

Table 1.1 Surface Science Techniques (page 19-28)

Acronym	Name	Description	Primary Surface Information
	Adsorption or selective chemisorption (1)	Atoms or molecules are physisorbed into a porous structure—such as zeolite or a sample of coal—or on to a surface and the amount of gas adsorbed is a measure of the surface area available for adsorption. Chemisorption of atoms or molecules on surfaces yields surface concentration of selected elements or adsorption sites.	Surface area, adsorption site concentration
AD	Atom or helium diffraction (2-13)	Monoenergetic beams of atoms are scattered from ordered surfaces and detected as a function of scattering angle. This gives structural information on the outermost layer of the surface. Atom diffraction is extremely sensitive to surface ordering and defects.	Surface structure
AEAPS	Auger electron appearance potential spectroscopy (2-4, 14-17)	A monoenergetic beam of electrons is used to excite atoms in the near surface region. As the beam energy is swept, variations in the sample emission current occur as the beam energy sweeps over the energy of an Auger transition in the sample. Also known as APAES.	Chemical composition
AES	Auger electron spectroscopy (2-4, 14, 16, 18-29)	Core-hole excitations are created, usually by 1 to 10-keV incident electrons; Auger electrons of characteristic energies are emitted through a two-electron process as excited atoms decay to their ground state. AES gives information on the near-surface chemical composition.	Chemical composition
AFM	Atomic force microscopy (30-37)	Very similar to scanning tunneling microscopy (STM). In this technique, however, the attractive van der Waals forces between the surface and the probe cause a bending of the probe. This deflection is measurable by variety of means. Because this technique does not require a current between the probe and the surface, nonconducting surfaces may be imaged.	Surface structure
APAES	Appearance potential auger electron spectroscopy	See AEAPS.	
APXPS	Appearance potential X-ray photoemission spectroscopy (2-4, 16)	The EAPFS excitation cross section is monitored by fluorescence from core hole decay (also known as SXAPS).	Chemical composition
ARAES	Angle-resolved auger electron spectroscopy (38)	Auger electrons are detected as a function of angle to provide information on the spatial distribution or environment of the excited atoms (see AES).	Surface structure
ARPEFS	Angle-resolved	Electrons are detected at given angles after	Surface structure

	photoemission extended fine structure (38-40)	being photoemitted by polarized synchrotron radiation. The interference in the detected photoemission intensity as a function of the electron energy ≈ 100 -500 eV above the excitation threshold gives structural information.	
ARPES	Angle-resolved photoemission spectroscopy (3, 24, 41-44)	A general term for structure-sensitive photoemission techniques, including ARPEFS, ARXPS, ARUPS, and ARXPD.	Electronic structure, surface, surface structure
ARUPS	Angle-resolved ultraviolet photoemission spectroscopy (3, 42, 45-48)	Electrons photoemitted from the valence and conduction bands of a surface are detected as a function of angle. This gives information on the dispersion of these bands (which is related to surface structure) and also gives structural information from the diffraction on the emitted electrons.	Valance band structure, bonding
ARXPD	Angle-resolved X-ray photo-electron diffraction (3, 38, 39, 49-51)	Similar to ARXPS and ARPEFS. The angular variation in the photoemission intensity is measured at a fixed energy above the excitation threshold to provide structural information.	Surface structure
ARXPS	Angle-resolved X-ray photoemission spectroscopy (3, 38, 39, 49, 50)	The diffraction of electrons photoemitted from core levels gives structural information on the surface.	Surface structure
CEM	Conversion electron Mossbauer spectroscopy (4, 52-55)	A surface-sensitive version of Mossbauer spectroscopy. Like Mossbauer spectroscopy, this technique is limited to some isotopes of certain metals. After a nucleus is excited by γ -ray absorption, it can undergo inverse β -decay, creating a core hole. The decay of core holes by Auger processes within an electron mean free path of the surface produces a signal. Detecting emitted electrons as a function of energy gives some depth-profile information because the changing mean free path.	Chemical environment, oxidation state
DAPS	Disappearance potential spectroscopy (2-4, 16)	The EAPFS cross section is monitored by variations in the intensity of electrons back-scattered from surface.	Chemical composition
EAPFS	Electron appearance potential fine structure (3, 56)	A fine structure technique (see EXAFS). Core holes excited by monoenergetic electrons. The modulation in the excitation cross section as the beam energy is varied may be monitored through absorption, fluorescence, or AUGER emission.	Surface structure
ELNES	Electron energy loss near edge structure	Similar to NEXAFS, except monoenergetic high-energy electrons ≈ 60 -300 keV excite core holes.	Surface structure
ELS or EELS	Electron energy loss spectroscopy (3, 4,	Monoenergetic electrons are scattered off a surface, and the energy losses are	Electronic structure, surface structure

