamination and then understand the true chemical nature of the underlying nitrides.

Number of materials: 6
Number of spectra: >100
Form of sample: powders, chips, wafers, coatings
Electrical behavior: insulator
Class of material: inorganic
Special treatment: fresh fractured to expose bulk or ion etched to expose bulk or pressed into thin 3 mm diameter disks
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: (as needed to remove surface contaminants)
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X- & S-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Oxides - binary

Name of directory: Oxid_Bin

Proper name: Binary metal oxides – commercially pure (99.99+%)

Purpose of spectra: To reveal the typical surface chemical composition of binary metal oxides.

Overview: Nearly all of the oxides and sub-oxide samples were purchased from the Aldrich Chemical Co. as powders with very high purity, typically 99.99+% based on ICP analyses. Lot numbers, which were provided with the samples from Aldrich, are reported on each spectrum along with the purity statement. Aldrich normally supplies ICP summaries with their high purity materials.

These high purity powders were pressed into 3 mm diameter thin disks (<1 mm thick) by a technique which avoided contaminating the surface with iron (Fe) or chromium (Cr) metals which typically occurs by using the standard pressing method. To avoid contaminating the surfaces of the thin disks we used a shiny side of a freshly cleaned piece of aluminum foil (kitchen grade). (Cleaning was done with isopropanol or ethanol.) Each thin disk was bonded to a small dish by using silver paint to ensure conduction if the oxide behaved as a conductor or semi-conductor.

We have included spectra from natural minerals which are simple binary metal oxides and have kept their original mineral names.

Wherever possible we included sub-oxides if they were commercially available. Some sub-oxide samples were bought from other sources, i.e. Rare Metallics Co or Cerac. Those samples were reported to be 99+% pure, but XPS of the surfaces of those powders or chips suggest they were mainly or only the thermodynamically stable full oxide. Until new sub-oxide samples are analyzed from other sources, it is difficult to be certain of the BEs derived from those some of the sub-oxides.

Materials: AgO, Ag₂O, Al₂O₃, As₂O₃, Au₂O₃, B₂O₃, BeO, Bi₂O₃, CaO, CdO, CoO, Co₃O₄, CrO₃, Cr₂O₃, Cu₂O, CuO, FeO, a-Fe₂O₃, g-Fe₂O₃, Fe₃O₄, Ga₂O₃, GeO₂, HfO₂, HgO, In₂O₃, IrO₂, MgO, MnO, Mn₂O₃, MoO₃, Nb₂O₅, NiO, PbO, PbO₂, PdO, PtO₂-nH₂O, Re₂O₇, Rh₂O₃, RuO₂, Sb₂O₃, Sb₂O₅, Sc₂O₃, SiO, SiO₂, SnO, SnO₂, Ta₂O₅, TiO, Ti₂O₃, Tl₂O₃, VO₂, V₂O₃, V₂O₅, WO₃, Y₂O₃, ZnO, ZrO₂, Anatase (TiO₂), Brookite (TiO₂), Cassiterite (SnO₂), Corundum (Al₂O₃), Cuprite (Cu₂O), Hausmannite (Mn₃O₄), Hematite (a-Fe₂O₃), Rutile (TiO₂), Rutilated Quartz (SiO₂ with TiO₂), and Sapphire (Al₂O₃).

Observations: Based on the peak-fitting methodology used to peak-fit the entire set of binary oxides, we have observed a general trend which indicates that the FWHM of the metal signal, the C (1s), and the O (1s) signal are all nearly the same (i.e. FWHM = 1.0-1.3 eV) if charge compensation is good.

We have also observed that the FWHM of the hydrocarbon C (1s) signal seems to be a good indicator of whether or not the charge compensation is good or not so good. When the FWHM of the C (1s) is small (e.g. 1.0-1.3 eV), then the main metal signal and the O (1s) signal seem to be small. When the FWHM of the C (1s) is relatively large (e.g. 1.5-1.8 eV), then the FWHM of the main metal signal and the O (1s) signals also are relatively large (e.g. 1.5-2.3 eV).

Most dark colored oxides behaved as conductors. All white colored oxides behaved as true insulators.

Some metal oxides which were expected to behave as insulators were found to behave as conductors or semi-conductors. The cause of this effect is uncertain but may be related to the many defects that exist in powders that are pressed into thin hard, smooth disks, which was the standard method used to analyze powdered samples because that approach minimized charging problems and increased the count-rate without causing any observable contamination.

Number of materials: 80
Number of spectra: >900
Form of sample: powders or crystalline chips
Electrical behavior: insulator and conductor
Class of material: inorganic
Special treatment: pressed into thin 3mm diameter disks and bonded to a small metal dish by using silver (Ag) paint or freshly fractured if the sample was a natural mineral

Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Oxides - native on elements

Name of directory: Oxid_Ntv

Proper name: Native oxides of the elements

Purpose of spectra: To reveal the typical surface chemical composition of native oxides.

Overview: Includes wide scan spectra, and principal signal of element high energy resolution spectra, carbon (1s) high energy resolution spectra, and oxygen (1s) high energy resolution spectra found in/on naturally formed native oxides of the elements.

The native oxide films in this collection were thin enough (10-70 Ang) that it was possible to observe the pure metal under the native oxide. The 90 degree TOA helped to reveal the metal signal for a few of the materials.

The metals which formed very thick (>100 Ang) native oxides were scraped in air to allow a fresh native oxide to develop. Those metals were Mg, Pb, Sb, Tl, V, and Y.

The reason to analyze thin native oxides was to try to make a logical and traceable connection between the BE of the pure metal signal and the most thermodynamically stable oxide of each metal. In most cases it appears that it is reasonable to use the BEs of the oxides as the true BEs for the oxides, but in some cases (e.g. Al₂O₃, MgO) there is some difficulty to make a logical and traceable connection because the oxides, even freshly formed films, appears to act as true insulators despite being thin enough to expect electron tunneling through the oxide films.

