Chemical Characterization Techniques of Qubits

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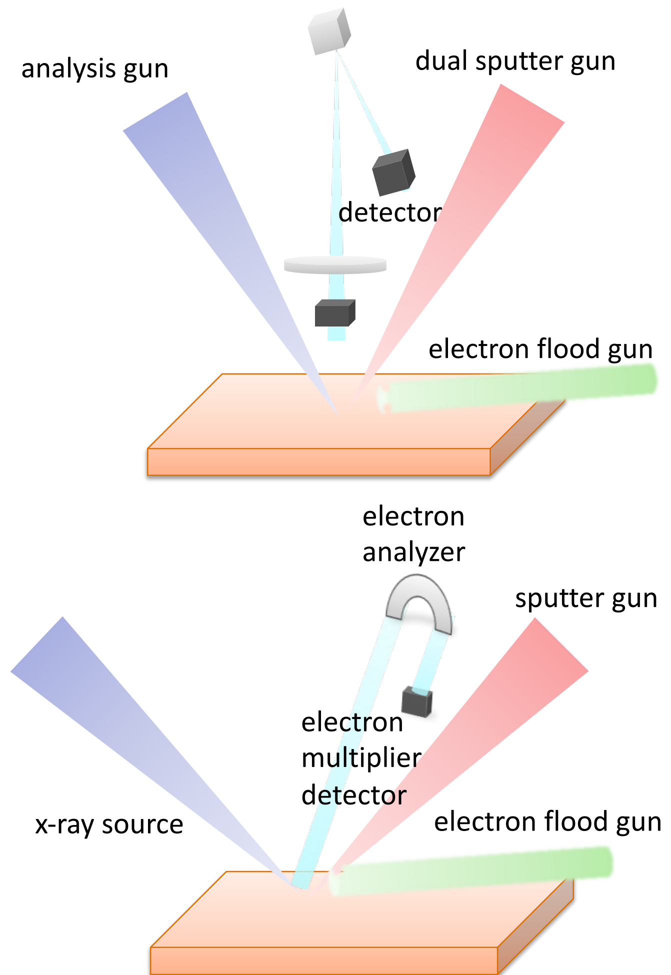
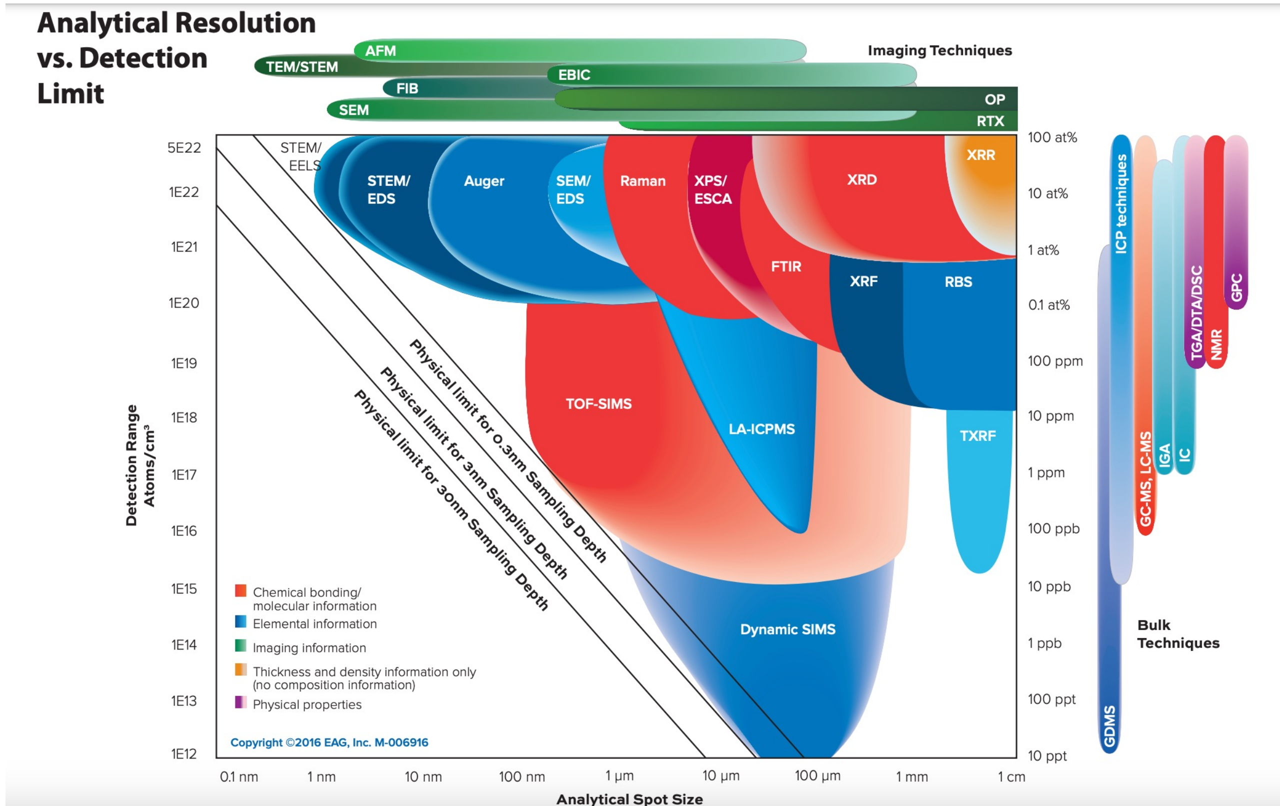
August 14th, 2023

Outline

- Overview of Chemical Characterization Techniques
- Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS)
- X-ray Photoelectron Spectroscopy (XPS)

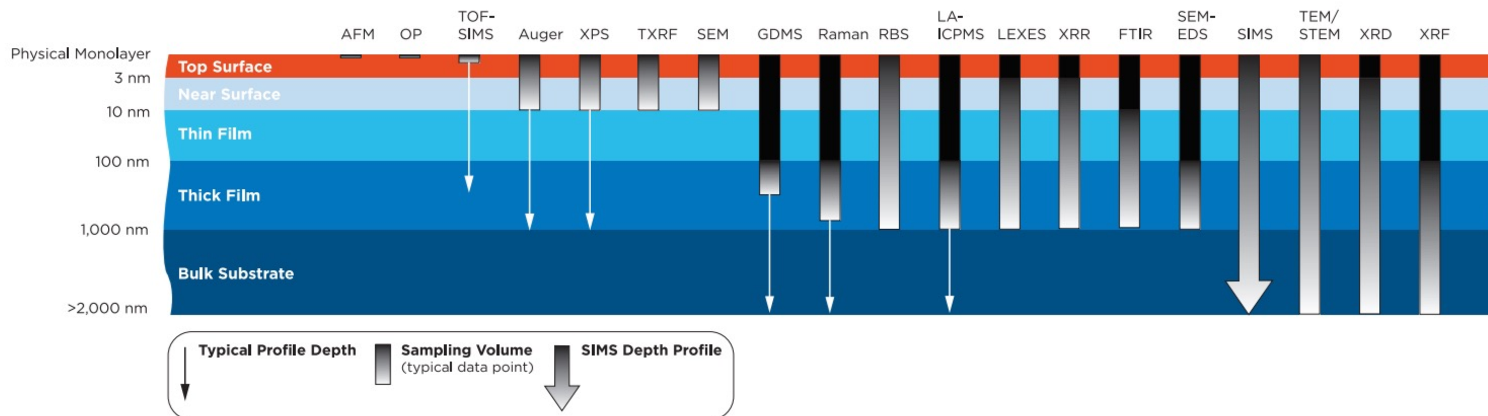


Chemical Characterization Techniques



Source: EAG

Chemical Characterization Techniques



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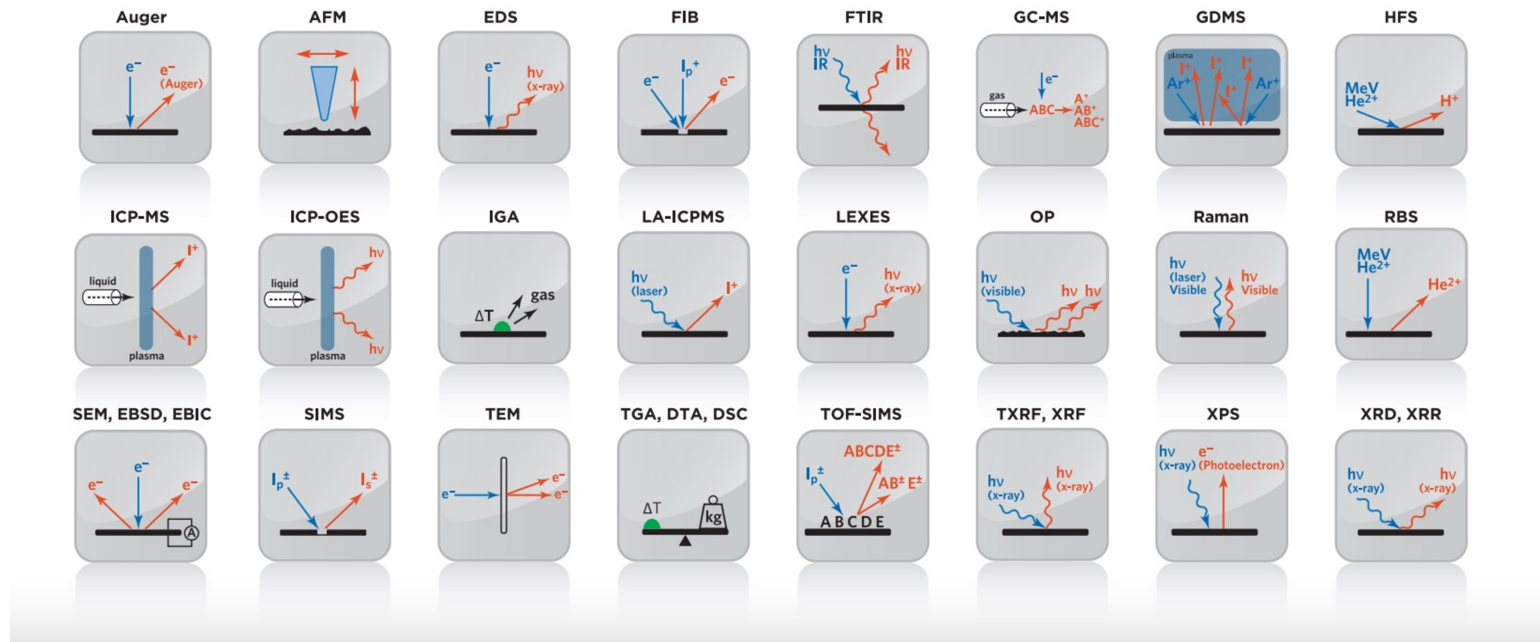
Chemical Characterization Techniques