Materials: Naturally formed "native oxides" on Ag, Al, As, B, Be, Bi, Cd, Co, Cu, Fe, Ga, Ge, Hf, In, Ir, Mg, Mn, Mo, Nb, Ni, Pb, Pd, Pt, Re, Rh, Ru, Sb, Sc, Se, Sn, Ta, Te, Ti, Tl, V, W, Y, Zn, and Zr.

Observations: Atomic percentage tables of surface composition reveal the natural oxidative tendencies of the elements and the tendencies of these elements to capture various gases from the air and/or various contaminants introduced to the surface from handling by the original chemical producers.

The tendency of the C (1s) BE of the adventitious hydrocarbons to be dependent on the native oxide substrate can be found by comparing these data. We also observed what appears to be a tendency for many materials to form carbonates but it is difficult to be certain.

Based on our rough analysis of the data and the rough reference data provided in the Handbook of XPS (Physical Electronics), it appears that the major oxide component of the native oxides tended to be the more thermodynamically stable oxide.

Number of materials:	41
Number of spectra:	200
Form of sample:	foils and chips and blocks
Electrical behavior:	conductor (oxide layer may be insulator)
Class of material:	mixed metal and inorganic
Special treatment:	none
Charge compensation:	none
Ion etching/cleaning:	none
Ref BE for Au (4f7):	83.96 eV (+/-0.078)
Ref BE for Cu (2p3):	932.47 eV (+/-0.078)
Ref BE for Cu (3s):	122.39 eV (+/-0.15)
Electron TOA:	90 degrees (maximum sampling depth)
Instrument used:	Surface Science Instruments X-Probe (model 206)
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Oxides – rare earth

Name of directory: Oxid_REO
Proper name: Rare Earth Oxides
Purpose of spectra: To reveal the typical surface chemical composition of rare earth oxides which were prepared as thin disks in the normal atmosphere of the laboratory.

Overview: Rare earth oxides easily capture CO₂ from the air and/or water to form carbonates and/or hydroxides. Therefore, the data in this directory represent data that is readily obtained in any lab and do not reflect the optimum results which could be obtained if a glovebox had been used.

Materials: CeO₂, Dy₂O₃, Er₂O₃, Eu₂O₃, Gd₂O₃, Ho₂O₃, Lu₂O₃, Pr₂O₅, Sm₂O₃, Tb₃O₇, Tm₂O₃, Yb₂O₃

Observations: Several REO, which were dark in color, behaved as conductors. Based on the maker's warnings these REOs did indeed easily collect CO₂ and/or water from the air during the time needed to press the pellets and enter the sample into the prep chamber. As a result the C (1s) spectra showed carbonate signals and the O (1s) signals should high BE peaks that correspond with the presence of carbonates and absorbed water.

Number of materials: 12
Number of spectra: 90
Form of sample: powders pressed into thin disks
Electrical behavior: insulators (except for those which were dark in color)
Class of material: inorganic
Special treatment: pressed into thin 3mm diameter disks in normal lab air
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.98 eV (+/-0.05)
Ref BE for Cu (2p₃): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Oxides – ternary (mixed oxides)

Name of directory: Oxid_Mix
Proper name: Ternary Oxides (Mixed Oxides)
Purpose of spectra: To reveal the typical surface chemical composition of ternary metal oxides (mixed oxides).

Overview: Ternary oxides are composed of 2 metallic elements and oxygen.

Materials: X:Y:Z series of PbO:GeO₂:PbF₂, K₂CrO₄, K₂Ti₄O₉, Li₂OteO₂, Li₂WO₄, Na₂OteO₂, Na₂S₂O₃, Na₂W₂O₇, Na₂WO₄, X:Y:Z series of TeO₂:PbO:PbF₂

Observations: none

Number of materials: 15
Number of spectra: 120
Form of sample: glasses
Electrical behavior: insulator
Class of material: inorganic
Special treatment: freshly fractured in air to expose bulk
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Paper, fiber, and ink samples

Name of directory: Papr&ink
Proper name: Paper, fiber, and ink samples
Purpose of spectra: To reveal the typical surface chemical composition of various types of papers, fibers, and inks.

Overview: The surface chemistry of papers and fibers used for printing or writing directly affects the sharpness of the lettering or pictures made on the papers and fibers. A wide variety of chemicals can be added to papers and fibers that improve the sharpness of the lettering and pictures. These chemicals must be present at the surface of at least one side. To understand the effect of these chemicals we have analyzed both sides of many of the papers and fibers in this collection so that the user can understand the chemistry needed to improve printing quality.

Some papers in this data set are designed to absorb gases from the air and to stop those gases from attacking (corroding) a material that is wrapped in those papers. These sorts of papers are used in the semiconductor industry and the jewelry business.

Some of the fibers (e.g. rice, wheat, tokusa) are included because one professor was studying the silicon nitride content of those fibers which should help makers to produce better printing paper for inkjet printers.

Materials: Alumitex wrapping paper, antistatic spray, Canon(Japanese) printer paper, cellulose powder, cleanroom paper, calendar paper, Coppertex wrapping paper, double-sided adhesive tape (3M Brand), envelop paper, Whatman filter paper, Fox River bond paper, Hoto (Japanese) printer paper, HP thermal printer paper, dried ink on calendar paper, HP inkjet paper for Paintjet, Kimwipe paper, Kokuyo (Japanese) printer paper, Asahi Lint-free paper, Nakabaya (Japanese) printer paper, nitrocellulose filter paper, Pilot (Japanese) printer paper, SilverSaver wrapping paper, Thermal printer paper, Tokusa stem, wax paper, wheat stem

Observations: The surface chemistry of the front side and the back side of various man-made papers and wraps are different.

Number of materials: 43
Number of spectra: >250
Form of sample: films
Electrical behavior: insulators
Class of material: organic
Special treatment: none
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.98 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Pellets (thin disks) from powders

Name of directory: Pellet_R
Proper name: Research on making pellets (thin disks) from powders
Purpose of spectra: To show the results of trying to find a quick easy, safe and clean method of producing thin disks which are easier to charge compensate and give stronger signal.

Overview: Differential charging of samples is directly linked with surface roughness. As a result powders are very often difficult to analyze by XPS. We have previously used double sided tape or Indium metal foil, and pressed the powders on to the tape or the Indium metal and leaving a large amount of the powder so that we could get better XPS data with less charging. Based on those results, we have experimented with a pellet press device that was designed to make KBr pellets (thin disks) for Infrared spectroscopy analyses. We purchased a hand operated press (Quik Handi-Press) which was made by the Spectra-Tech company and sold by the Aldrich Chemical Co.. We used that press to make thin disks which had smooth surfaces and showed minimal differential charging effects. The problem with this approach was that some of the powders would react with the stainless steel anvil by some unknown mechanism and the resulting thin disk ended up with traces of iron (Fe) or chromium (Cr) on the surface of the thin disk. We assumed that the iron or chromium contamination was due to a pressure-induced reaction whereby tiny particles were transferred onto the disk or there was a true solid-state reaction of some sort. Due to this problem we searched for a method that would stop the thin disks from being contaminated. The data in this directory are the results of our efforts which led us to use two materials that are very convenient and inexpensive. Those materials (aluminum foil cleaned with isopropanol or glycine paper) helped us to avoid the iron and chromium contamination problem.

Materials: Aluminum kitchen grade foil, copper foil, glycine (weighing) paper, high density poly(ethylene) film, Scotch Brand Magic Tape, Teflon film, and wax paper.

Observations: Aluminum kitchen grade foil was found, by trial and error process, to be an excellent choice for the production of thin disks. This was done by placing a freshly cleaned piece of it between the powder to be pressed and the stainless steel anvil of the mini hand press. Experiments showed that it was best to clean the surface of the shiny side of the aluminum foil with either isopropanol or ethanol to remove any contaminants just prior to using the foil. Even though the aluminum foil was usually the best choice, we did find that some oxides (powders) and other materials would react with the aluminum foil that made it impossible to separate the thin disk from the aluminum foil.

As an alternative, it was found that glycine (weighing) paper was another good choice, but it was found to sometimes transfer a trace amount of carbon and/or nitrogen to the surface of the thin disk.

Based on some rough observations, it seemed that the chance for the aluminum foil to stick to the thin disk was dependent on the amount of hand pressure used to press the thin disk. Based on some rough tests on the glycine paper, it seemed that the amount of carbon and nitrogen was also dependent on the amount of pressure used to make the thin disks.

Number of materials: 7
Number of spectra: 40
Form of sample: powders
Electrical behavior: insulators
Class of material: inorganic
Special treatment: pressed into thin 3 mm diameter disks
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none

Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Phosphides

Name of directory: Phosphid
Proper name: Metal phosphides
Purpose of spectra: To reveal the typical surface chemical composition of metal phosphides.

Overview: Metal phosphides have various uses in the semiconductor industry so we have studied them as received, freshly fractured to expose the bulk, and after ion etching to see the effects of ion etching. We were fortunate enough to obtain two different crystalline forms of GaP.

Materials: GaP <100>, Ga <111>, and InP

Observations: Ion etching causes a shift in the peaks due to some inherent change in the electronic structure which is due to either implanting of Argon ions or localized amorphization due to the ion etching.

Number of materials: 7
Number of spectra: >60
Form of sample: wafers
Electrical behavior: conductor
Class of material: semiconductor
Special treatment: freshly fractured to expose bulk or ion etched
Charge compensation: none
Ion etching/cleaning: used to show effects of ion etching
Ref BE for Au (4f7): 83.99 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Phosphorus silicate glass on silicon wafers

Name of directory: PSG_Si
Proper name: Phosphorus silicate glass on silicon
Purpose of spectra: To reveal the typical surface chemical composition of a series of phosphorus silicate glasses with different levels of phosphorus.

Overview: The concentration of phosphorus in phosphorus silicate glass is a key factor in determining how uniformly the PSG glass forms on top of the silicon.

Materials: Phosphorus doped silicate glass with phosphorus concentrations ranging from 0% to 10%.

Observations: none

Number of materials: 9
Number of spectra: 58
Form of sample: wafers
Electrical behavior: insulator
Class of material: inorganic
Special treatment: rinsed in dilute HF for 1 minute
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.98 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Polymers – part 1

Name of directory: Polymer1
Proper name: Polymers
Purpose of spectra: To reveal the typical surface chemical composition of highly purified polymer films.

Overview: These samples were prepared and analyzed by the scientists at the National ESCA Center for Surface Chemical Analysis at the University of Washington under the direction of Buddy Ratner and David Castner on an SSI XPS system.

Materials: poly-ethylene (PE), poly-vinyl chloride (PVC), poly-vinylidene di-fluoride (PVDF), poly-tetrafluoroethylene (PTFE), poly-styrene (PS), poly-a-methyl styrene (AMPS), poly-4-methyl styrene (4MPS), poly-4-octylstyrene (POS), poly-4-hydroxystyrene (PHS), poly-4-hydroxystyrene-derviatized with trifluoro acetic anhydride, poly-4-ethoxystyrene (PES), poly-4,4'-dimethoxy benzophenone (4DBP), poly-ether ether ketone (PEEK), poly-ethylene terephthalate (PET), poly-ethyl acrylate (PEA), poly-mehtyle acrylate (PMA), poly-methyl methacrylate (PMMA) on copper, poly-ethyl methacrylate (EMA), poly-2-hydroxyl methacrylate (HEMA), poly-trimethyl silane hydroxyethyl methacrylate (CLMA), poly-ethylene glycol (PEG), poly-propylene glycol (PPG), poly-tetramethylene glycol (PTMG), poly-vinyl alcohol (PVA), Biomer™, poly-methylene diisocyanate/propane-diamine copolymer (MDPD), poly-methylene diisocyanate/butane-diol copolymer (MDBD), poly-methylene diisocyanate/propane-diamine/butane-diol terpolymer (MDBP), poly-dimethyl siloxane (PDMS) and Whatman™ filter paper (cellulose)

Observations: The University of Washington group used a 284.6 eV value as the hydrocarbon C (1s) BE. Based on our research XPS International prefers to use a 285.0 eV value for the C (1s) BE of sp³ type hydrocarbons.