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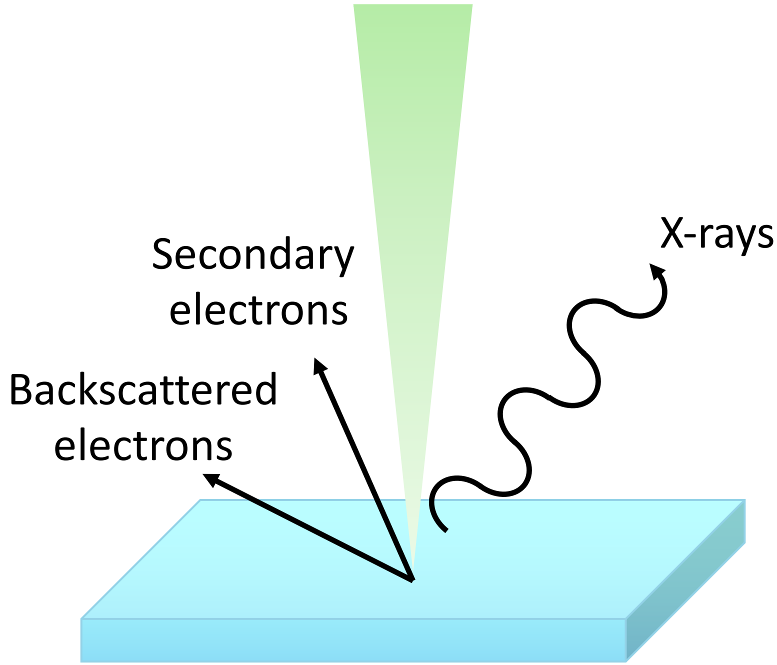
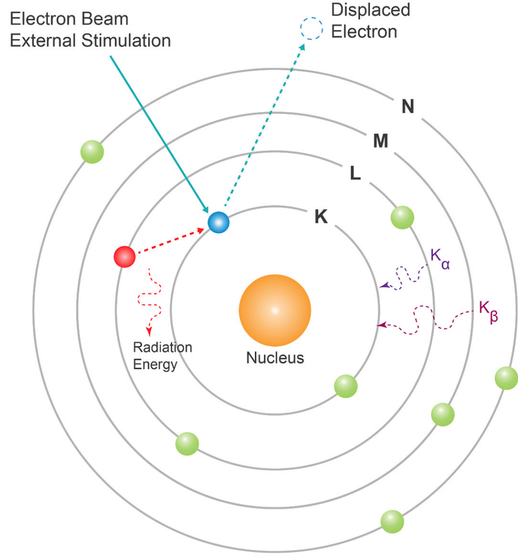
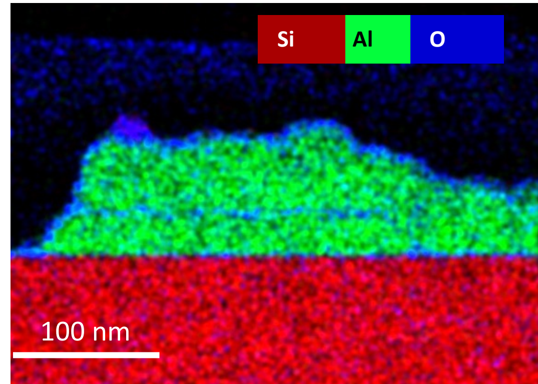
Chemical Characterization Techniques - EDS

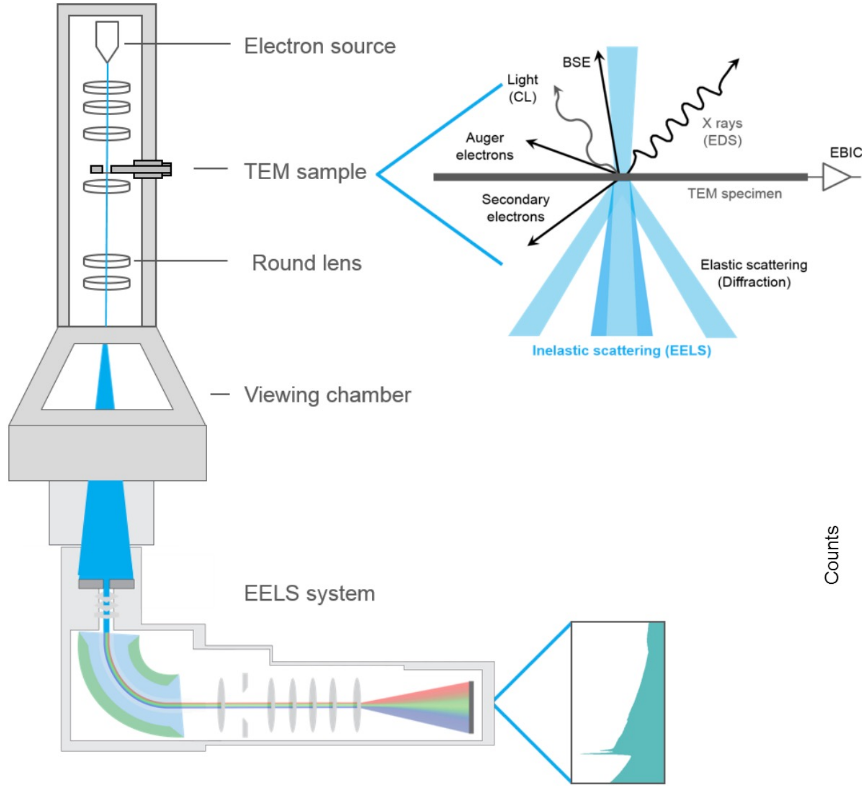




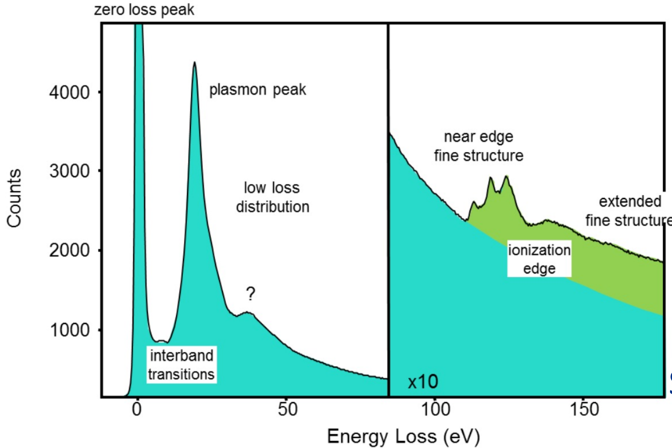


Courtesy of Prof. Lin Zhou

Chemical Characterization Techniques - EELS

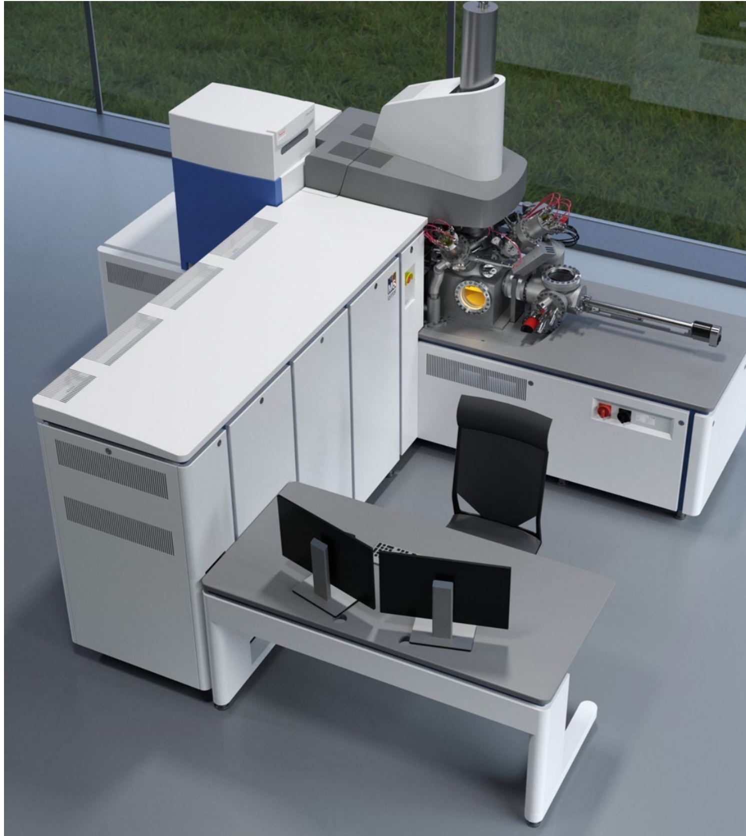


Bonding and oxidation state (density of unoccupied states)



Source: Gatan

ToF-SIMS



analysis gun

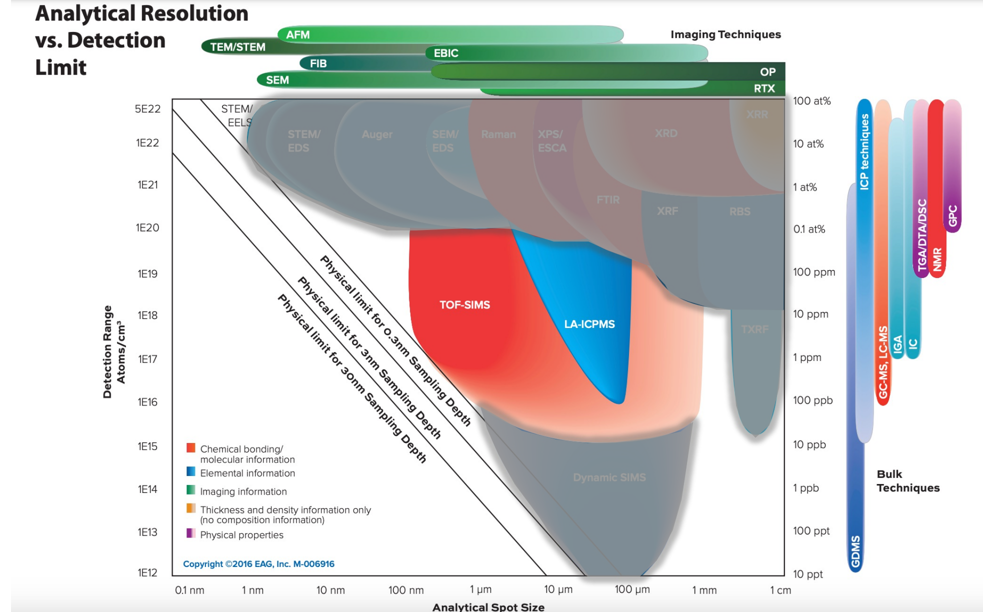
dual sputter gun

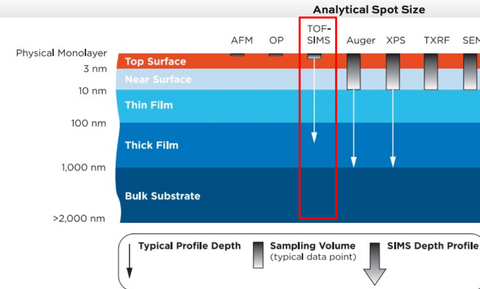
detector

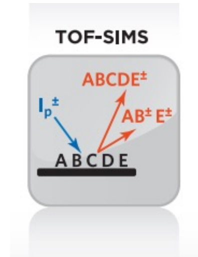
electron flood gun

ToF-SIMS: Basics

- Very sensitive surface analytical technique
- Provides elemental & molecular information
- 3D analysis
- Detection of low atomic number elements



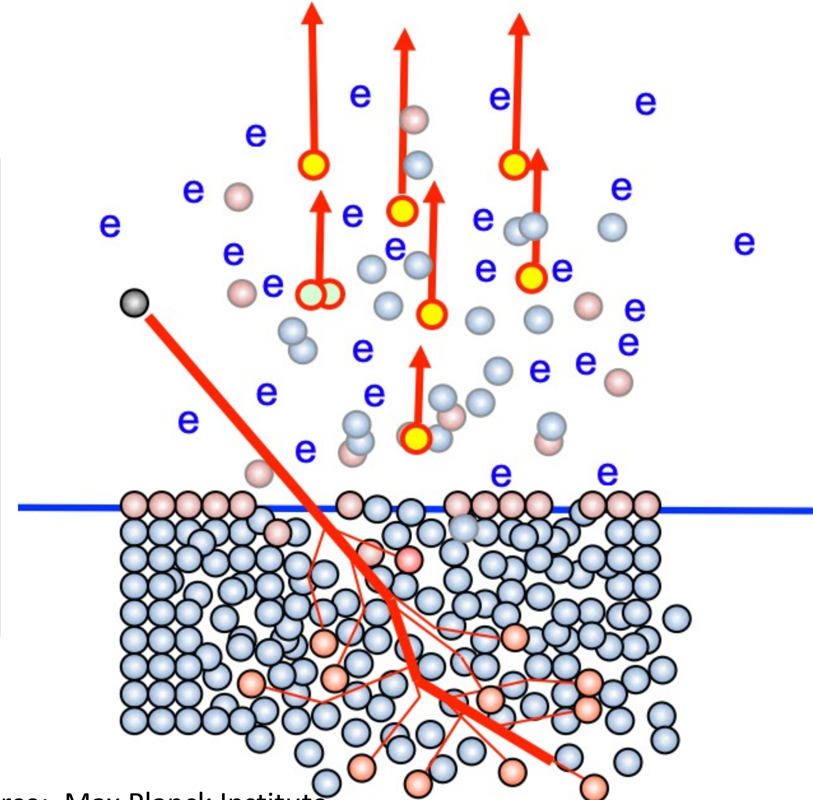




ToF-SIMS: Surface Bombardment

- Surface is bombarded by 30 keV primary ions
- Primary ion energy transferred to surface atoms and molecular compounds through atomic collisions

  → secondary ions overcome surface binding energy

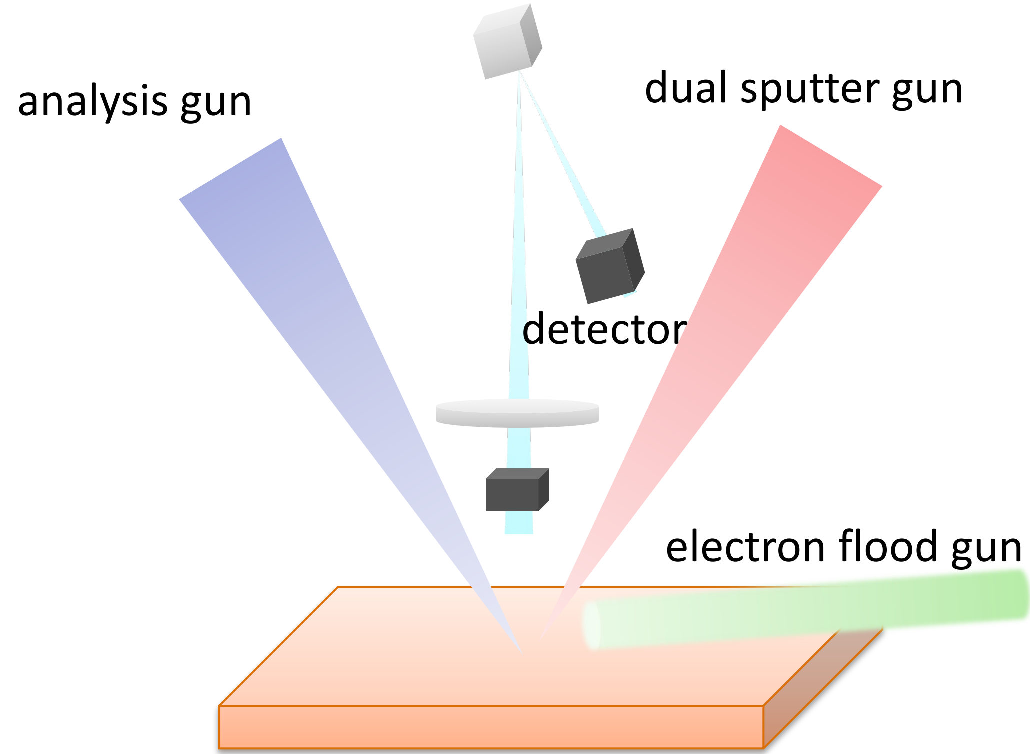


Source: Max Planck Institute

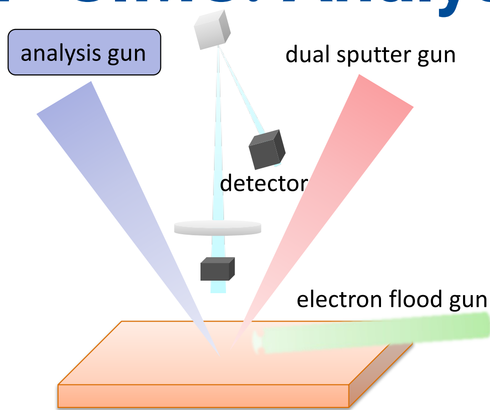
Fermilab

ToF-SIMS

- Analysis gun
- Dual sputter gun
- Electron flood gun
- Detector



ToF-SIMS: Analysis Gun - Source



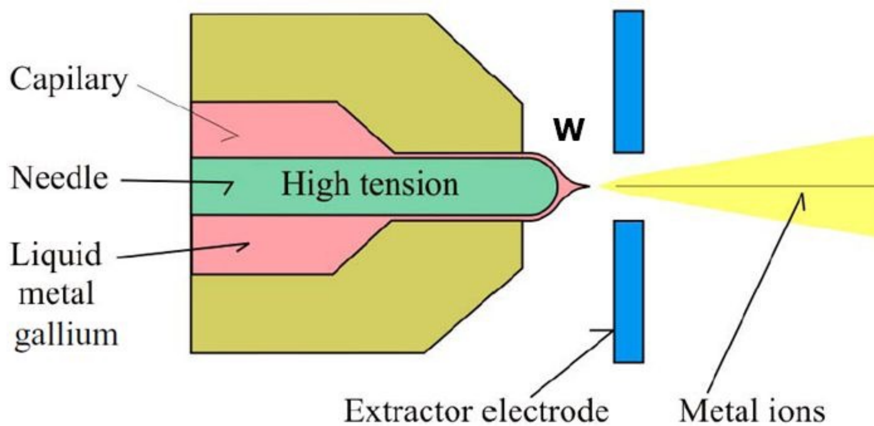
Periodic Table of the Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.008																	2 He Helium 4.003
2	3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
3	11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
4	19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798
5	37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.293
6	55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
7	87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [278]	110 Ds Darmstadtium [281]	111 Rg Roentgenium [280]	112 Cn Copernicium [285]	113 Nh Nihonium [286]	114 Fl Flerovium [289]	115 Mc Moscovium [289]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]

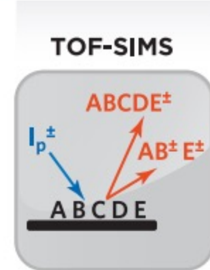
Series															
Lanthanide Series	57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Key: Number / Symbol / Name / Mass

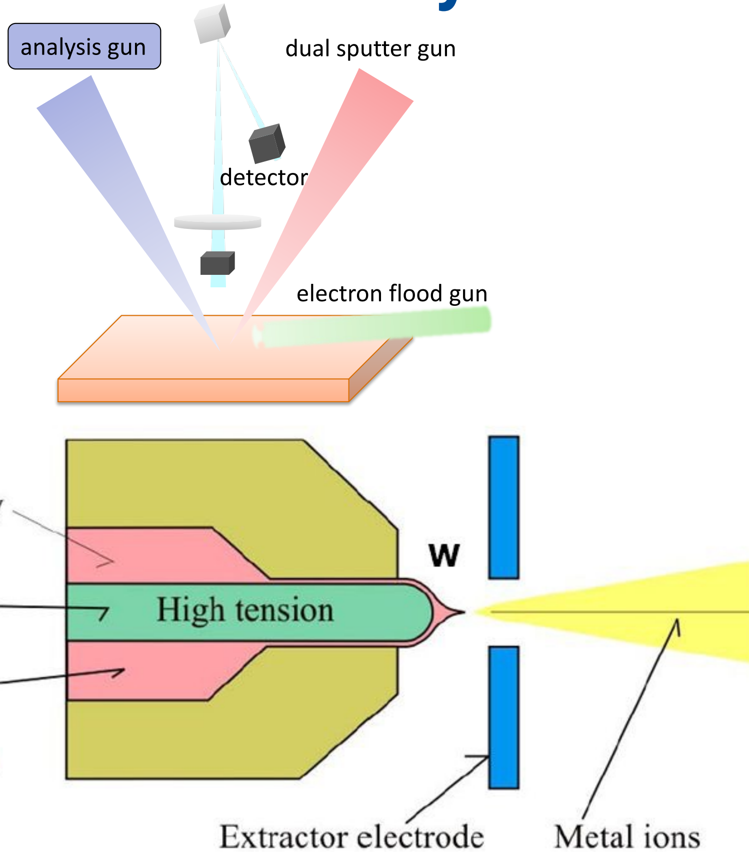
Legend: Alkali Metal | Alkaline Earth | Transition Metal | Basic Metal | Metalloid | Nonmetal | Halogen | Noble Gas | Lanthanide | Actinide

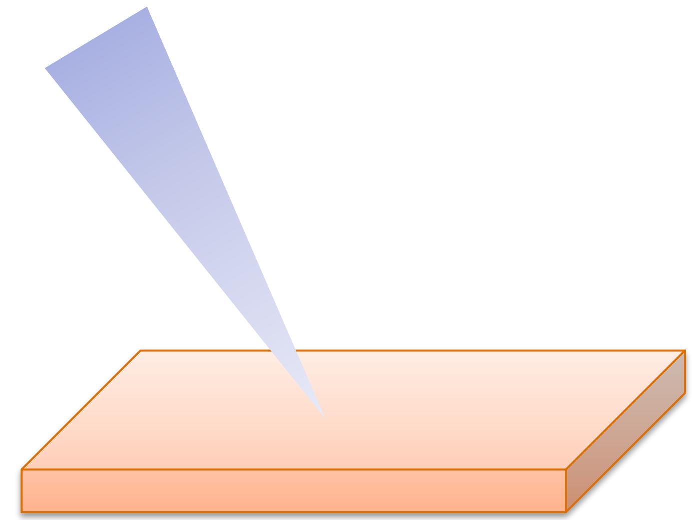


- Beam Energy: ~ 10-30keV
- Probe Size: <1um
- Information Depth: ~ 1-2 nm

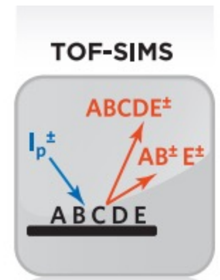


ToF-SIMS: Analysis Gun - Source

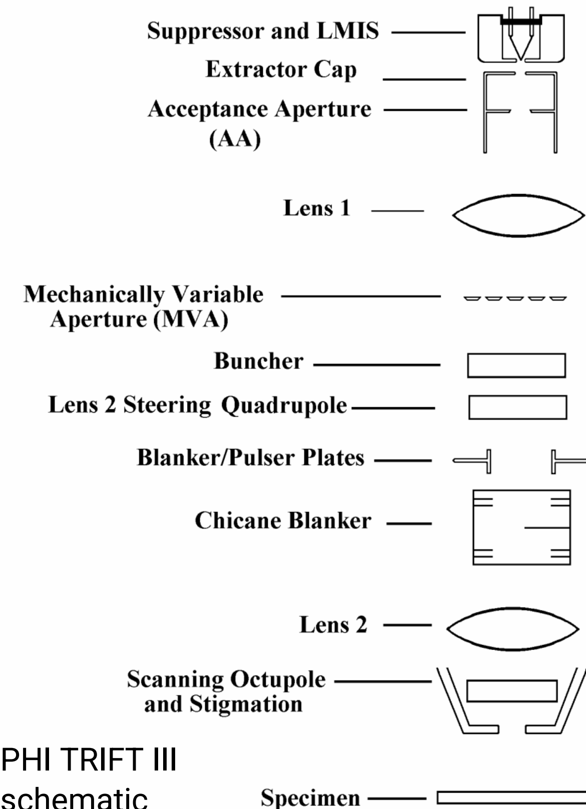




- Pulsed ion beam → reduce damage to sample surface
- Pulse length ~ 500 ps



ToF-SIMS: Analysis Gun - Optics



PHI TRIFT III schematic

Extractor: Accelerating voltage used to extract ions from source and generate ion beam