Number of materials: 30
Number of spectra: 104
Form of sample: thin films
Electrical behavior: insulators
Class of material: organic polymers
Special treatment: cast into thin films after extensive purification
Charge compensation: yes, flood gun
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: National ESCA Center for Surface Chemical Analysis
Various students at the University of Washington under the guidance of Prof. Buddy Ratner & Dr. David Castner

Polymers – part 2

Name of directory: Polymer2

Proper name: Polymers

Purpose of spectra: To reveal the typical surface chemical composition of organic polymers as received and as a function of time that the polymer is exposed to mono X-rays for >10 hours.

Overview: This data set contains polymers that were studied as received and also as a part of a X-ray induced damage study which was to be compared to the results obtained by Ishitani (Toray Research Center, Japan) who used a non-mono XPS system to study some of the same polymers.

Damage is perhaps better described as "change". This study was done to reveal the changes that occur due to long term (10-14 hr) exposure to monochromatic X-rays. Based on a reference book on polymer degradation (W. Schnabel) we learned that changes can be synergistically due to heat, electrons, X-rays, and Bremmstrahlung from non-mono sources. The Schnabel book also explained that hydrocarbon polymers can lose hydrogen, and that polymers with benzene rings are more stable to X-rays.

Materials: The polymers used for the X-ray damage study are described by their monomeric names: Acetal, Acrylic acid, Amide, Butene, Carbonate, HDPE (Ethylene), Iso-hexene, Kapton, Nitrocellulose based filter paper, Nylon 6, Acrylonitrile (PAN), Ethylene Oxide (PEO), Ethylene terephthalate (PET, Mylar), Methyl methacrylate (PMMA), Phenylene sulfide (PPS), Propylene (industrial grade), Vinyl acetate (PVA), Vinyl chloride (PVC), Vinylidene di-fluoride (PVDF), Styrene, Sulphone, Tetrafluoroethylene (Teflon). Most of these polymers were obtained in powder form as part of a sample kit of 100 different polymer samples purchased from the Scientific Polymer Products Company.

The other polymers, which were studied just as reference spectra, are: Gladwrap (brand name), Low density linear poly(ethylene) (Lldpe), Nomex (brand name), printed circuit board anti-static bag (Pcb_bag), poly(4-chlorostyrene) (Pcl_ar) irradiated by argon laser, poly(ethylene) interface (Pe_if), industrial grade poly(propylene) as received (Pp_as recd), fresh exposed bulk of industrial grade poly(propylene) (Pp_bulk), control sample of poly(styrene) (Ps_contr), poly(styrene) after exposed to Gamma radiation (Ps_gamma), poly(styrene) after oxidation (Ps_ox), poly(styrene) after being oxidized and exposed to Gamma radiation (Ps_ox_gm), poly(vinylnaphthelene) exposed to UV laser (Pvn_uv), poly(vinylpyridine), Saran, dimethyl silicone, and Ziploc (brand name)

Observations: The changes that occurred fell into two basic groups. Group 1 is described as the loss of one or more elements or a chemical species group. Group 2 is described as a rearrangement of the chemical bonds with or without the loss on one or more elements. We observed that HDPE and other pure hydrocarbons lost hydrogen and that there was a shift in BE peak max to lower BE indicating the formation of sp² (double bond) type carbons. We also observed that polymers with benzene rings and the cyano group (CN) were relatively stable to long term exposure. The X-ray energy is somehow absorbed by the benzene ring and CN group and dissipated in a "harmless" manner.

Many polymers are contaminated at the surface of the pellet or final film by silicone oil and or various agents that inhibit "caking" or "static" charge-buildup or "drying agents" or "slip agents". These agents appear at the surface because they act as foreign bodies that are push to the surface of a polymer solution because they disrupt the regular structure of the polymer film which is influenced by various electrical properties.

Number of materials:	48
Number of spectra:	>600
Form of sample:	pellets, beads, films, powders
Electrical behavior:	insulators (unless made as a thin film on aluminium)
Class of material:	polymer
Special treatment:	freshly cut with a cleaned razor to expose pure bulk
Charge compensation:	yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning:	none
Ref BE for Au (4f7):	83.96 eV (+/-0.078)
Ref BE for Cu (2p3):	932.47 eV (+/-0.078)
Ref BE for Cu (3s):	122.39 eV (+/-0.15)
Electron TOA:	90 degrees (maximum sampling depth)
Instrument used:	Surface Science Instruments S-Probe (model 2703)
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Reliable scale calibrations for Ref_BE_1

Name of directory: Ref_BE_2
Proper name: Energy scale calibration checks and adjustments
Purpose of spectra: To check the reference energies of the Cu (2p3), Cu (3s), and Au (4f7) and to use those to make corrections in the energy scale if needed. These spectra were used to help produce reliable reference energies for the 52 elements listed in the directory called "Ref_BE_1".

Overview: These spectra are the proof that the energy scale of the SSI system was adjusted so that it produced reliable reference energies for the 52 elements listed in the directory called "Ref_BE_1". The step size for the Cu (2p3), Cu (3s) and Au (4f7) signals was set to 0.02 eV/step so as to maximize the accuracy and reliability of the results.

Materials: Copper (Cu) and Gold (Au)

Observations: none

Number of materials: 2
Number of spectra: >300
Form of sample: foil
Electrical behavior: conductor
Class of material: metals
Special treatment: copper was ion etched clean at >2 KeV for more than 60 seconds at a minimum, while the gold was ion etched for 20 seconds at minimum
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.98 eV (+/-0.02)
Ref BE for Cu (2p3): 932.67 eV (+/-0.02)
Ref BE for Cu (3s): 122.45 eV (+/-0.05)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Reliable secondary reference energies

Name of directory: Ref_BE_1

Proper name: Reliable secondary reference energies for pure elements

Purpose of spectra: To obtain reliable secondary reference energies and to provide user with wide scan spectra, narrow scan spectra, and valence band without any sort of contamination.

Overview: The objective of this data set was to provide users with wide scan spectra that were reliable and free of contamination with the exception of argon that was implanted by the ion etching process.

The objective of this data set was to also provide high energy resolution spectra of the main XPS signals so that the BE and FWHM of those signals could be used to peak-fit other materials. The BE of that main signal can be used as a reference energy because we checked and adjusted if necessary the reference energies for copper and/or gold juts prior to and just after collecting each set of spectra. The copper and gold spectra were collected with 0.02 eV per channel resolution (step size). To the best of our knowledge the BE derived from these 52 elements represent the best values available with the exception of the gold and copper and silver samples which have been carefully studied by the National Physical Laboratory in the UK.

This series of spectra were collected in response to a request from Cedric J. Powell at the National Institute of Science and Technology in the USA who carried out a mini-round robin study of BEs obtained by measuring elements under conditions that should provide reliable BEs. The results of that mini-round robin were published in the journal of "Applied Surface Science" Vol. 89, pp 141-149 (1995).

The objective of this data set was to also provide users with high energy resolution valence band spectra for the elements that were analyzed which may be useful to theoretical studies of the density of states (DOS) of pure elements.

Materials: Ag, Al, Ar/C, As, Au, B, Be, Bi, C, Cd, Co, Cr, Cu, Dy, Er, Fe, Ga, Gd, Ge, Hf, Hg, Ho, In, Ir, Kr, Lu, Mg, Mn, Mo, Nb, Ni, Pb, Pd, Pt, Re, Rh, Ru, Sb, Sc, Se, Si, Sn, Ta, Tb, Te, Ti, Tl, Tm, V, W, Y, Yb, Zn, and Zr.

Observations: We have found that ion etching to make an element clean causes that element, if it behaves as a semiconductor, to suffer a shift in its BE which is caused by the implantation of the argon ions. As an example, un-doped silicon give a Si (2p) BE of 99.80 eV before it is ion etched. After ion etching the un-doped Si (2p) BE drops to 99.40 eV. This behavior was also observed for B, Te, and Se, which are semiconductors.

By adding together the spectra that were obtained by repeatedly ion etching a pure element within a short time and with very high energy resolution conditions we were able to experimentally measure FWHM which may be the best values available by using a commercially made instrument.

Repeated ion etching of some metals caused a very small energy shift (0.03 to 0.06 eV) towards lower BE when the first etch cycle data was compared to the last etch cycle data. For example: Copper (2p_{3/2}) was at 932.68 eV after the first etch cycle but appeared at 932.64 eV after the last etch cycle. This effect indicates that the surface of some metals has become more disordered and thus it is easier for the photoelectrons to escape the surface. This shift toward lower BE as etching was continued is most notable when comparing initial etch cycles with later etch cycles. The shift did not seem to be a progressive shift with more etching.

Number of materials: 52
Number of spectra: 189
Form of sample: foils and chips and blocks and rods
Electrical behavior: conductor
Class of material: metals
Special treatment: scraped in air to expose fresh bulk
Charge compensation: none
Ion etching/cleaning: most samples were repeatedly ion etched to keep surface clean while some samples were ion etched for 30-40 minutes one day and then let in UHV overnight and etched again for 5 minutes to produce clean surface that would stay clean for 1 hour

Ref BE for Au (4f7): 83.98 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Residues

Name of directory: Residue
Proper name: Residues from various solutions
Purpose of spectra: To reveal the typical surface chemical composition of residues left by tap water and other solutions used to clean or protect glass.

Overview: A very small study of residues.

Materials: Armorall silicone oil protective solution. Microlab cleaning solution that should remove silicone oil, and tap water residues from California

Observations: None.

Number of materials: 4
Number of spectra: 26
Form of sample: thin film
Electrical behavior: insulator
Class of material: inorganic
Special treatment: solution allowed to concentrate by evaporation
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Semiconductor materials

Name of directory: SemiCon1
Proper name: Semiconductor materials (cleaved or etched or as rec'd)
Purpose of spectra: To reveal the typical surface chemical composition of semiconductors in various states of preparation.

Overview: The study of semiconductors is critical to be able to understand problems in production and how to develop new devices. The spectra in this directory are useful for those purposes. We have included valence band spectra which are very important to the semiconductor scientists because they reveal the subtle physics of the conduction band.

A second directory called "SemiCon2" includes metals and insulator materials that are commonly used in the semiconductor industry but are not semiconductive. These spectra act as support information. Many of our semiconductor samples were generously provided by the large companies here in Japan who make and sell semiconductor samples. Their names are listed in each individual data-file. The doping nature and doping level of many of our samples is unknown, but a few data-files do provide that kind of useful information.

Materials: AlGaAs, AlN, BeO, BN, C, CdO, CdSe, Cu₂O, CuCl, Diamond, GaAs, GaInAs, GaP (100), GaP (111), GaSb, GeSe, GeSe₂, HgS, HgTe, HOPG, InP, InSb, InSnOx (ITO), n-Si, p-Si, undoped Si, NBS p-Si, NiO, Pb₂O₃, PbO₂, PbO, PbS, SbTe, Se, Si₃N₄, SnO₂, Te, WO₃, ZnO.

Observations: 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. We have observed only a subtle energy difference between n-Si and p-Si because our samples were not heavily doped. As a result we did not observe the large 0.8 eV shift difference that other groups have observed.

Number of materials: >70
Number of spectra: >650
Form of sample: wafers, chips, powders
Electrical behavior: semiconductor
Class of material: semiconductor
Special treatment: pressed into thin 3mm diameter disks if in powder form
cleaved in air to expose fresh bulk if in wafer form
ion etched to see the effects of etching on composition and chemical shifts
Charge compensation: flood gun not used because it may bias the BEs
Ion etching/cleaning: as needed to study chemical shifts and physics
Ref BE for Au (4f7): 83.98 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Semiconductors - related materials

Name of directory: SemiCon2
Proper name: Semiconductor related materials
Purpose of spectra: To reveal the typical surface chemical composition of materials that are not semiconductive but are used in the production of semiconductor devices.

Overview: The study of semiconductors is critical to be able to understand problems in production and how to develop new devices. The materials analyzed in this directory are used for the semiconductor industry but are not semiconductive. These spectra act as support information.