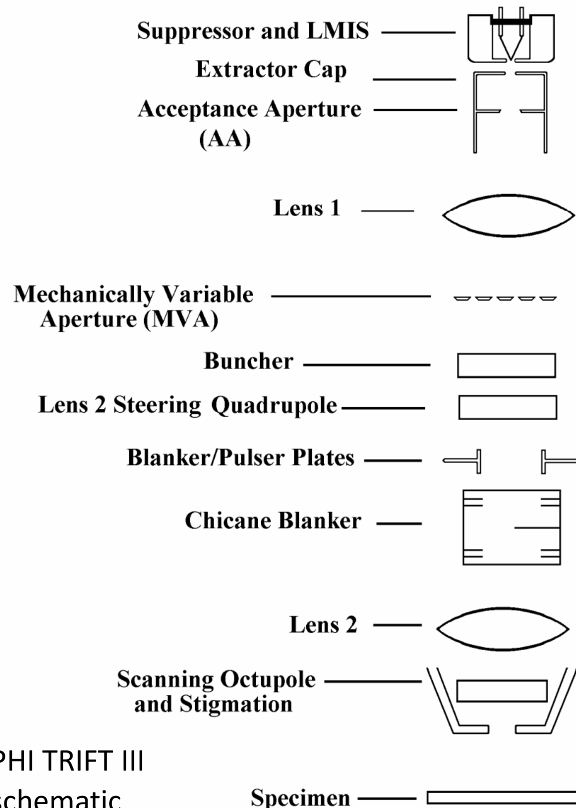
Suppressor: Voltage used to improve distribution of extracted ions

Lens 1 (Condenser Lens): Parallelizes ion beam to form an ion probe

Mechanically Variable Aperture: Defines ion current – array of apertures used to set probe size

Fermilab

ToF-SIMS: Analysis Gun - Optics



PHI TRIFT III schematic

Blanker/Pulser Plates: Pulses ion beam to reduce surface damage

Lens 2 (Objective Lens): Focuses ion beam onto sample

Scanning Octupole: Allows for rastering ion beam across region of interest

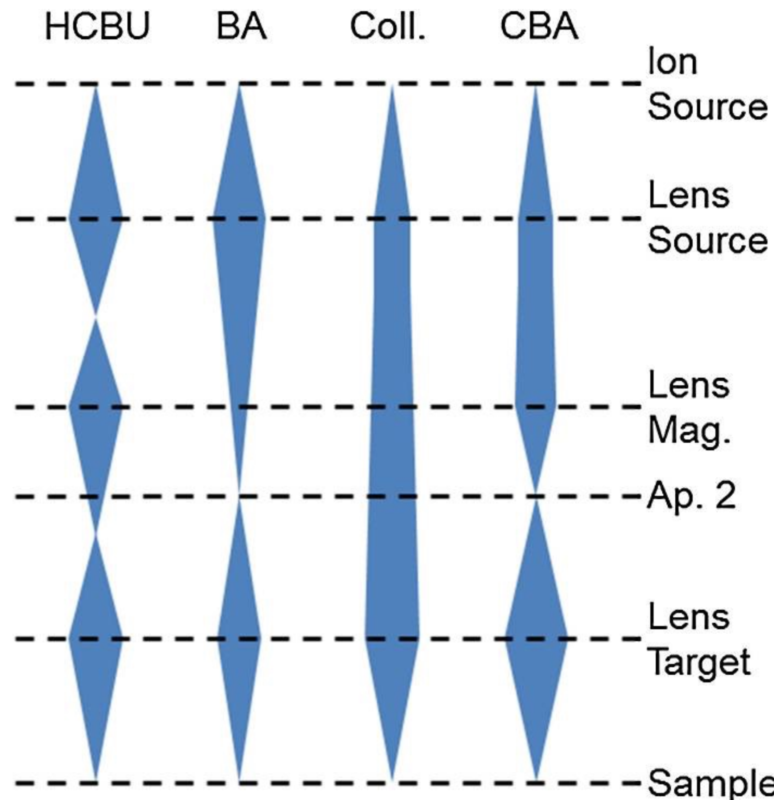
Stigmation: Applies weak electric field to reduce astigmatism in ion beam

Fermilab

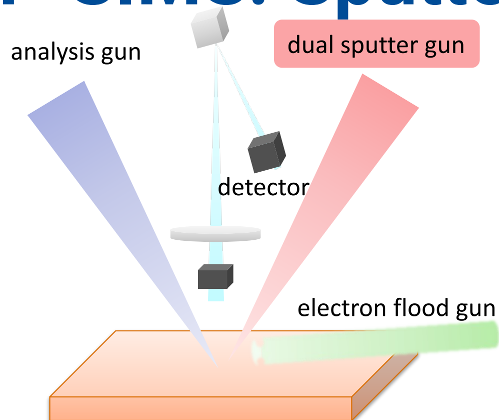
ToF-SIMS: Analysis Gun – Different Modes

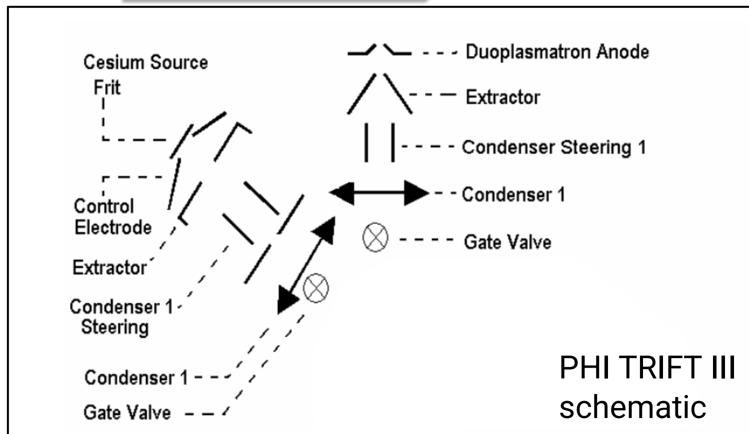
Operation mode	HCBU	BA	Collimated	CBA
Lens Source	~3150 V	~3300 V	~3900 V	~3750 V
Lens Mag	~14.8 kV	0 V	0 V	12–13 kV
DC-current	~15 nA	0.4–0.7 nA	50 pA	70–100 pA
Crossovers	2	1	0	1
Lateral resolution	2–10 μm	~250 nm	~100 nm	~100 nm
Mass resolution	~11,000	~200	~200	~200

Kubicek M, et al. Appl Surf Sci. 2014 Jan 15;289(100):407-416. doi: 10.1016/j.apsusc.2013.10.177. PMID: 24748701; PMCID: PMC3990430.



ToF-SIMS: Sputter Gun - Source



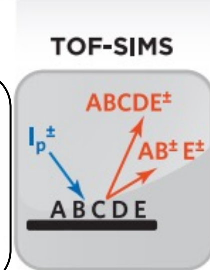


PHI TRIFT III schematic

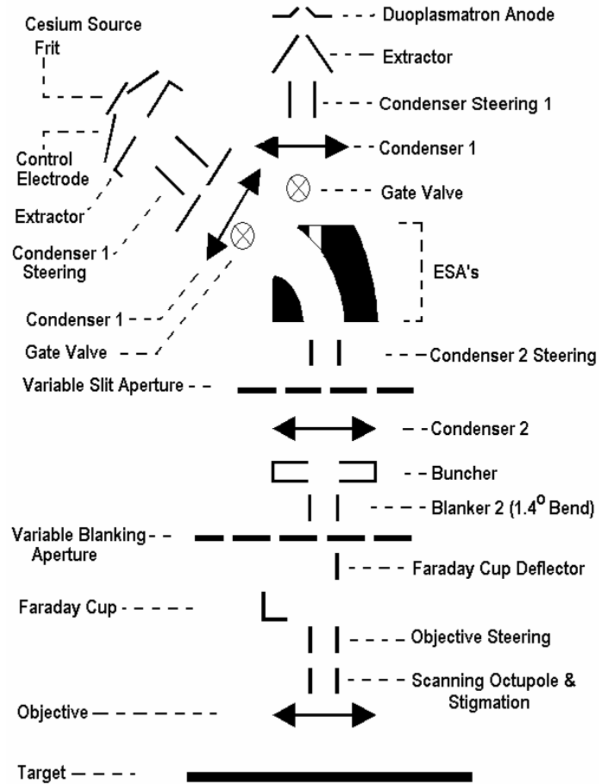
Periodic Table of the Elements

Alkali Metal | Alkaline Earth | Transition Metal | Basic Metal | Metalloid | Nonmetal | Halogen | Noble Gas | Lanthanide | Actinide