Materials: Ag, Al, Al₂O₃, Al(OH)₃, Ar, As, As₂O₃, Au, Au₂O₃, B, BeO₃, BeO, C, Diamond, Cr, Cu, Cu(OH)₂, Cu₂O, CuO, Ga, Ga₂O₃, GeO₂, HOPG, In, In₂O₃, MgO, Ni, NiO, Ni(OH)₂, Pb₂O₃, PbO, PbO₂, PdO, Pt, PtO₂, Si₃N₄, Silicone oil, SiO, SiO₂, SnO, SnO₂, Te, TeO₂, Ti, W, WO₃

Observations: none

Number of materials: 48
Number of spectra: >450
Form of sample: varied
Electrical behavior: conductors and insulators
Class of material: metals, inorganics
Special treatment: pressed into thin 3mm diameter disks if in powder form
cleaved in air to expose fresh bulk if in wafer form
ion etched to see the effects of etching on composition
and chemical shifts
Charge compensation: flood gun used as necessary with mesh-screen
Ion etching/cleaning: as needed to study chemical shifts and physics
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments X-Probe (model 206)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Silicides

Name of directory: Silicide
Proper name: Binary metal silicides
Purpose of spectra: To reveal the typical surface chemical composition of binary metal silicides.

Overview: Silicides are used in the semiconductor industry which needs to understand the electronic characteristics of silicides. We have analyzed only 2 silicides so far, but have analyzed them as received, after freshly exposing the bulk and after ion etching.

Materials: CrSi thin film, TiSi thin film

Observations: none

Number of materials: 2
Number of spectra: 50
Form of sample: thin films
Electrical behavior: conductor
Class of material: semiconductor
Special treatment: as received, freshly exposed bulk, or ion etched
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Sulfides

Name of directory: Sulfide
Proper name: Binary metal sulfides
Purpose of spectra: To reveal the typical surface chemical composition of binary metal sulfides.

Overview: A variety of binary metal sulfides are available as natural minerals in high purity. These minerals can be fractured and analyzed without any significant amount of contamination from the air. Many binary sulfides act as good conductors as long as the color is dark or black.

Materials: Ag₂S (Argentite), As₂S₃ (Orpiment), AsS (Realgar), CuS (Covellite), FeS₂ (Pyrite), MoS₂ (Molybdenite), PbS (Galena), TaS₂, and ZnS

Observations: None

Number of materials: 10
Number of spectra: 100
Form of sample: chips from natural minerals
Electrical behavior: conductor or insulator
Class of material: inorganic
Special treatment: freshly fractured in air just prior to analysis
Charge compensation: varied (when needed, used 4 eV FG with mesh-screen)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.98 eV (+/-0.05)
Ref BE for Cu (2p₃): 932.67 eV (+/-0.05)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Superconductors-high temperature ceramic

Name of directory: SuperCon
Proper name: High temperature ceramic superconductors
Purpose of spectra: To reveal the typical surface chemical composition of high temperature ceramic superconductors and related materials.

Overview: This data set includes just a few samples of superconductive mixed oxides. We have provided data from various Japanese sources in the as received state, scraped state, and freshly scraped state if possible.

Materials: BiSrCuOx (Tokyo Univ), BiSrCaCuOx, YBaCuOx (CPS Co.) and YBaCuOx 2115.

Observations: It was revealed by Richard Brundle (IBM) that it was necessary to scrape the surface of some of the oxides while the sample was inside UHV to be able to study the chemical species that seemed to be producing the superconductivity. We have also provided some results from our Laser XPS research which showed that a CW dye laser could be used to partially clean the surface of the sample. This cleaning was presumed to occur by a photo-thermal effect.

Number of materials: 5
Number of spectra: 80
Form of sample: crystalline or pressed powder
Electrical behavior: semiconductor or insulator
Class of material: inorganic
Special treatment: freshly scraped to expose bulk or pressed into thin 3mm diameter disks (exposed to CW laser for cleaning)
Charge compensation: if needed, flood gun (ca. 4 eV) and nickel mesh-screen
Ion etching/cleaning: as needed to study the sub-surface composition
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X- & S-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

System behavior checks

Name of directory: SystemChk

Proper name: Checks done on system behavior

Purpose of spectra: To reveal the behavior of the instruments under various conditions that should reveal the ability of the instruments to produce reliable results and to reveal the basic performance of the instruments used to produce the database.

Overview: The details provided by the spectra in this directory are summarized in the introduction to all of our handbooks and the paper version of the index to our complete library of XPS spectra. That summary can be downloaded from our FTP site at "xpsdata.com".

As a part of an international round robin test sponsored by the National Physical Laboratory in England, we submitted a set of spectra obtained from pure copper (Cu) that were measured at different pass energies and with different X-ray spot sizes. Those spectra were submitted in ASCII format to Dr. Martin P. Seah so that the "*instrument response function*" (transmission function) of the SSI X-Probe system (model 206) could be established. The results of that study are published in "Surface and Interface Analysis" Vol. 20, pp. 243-266 (1993)

As a part of an international round robin test sponsored by the National Institute of Science and Technology (NIST), we submitted a set of spectra obtained from the gold (Au), copper (Cu) and silver (Ag) samples supplied to us by the NIST for this study. Those spectra were submitted in ASCII format to Dr. Cedric J. Powell so that the instrument could be tested for "*reproducibility*" and "*repeatability*".

We have also determined: (A) the Signal/Background behavior of the S-Probe instrument, (B) the Signal/Noise behavior, (C) sensitivity to temperature changes, and (D) the effect of defocusing the monochromator crystal.

Materials: Ag/Si, Cu, Au

Observations: The random error checks performed for the NIST study have not yet been published, but the initial results indicated that the error due to random effects was nominal.

The focus of the SSI systems is very sharp and it is easy to decide if the sample is correctly focused by checking the count rate. The sharpness of this focus helps the user to avoid various energy scale and count-rate problems that occur in lense systems that allow a much large depth of field.

The Signal/Background ratio depends on pass energy settings. Signal/Background ratios were found to improve as the pass energy setting decrease.

We have also determined useful "exponent factors" that are used to modify the relative sensitivity factors (RSF) that are used in the SSI systems. Those RSF numbers are based on the photoionization cross-sections that were theoretically calculated by J. Scofield in 1976. We have tested the resulting Scofield based RSFs to see if they can used in a routine manner. Our results indicate that the Scofield numbers produce an error range that ranges from +/- 10% to +/-30% depending on the signal being used. We have found that the weaker XPS signals seem to be more susceptible to error. We have therefore suggested to the ASTM E-42 committee and the ISO TC/201 committee to study the Scofield RSFs to determine to what extent they are reliable especially since many users around the world are using the Scofield numbers.

The silver on silicon sample supplied by NIST was found to contain chlorine even after ion etching which may or may not have affected the results. That same sample had a surface roughness that was easy to observe through a 50X optical microscope.

Number of materials:	3
Number of spectra:	250
Form of sample:	foils
Electrical behavior:	conductor
Class of material:	metals
Special treatment:	as received or ion etched clean as per procedure
Charge compensation:	none
Ion etching/cleaning:	none
Ref BE for Au (4f7):	83.98 eV (+/-0.05)
Ref BE for Cu (2p3):	932.67 eV (+/-0.05)
Ref BE for Cu (3s):	122.45 eV (+/-0.1)
Electron TOA:	35 degrees (unless otherwise specified)
Instrument used:	Surface Science Instruments X- and S-Probe
X-ray source:	monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator:	B. Vincent Crist (XPS International, Inc.)

Titanates

Name of directory: Titanate

Proper name: Metal titanates

Purpose of spectra: To reveal the typical surface chemical composition of metal titanates.

Overview: Titanates are useful materials because their crystal structure allows other materials to be easily deposited on them. Titanates are used in the Semiconductor industry and the Hard Disk Magnetic Memory industry.

Materials: CaTiO₃, K₂Ti₄O₉, SrTiO₃

Observations: Easily cleaved and stay clean after cleaving (fracturing) in air.

Number of materials: 3

Number of spectra: 31

Form of sample: crystalline or polymorphic crystals

Electrical behavior: insulator

Class of material: inorganic

Special treatment: freshly fractured to expose bulk

Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)

Ion etching/cleaning: none

Ref BE for Au (4f₇): 83.98 eV (+/-0.05)

Ref BE for Cu (2p₃): 932.67 eV (+/-0.05)

Ref BE for Cu (3s): 122.45 eV (+/-0.1)

Electron TOA: 90 degrees (maximum sampling depth)

Instrument used: Surface Science Instruments S-Probe (model 2703)

X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)

Operator: B. Vincent Crist (XPS International, Inc.)

Transmission function studies

Name of directory: Transmis
Proper name: Transmission function studies
Purpose of spectra: To study the transmission function behavior (instrument response function) of the SSI XPS systems.

Overview: The transmission function of an instrument is important to correct for so that users can maximize the reliability of the quantitative results obtained from any XPS system. We have studied the transmission function of the SSI systems and have corrected for the transmission function effect and other effects by a trial and error method which produced a set of modified relative sensitivity factors that are based on Scofield's theoretically measured photoionization cross-sections. We have analyzed a variety of very high purity materials to determine if we had or had not corrected for the transmission behavior and produced useful RSF values.

As a part of an international round robin test sponsored by the National Physical Laboratory in England, we submitted a set of spectra obtained from pure copper (Cu) that were measured at different pass energies and with different X-ray spot sizes. Those spectra were submitted in ASCII format to Dr. Martin P. Seah so that the "*instrument response function*" (transmission function) of the SSI X-Probe system (model 206) could be established. The results of that study are published in "Surface and Interface Analysis" Vol 20, pp 243-266 (1993)

Materials: Copper (Cu) and Nickel (Ni) and zinc (Zn)

Observations: Our tests indicated that we could have quantitative results that were reliable to +/-10% of the expected values. We have tested the RSFs that were derived by this trial and error method and found that the uncertainties are somewhat larger when we measure non-principal XPS signals and signals that appear at very low BE (e.g. 0-30 eV) or very high BE (e.g. 1,150-1,450). The increase in uncertainty was estimated to be +/-20%.

Number of materials: 3
Number of spectra: 50
Form of sample: foil
Electrical behavior: conductor
Class of material: metal
Special treatment: ion etched until clean
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments X- & S-Probe
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Tribology studies

Name of directory: Tribolgy
Proper name: Tribology studies on metal bearings
Purpose of spectra: To reveal the typical surface chemical composition of metal bearing before and after being used.

Overview: These spectra are from real world materials used under harsh conditions with heavy friction that might cause material transfer or high levels of heat.

Materials: Wear Spot on Ball Bearing after Freon Cleaning, Normal Area on Ball Bearing (near wear marks), Wear Track area on Ball Bearing #2 (ion etched), Bearings #1 and #2 (as received), Normal Area on Race #1 (after 40 angstrom etch), Normal Area on Race #1 (as received), Wear Area on Race #1 (after 40 sec ion etch with Xe+), Showa NO.1 Bearing (as received), NO.2 Bearing (as received)

Observations: none

Number of materials: 6
Number of spectra: 50
Form of sample: balls or metal tracks
Electrical behavior: conductor (unless heavily contaminated with insulators)
Class of material: metal with lubricant
Special treatment: none
Charge compensation: none, unless needed
Ion etching/cleaning: ion etched after analyzing as received surface
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Tungstates

Name of directory: Tungstat
Proper name: Metal Tungstates
Purpose of spectra: To reveal the typical surface chemical composition of metal tungstates.

Overview: Sodium tungstate is a good source of WO₃ and tungsten metal. Pure crystals of Scheelite are used as scintillation counter phosphors for gamma-ray detectors

Materials: Li₂WO₄, Na₂W₂O₇, Na₂WO₄, CaWO₄ (Scheelite)

Observations: none

Number of materials: 4
Number of spectra: 33
Form of sample: polymorphic crystals
Electrical behavior: insulators
Class of material: inorganics
Special treatment: freshly fractures in air just prior to analysis
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

UV-ozone treatments of materials

Name of directory: UV_Ozone
Proper name: UV with Ozone treatments of materials
Purpose of spectra: To study the speed at which a surface becomes re-contaminated after being exposed to a UV-Ozone treatment.