- Beam Energy: ~ 0.5-2 keV
- Probe Size: >1um
- Depth Resolution: ~ 2-5 nm



ToF-SIMS: Sputter Gun - Optics

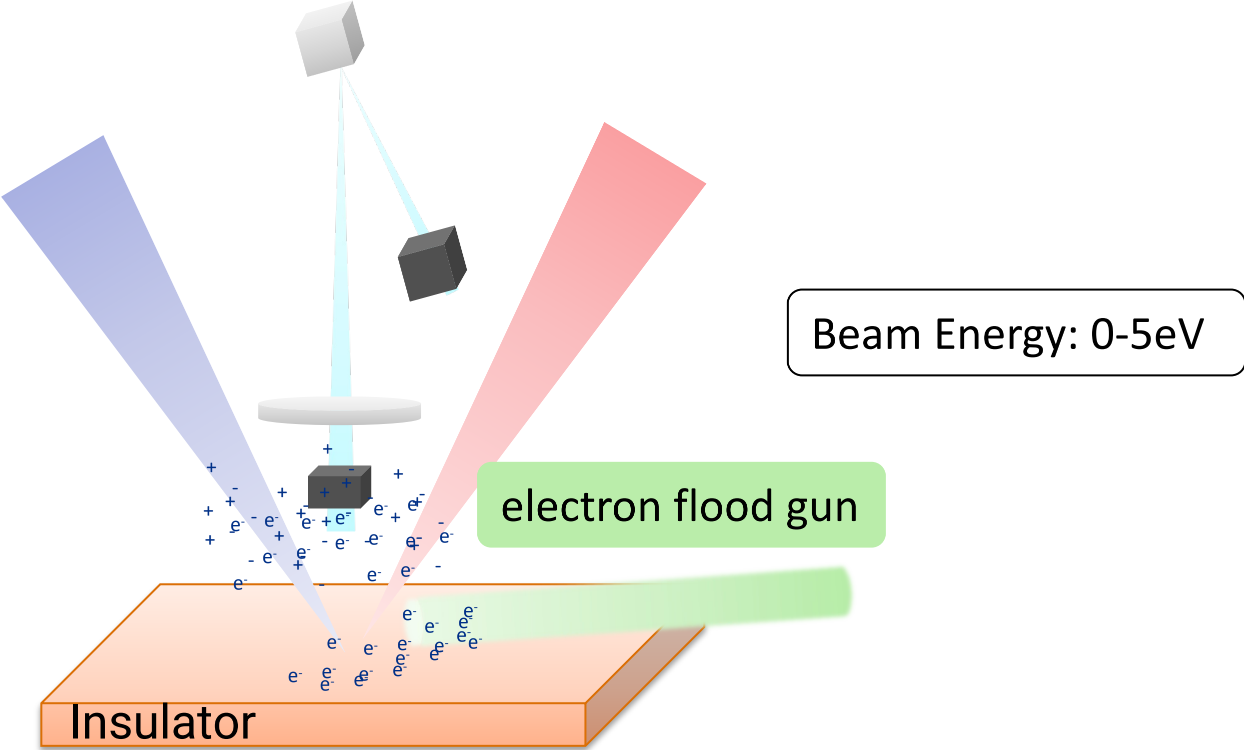


PHI TRIFT III schematic

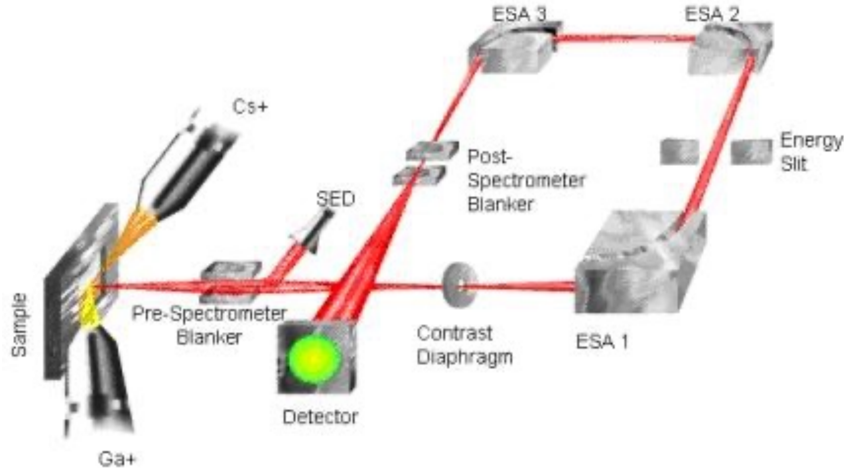
Similar to analysis gun optics

Fermilab

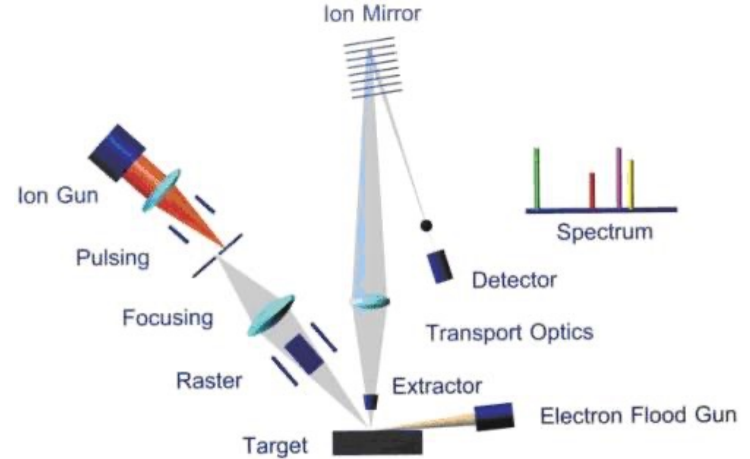
ToF-SIMS: Electron Flood Gun



ToF-SIMS: Mass Spectrometer – Flight Path

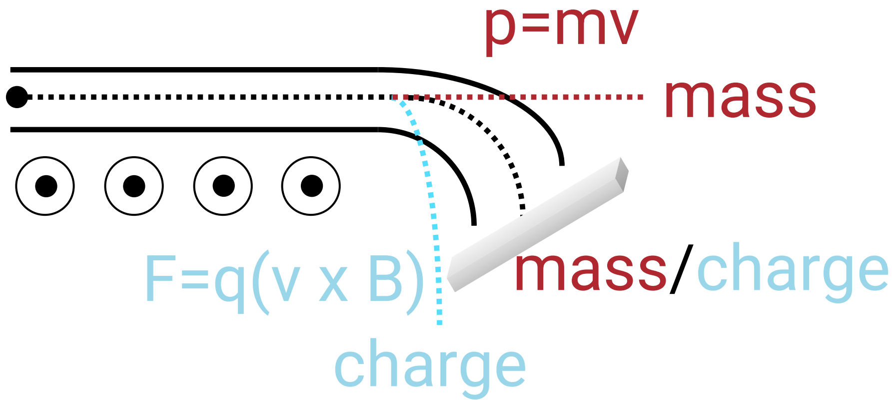


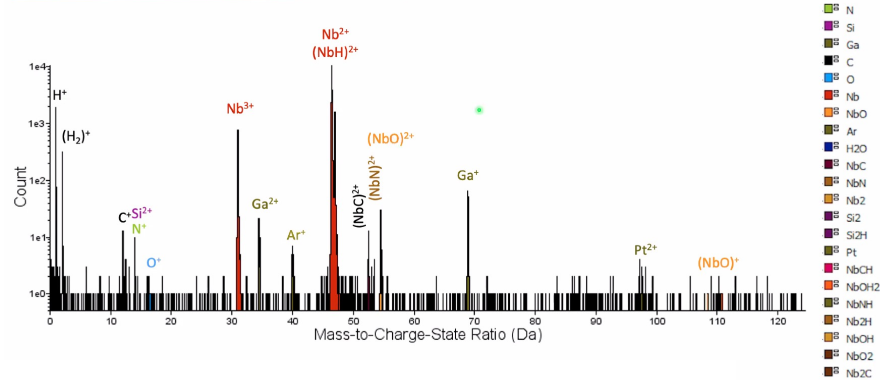
vs.



- Secondary ions directed using an extractor
- 2 main options in terms of flight paths:
  - Circular vs Linear

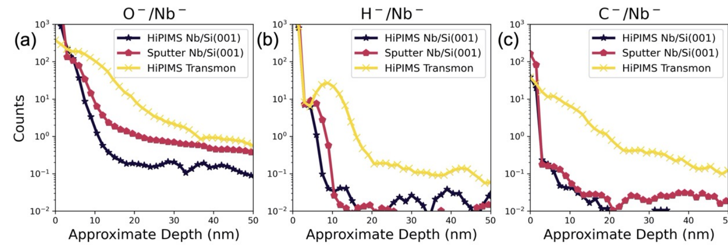
ToF-SIMS: Detector – Mass Spectrometer



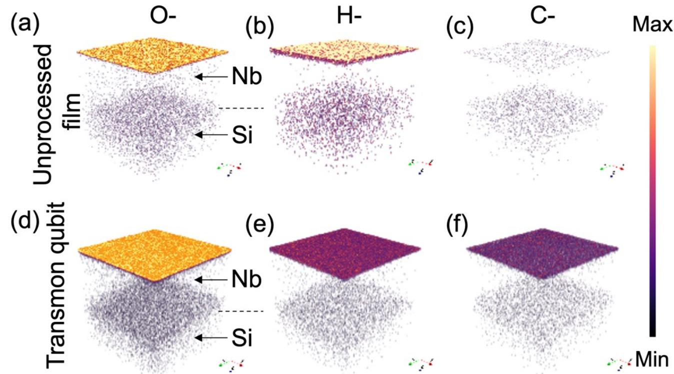


Detector measures m/z ratio

Highlight: Quantifying Impurities in Nb Qubit Films



Depth Profiles of impurities in Nb film



3D representation of impurity concentrations

- TOF-SIMS applied for the first time ever to 2D qubits reveal levels of contamination in the Nb pads
- Lithography steps during qubit fabrication lead to incorporation of impurity species including O^-, H^-, C^-, Cl^-, F^-, Na^+, Mg^+, and Ca^+
- Evaluating possible effects of the film purity on the microwave dissipation

Appl. Phys. Lett. **120** (4), 044002 (2022)