Overview: The combined use of UV light and Ozone gas has been used to clean the surfaces of various materials, and in some cases to oxidize the surface. The purpose of this study was to see how long it would take for the cleaned surfaces to become dirty again and what kind of dirt might return.

Materials: Si₃N₄/glass and Ta₂O₅/glass

Observations: Almost no difference could be observed for the time delays between measurements. This means that the surface composition observed 5 minutes after exposure was almost the same as the surface composition 24 hour later.

Number of materials: 2
Number of spectra: 6
Form of sample: thin film
Electrical behavior: insulator
Class of material: inorganic
Special treatment: exposed to UV light and Ozone (O₃) gas at the same time at 1 atm pressure outside the XPS instrument
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f₇): 83.96 eV (+/-0.078)
Ref BE for Cu (2p₃): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 35 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Valence band spectra – elements

Name of directory: VB_Elem
Proper name: Valence band spectra from pure elements
Purpose of spectra: To reveal the band structure of the density of states of the elements which have been ion etched clean without any subsequent annealing or other treatment.

Overview: These spectra should be helpful to scientists who want to study the density of states in the valence band. Some spectra are provided with medium energy resolution and some are provided with high energy resolution. Higher energy resolution spectra would require a lot of time on a synchrotron system which is using high quality X-ray monochromators.

These same spectra are provided elsewhere in this database within datafiles that include data from pure elements. We have collected the valence band spectra into this directory just for convenience.

Materials: Ag, Al, Au, Be, Bi, C, Cd, Co, Cr, Cu, Fe, Hf, In, Ir, Mn, Mo, Nb, Ni, Pb, Pt, Rh, Ru, Sb, Si, Sn, Ta, Te, Ti, Tl, V, W, Y, Zn, Zr.

Observations: The quality of valence band data depends on the energy resolution settings to some extent. Higher energy resolution spectra require several hours time to obtain high quality signal/noise ratios. The data presented here are effectively practical grade data with medium energy resolution.

Number of materials: 37
Number of spectra: 39
Form of sample: metal foils (amorphous) and pressed powder (Ru)
Electrical behavior: conductor
Class of material: metal
Special treatment: ion etched clean
Charge compensation: none
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.98 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.075)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 35 or 90 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Valence band spectra - semiconductors

Name of directory: VB_Semic
Proper name: Valence band spectra from semiconductors & related materials
Purpose of spectra: To reveal the band structure of the density of states of semiconductors and related materials as received, after fracturing to expose the bulk, or after ion etching.

Overview: These spectra should be helpful to scientists who want to study the density of states in the valence band. Some spectra are provided with medium energy resolution and some are provided with high energy resolution. Higher energy resolution spectra would require a lot of time on a synchrotron system which is using high quality X-ray monochromators.

These same spectra are provided elsewhere in this database within datafiles that include data from semiconductors and related materials. We have collected the valence band spectra into this directory just for convenience.

Materials: Ag, Au, C, InP, Si, SiO,

Observations: The quality of valence band data depends on the energy resolution settings to some extent. Higher energy resolution spectra require several hours time to obtain high quality signal/noise ratios. The data presented here are effectively practical grade data with medium energy resolution.

Number of materials: 10
Number of spectra: 10
Form of sample: wafers and chips
Electrical behavior: semiconductor and conductors and insulators
Class of material: semiconductor, metal, inorganic
Special treatment: as received, fractured in air, or ion etched clean
Charge compensation: none
Ion etching/cleaning: etched to remove contaminants
Ref BE for Au (4f7): 83.98 eV (+/-0.05)
Ref BE for Cu (2p3): 932.67 eV (+/-0.075)
Ref BE for Cu (3s): 122.45 eV (+/-0.1)
Electron TOA: 35 or 90 degrees
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)

Zeolites

Name of directory: Zeolite
Proper name: Zeolites (as received and after treatment)
Purpose of spectra: To reveal the typical surface chemical composition of zeolites and zeolite related materials.

Overview: Zeolites are often used in the catalyst industry and for purification of various chemicals. Chemical makers often add some chemicals or process the natural or man-made zeolites to improve the efficiency of the zeolites. This directory includes various man-made and natural zeolites as received and after treatment.

Materials: Carbon on 4 different Zeolites, Mordenite, MS-5a, Msn-25, Platinum on zeolite, Talcum, Zeolite X (Ca,Na exchanged) (WE-884), Zeolite X (Na exchanged) [WE-894], Zeolite Y (Na exchanged) [Mizuka sieve Y-500], Zeolite (1 μ M, cubic) pellet (gc press), Black colored zeolite (uncrushed, single chip), White Zeolite (pressed into pellet, used SSI mesh), Zeolite ZSM-5 (not-treated, pressed into pellet, screen, 90 TOA)

Observations: Zeolites seem to be sensitive to X-rays and sometimes change from a white color to a light or dark yellow color in the area hit by the X-rays, which implies some "minor" but perhaps significant change.

Number of materials: 14
Number of spectra: 60
Form of sample: powder or pellet or crystalline chip
Electrical behavior: insulator
Class of material: inorganic
Special treatment: pressed into thin 3mm diameter disks if powder or freshly fractured to expose bulk
Charge compensation: yes, flood gun (ca. 4 eV) and nickel mesh-screen (80% T)
Ion etching/cleaning: none
Ref BE for Au (4f7): 83.96 eV (+/-0.078)
Ref BE for Cu (2p3): 932.47 eV (+/-0.078)
Ref BE for Cu (3s): 122.39 eV (+/-0.15)
Electron TOA: 90 degrees (maximum sampling depth)
Instrument used: Surface Science Instruments S-Probe (model 2703)
X-ray source: monochromatic aluminium (1486.7 eV, 8.393 Angstroms)
Operator: B. Vincent Crist (XPS International, Inc.)