X-Ray Photoelectron Spectroscopy

electron analyzer

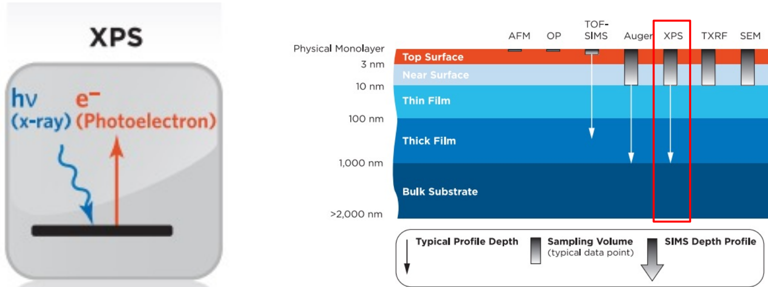
sputter gun

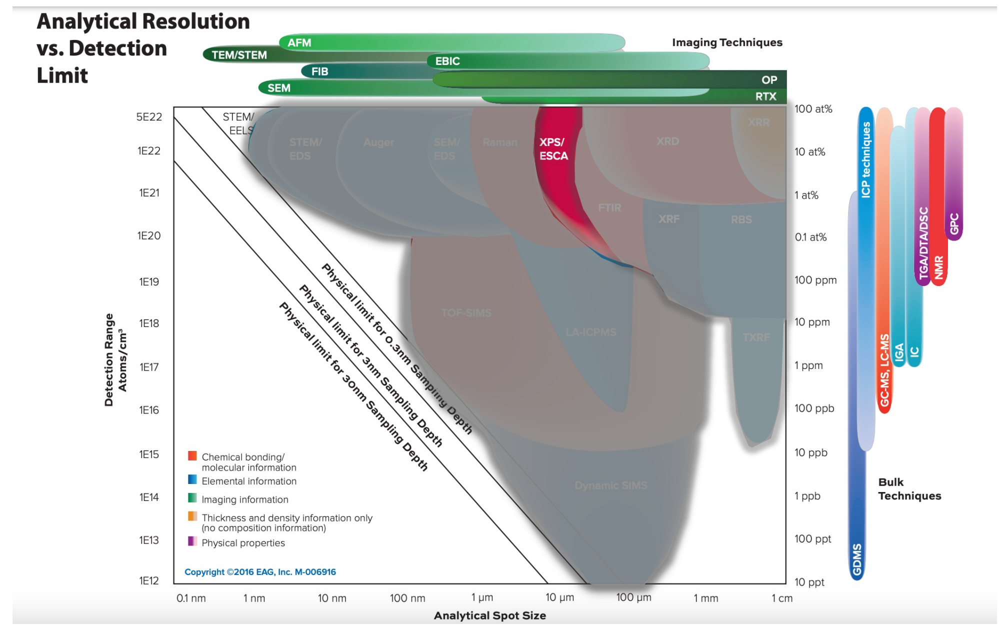
electron multiplier detector

x-ray source

electron flood gun

XPS Basics

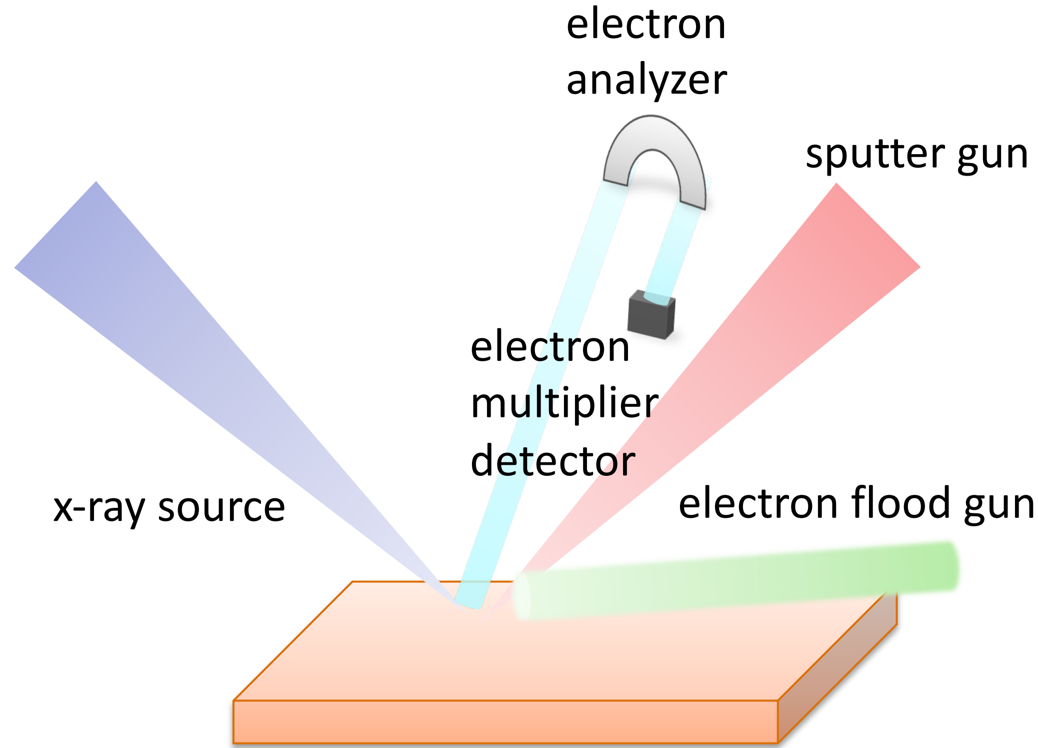




- Sensitive to atom%
- Provides elemental & bonding information
- Detection of low atomic number elements

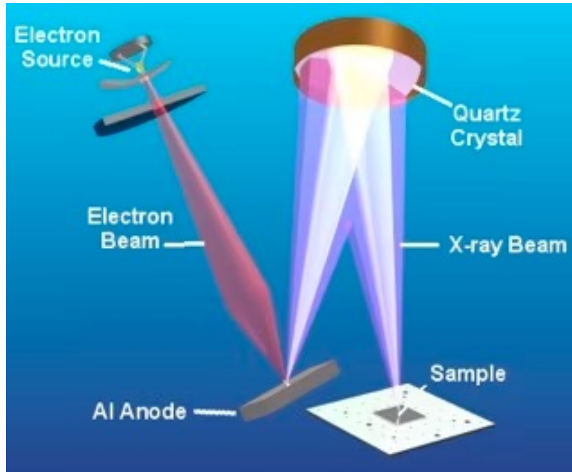
XPS Components

- X-Ray Source
- Sputter gun
- Electron flood gun
- Electron detector

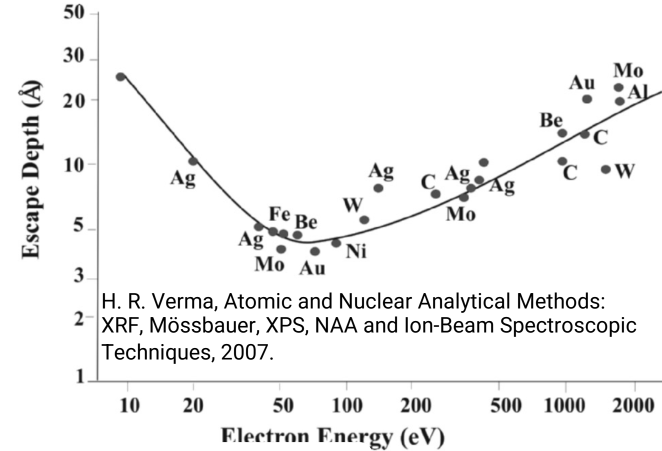


Fermilab

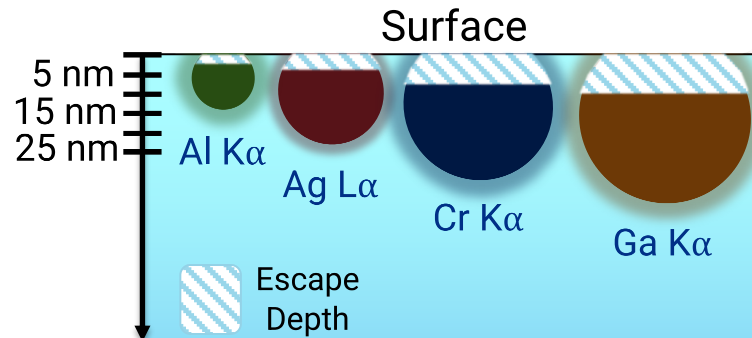
XPS: X-Ray Source



X-Ray Source	Energy (eV)
Al Kα	1486.6
Ag Lα	2984.3
Cr Kα	5414.8
Ga Kα	9251.7

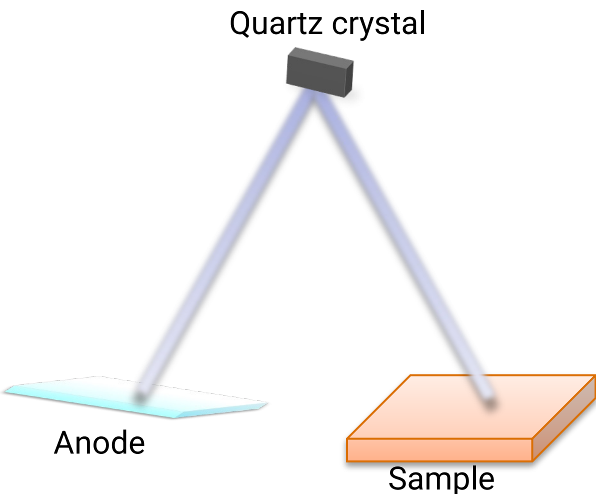


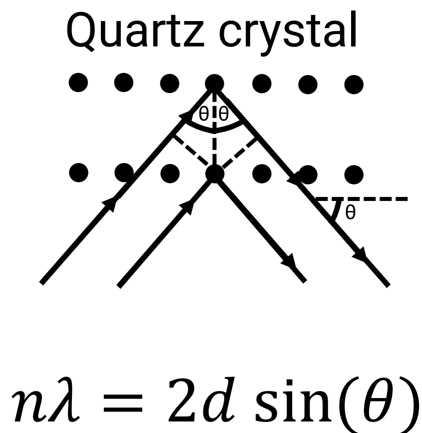
H. R. Verma, Atomic and Nuclear Analytical Methods: XRF, Mössbauer, XPS, NAA and Ion-Beam Spectroscopic Techniques, 2007.



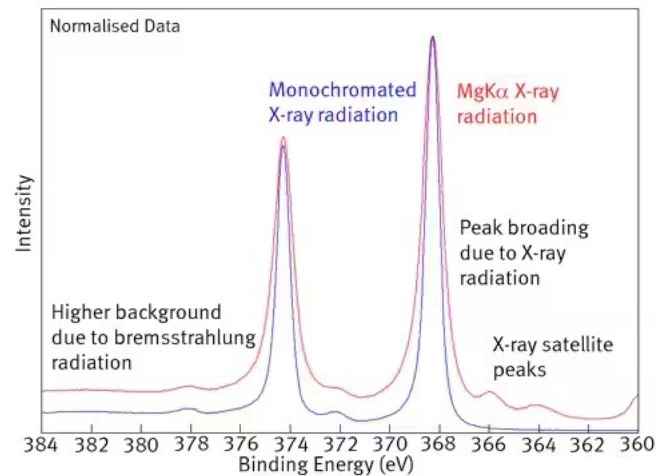
- Probe Size: ~500 um
- Information Depth: ~ 5-15 nm

XPS: X-Ray Monochromator



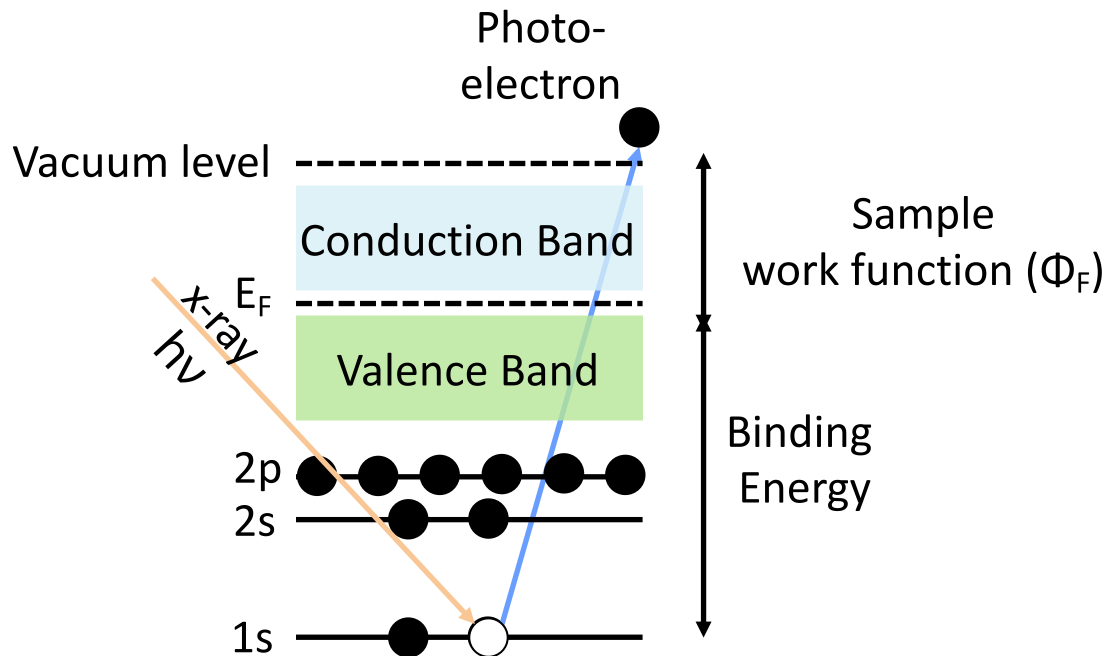


$$n\lambda = 2d\sin(\theta)$$



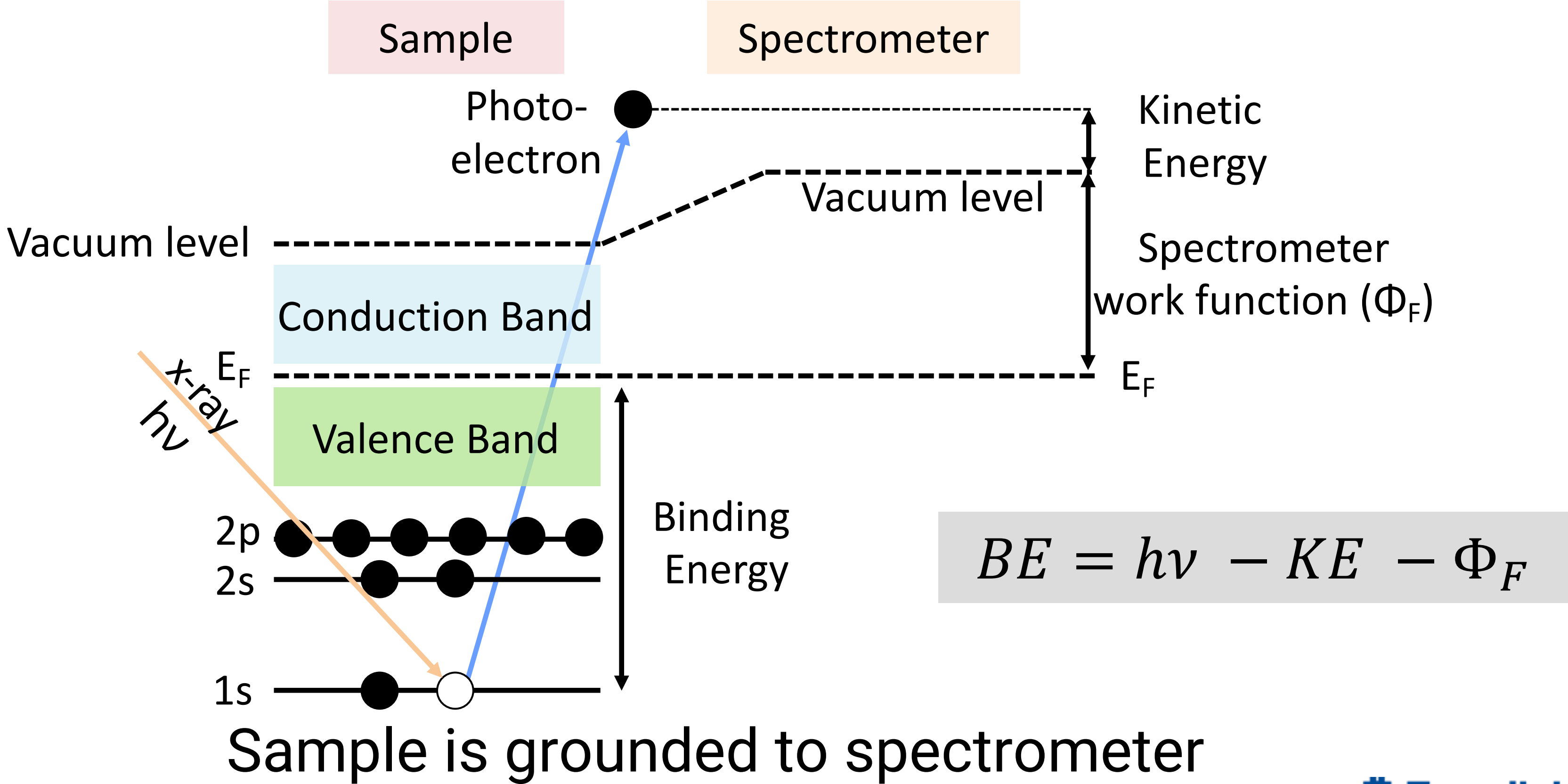
Source: Thermofisher

XPS: Photoelectric Effect

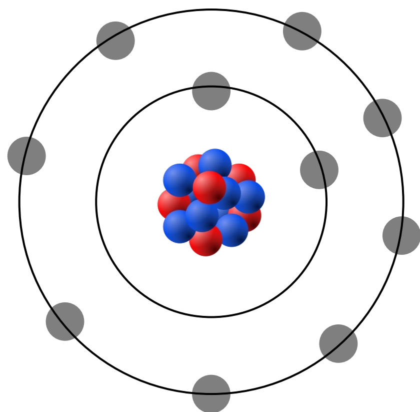


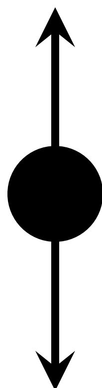
How does BE relate to Φ_F, hv, and KE of photoelectron?

XPS: Binding Energy



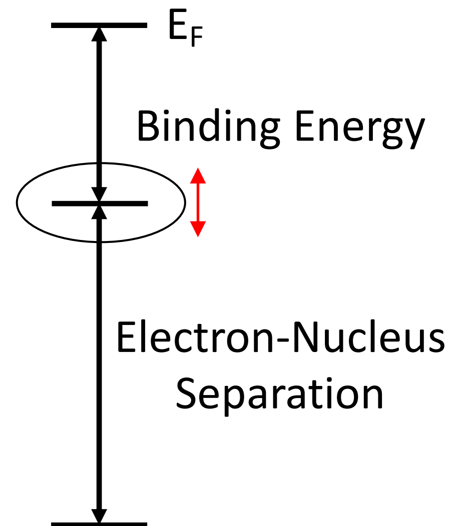
XPS: Local Changes to Binding Energy





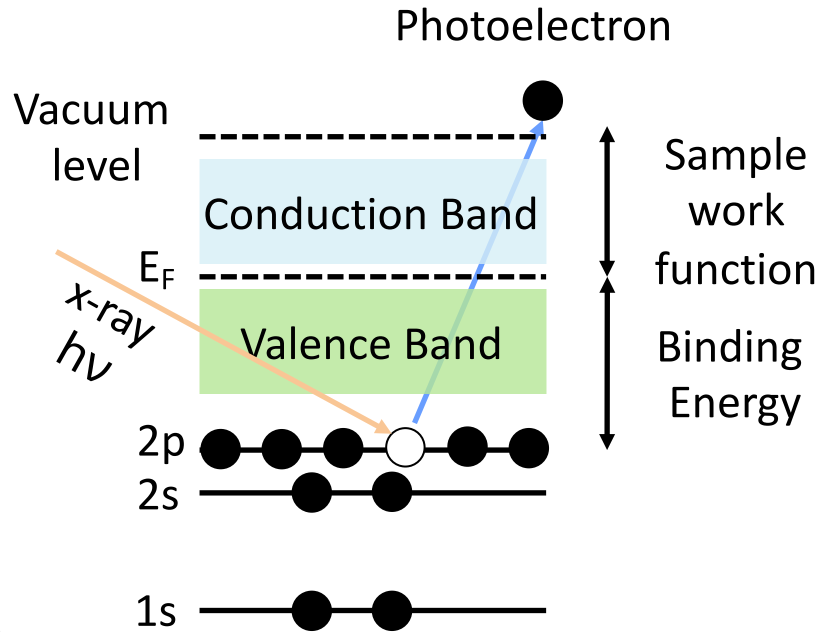
Electron-electron repulsion

Electron-nucleus attraction

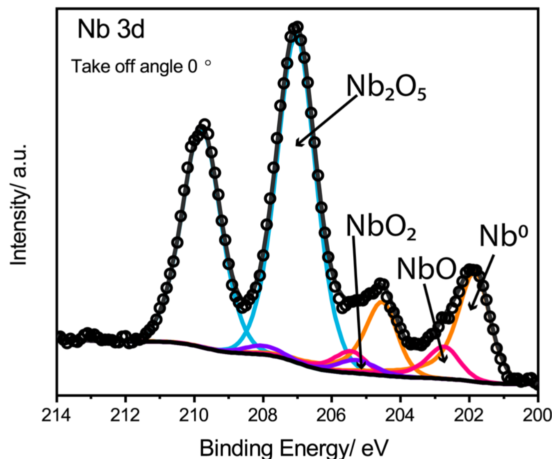


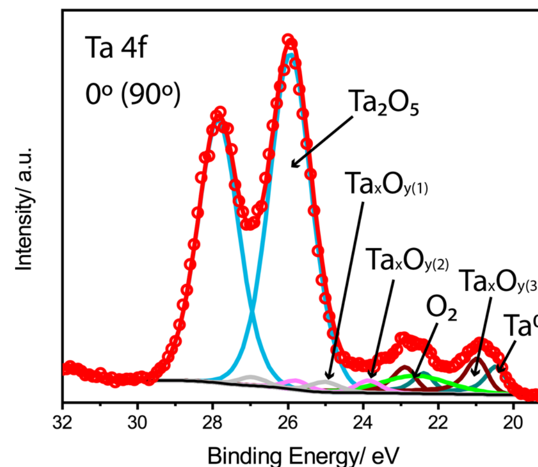
XPS: Local Changes to Binding Energy

Si
Si 2p
SiO_2
Si_3N_4
PEE5
PEE6
96 98 100 102 104 106 108
Binding Energy [eV]



Highlight: Quantifying Impurities in Nb Qubit Films



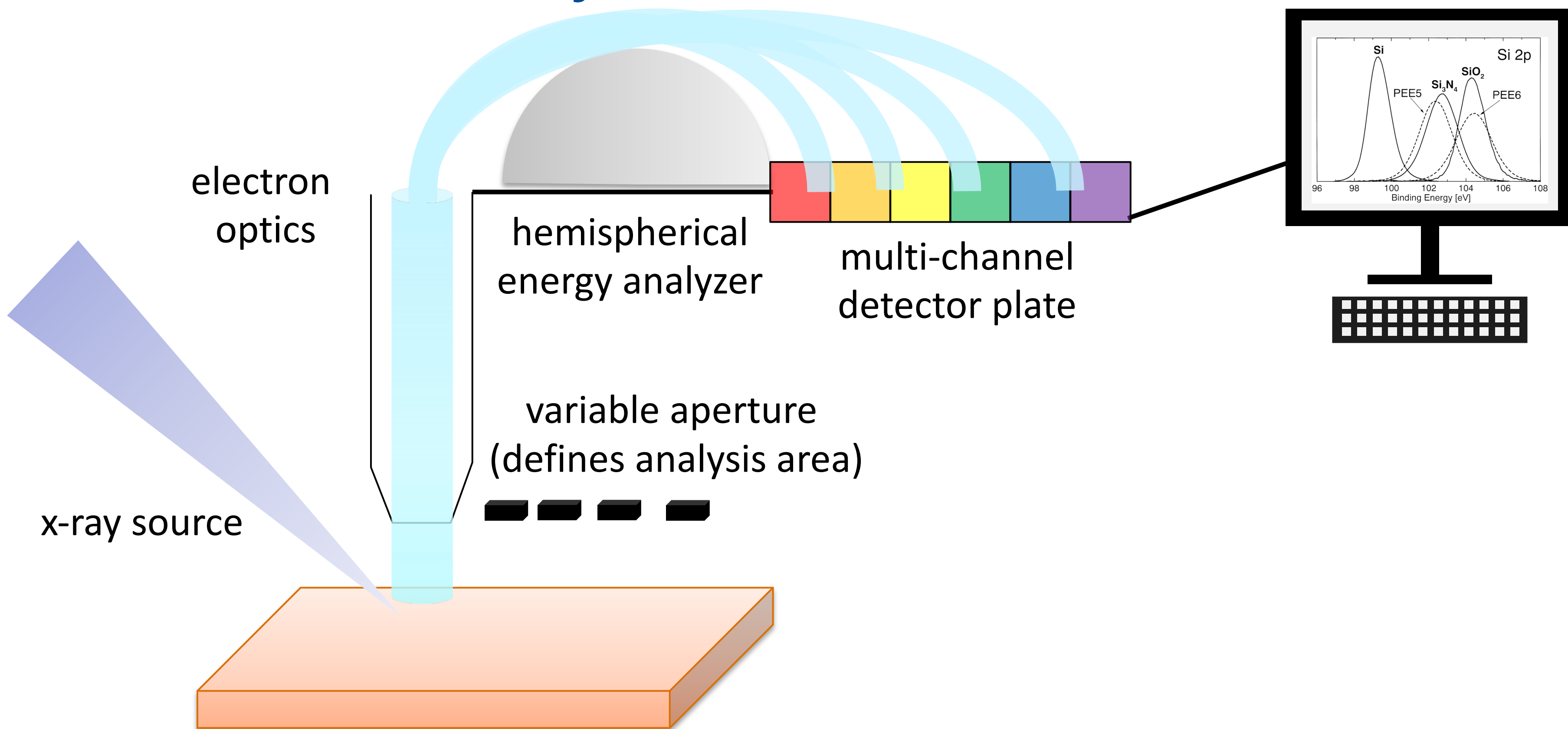


angle	0° (90)			
Species	**BE/ eV**	**ΔBE/ eV**	**FWHM/ eV**	**Q**
Nb^0	201.83	2.7	1.1	22.06
NbO	202.73	2.72	1.1	6.53
NbO_2	205.29	2.7	1.3	2.7
Nb_2O_5	207.03	2.76	1.3	68.7
ΔBE/ eV_{5-0}	5.2			

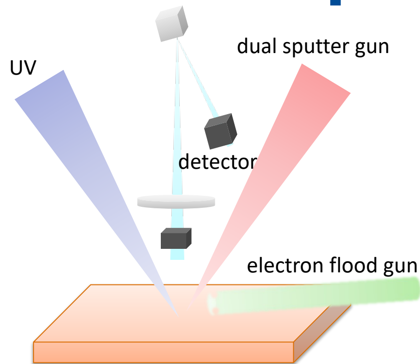
angle	0° (90)			
Species	**BE/ eV**	**ΔBE/ eV**	**FWHM/ eV**	**Q**
Ta^0	20.46	1.92	0.7	4.93
$Ta_xO_{y(1)}$	20.96	1.92	0.7	6.51
$Ta_xO_{y(2)}$	23.86	1.92	0.8	1.66
$Ta_xO_{y(3)}$	25.02	1.92	0.9	0.9
Ta_2O_5	25.94	1.92	1.3	85.99
ΔBE/ eV_{5-0}	5.48			

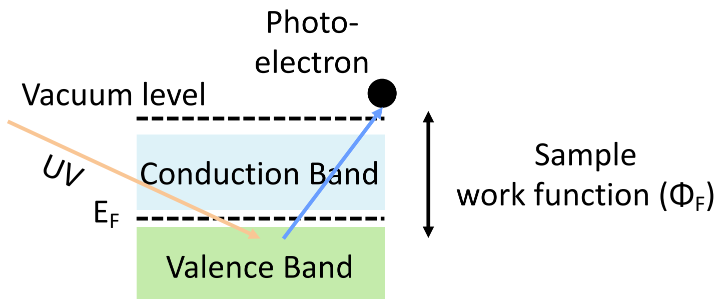
Fermilab

XPS: Electron Analyzer + Detector

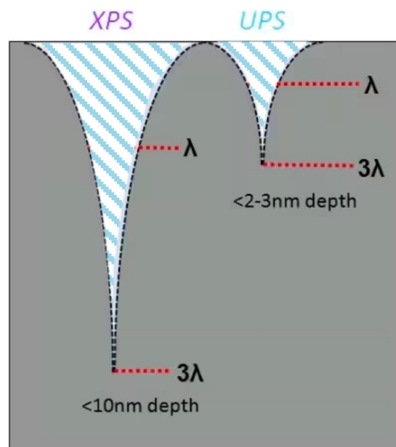


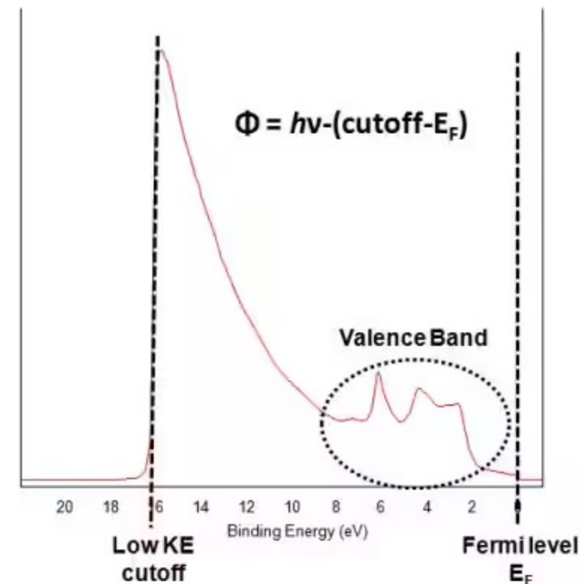
Related Topics: UV Photoelectron Spectroscopy





UV Source	Energy (eV)
He I	21.2
He II	40.8

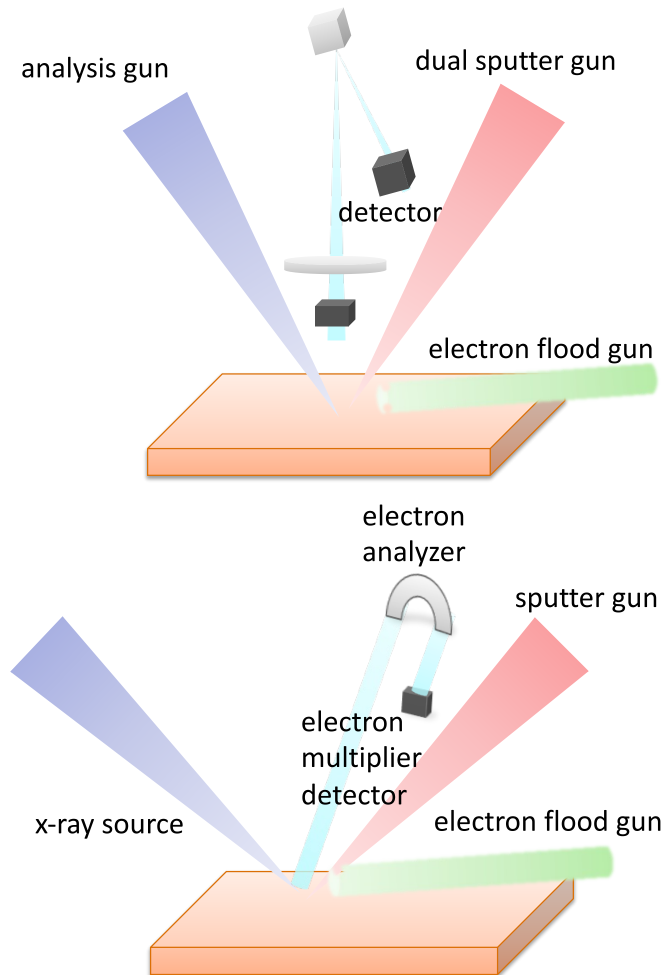




Source: Thermofisher

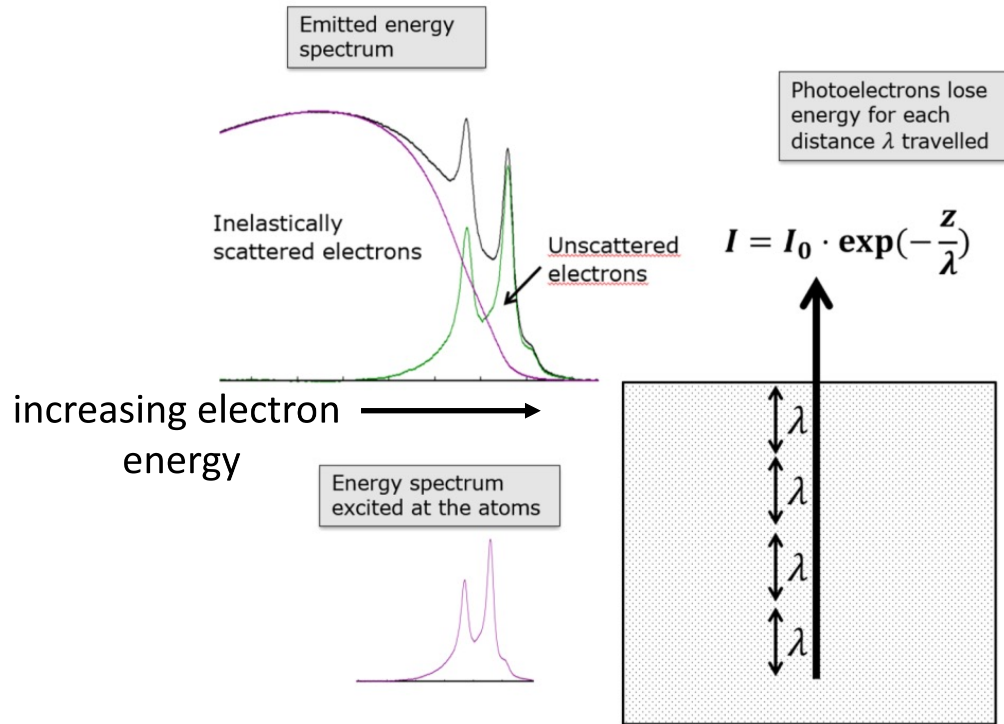
Summary

- ToF-SIMS
  - Very sensitive surface analytical technique
  - Allows detection of low Z elements
  - Useful for probing impurities in quantum devices
- XPS
  - Surface analytical technique sensitive to atom%
  - Allows detection of changes in bonding environment
  - Useful for characterizing surface stoichiometry in quantum devices



Appendix

Inelastic Scattering



Sven Tougaard; Practical guide to the use of backgrounds in quantitative XPS. Journal of Vacuum Science & Technology A 1 January 2021; 39 (1): 011201. https://doi.org/10.1116/6.0000661