	20, 23, 41, 57-60)	determined. This gives information on the electronic excitations of the surface and the adsorbed molecules.	
ESCA	Electron spectroscopy for chemical analysis (2-4, 16, 22, 61-63)	Now generally called XPS.	Composition, oxidation state
ESDIAD or PSD	Electron (photon)-stimulated ion angular distribution (2-4, 8, 64-69) Ellipsometry (70)	Electrons or photons break chemical bonds in adsorbed atoms or molecules, causing ionized atoms or radicals to be ejected from the surface along the axis of the broken bond by Coulomb repulsion. The angular distribution of these ions gives information on the bonding geometry of adsorbed molecules. Used to determine thickness of an adsorbed film. A circular polarized beam of light is reflected from a surface, and the change in the polarization characteristics of the light gives information about the surface film.	Bonding geometry, molecular orientation Layer thickness
EXAFS	Extended X-ray absorption fine structure (3, 8, 71-77)	Monoenergetic photons excite a core hole. The modulation of the absorption cross section with energy at 100-500 eV above the excitation threshold yields information on the radial distances on the neighboring atoms. The cross section can be measured by fluorescence as the core holes decay or by attenuation of the transmitted photon beam. EXAFS is one of the many "fine-structure" techniques.	Local surface structure and coordination numbers
EXELFS	Extended X-ray energy loss fine structure (3)	Monoenergetic electrons excite a core hole. The modulation of the absorption cross section with energy 100-500 eV above the excitation threshold yields information on the radial distances to the neighboring atoms. The cross section can be measured by fluorescence as the core holes decay or by attenuation of the transmitted photon beam.	Local surface structure and coordination numbers
FEM	Field emission microscopy (2-4, 11, 20, 22, 78, 79)	A strong electric field (on the order of volts/angstrom) is applied to the tip of sharp, single-crystal wire. The electrons tunnel into the vacuum and are accelerated along radial trajectories by Coulomb repulsion. When the electrons impinge on the fluorescent screen, variations of the electric field strength across the surface of the tip are displayed.	Surface structure
FIM	Field ionization microscopy (2-4, 11, 20, 22, 79, 80)	A strong electric field (on the order of volts/angstrom) is created at the tip of a sharp, single-crystal wire. Gas atoms, usually He, are polarized and attracted to the tip by the strong electric field, and are ionized by electrons tunneling from gas atoms into the tip. These ions, accelerated	Surface structure and surface diffusion

		along radial trajectories by Coulomb repulsion, map out the variations in the electric field strength across the surface, showing the surface topography with atomic resolution.	
FTIR	Fourier transform infrared spectroscopy (81-83)	Broad-band IRAS experiments are performed, and the IR adsorption spectrum is deconvoluted using a Doppler-shifted source and the Fourier analysis of the data. This technique is not restricted to surfaces.	Bonding geometry and strength
HEIS	High-energy ion scattering spectroscopy (3, 11, 84, 85)	High-energy ions, above ≈ 500 keV, are scattered off a single-crystal surface. The “channeling” and “blocking” of scattered ions within the crystal can be used to triangulate deviations from the bulk structure. HEIS has been especially used to study surface reconstructions and the thermal vibrations of surface atoms. See also MEIS and ISS.	Surface structure
HREELS	High-resolution electron energy loss spectroscopy (2, 3, 86-88)	A monoenergetic electron beam, ≈ 2 -10 eV is scattered off a surface; and the energy losses between ≈ 0.5 eV to bulk and surface phonons and vibrational excitations of adsorbates are measured as a function of angle and energy (also called EELS)	Bonding geometry, surface atom vibrations
INS	Ion-neutralizations spectroscopy (2, 3, 89)	Slow ionized atoms, usually He ⁺ , strike a surface, where they are neutralized in a two-electron process that can eject a surface electron—a process similar to Auger emission from the valence band. The ejected electrons are detected as a function of energy, and the surface density of states can be determined from the energy distribution. The interpretation is more complicated than for SPI or UPS.	Valence bands
IP	Inverse photoemission (90-95)	The absorption of electrons by surface is measured as a function of energy and angle. This technique gives information about conduction bands and unoccupied levels.	Electronic structure
IRAS	Infrared reflection adsorption spectroscopy (3, 59, 60, 83, 96, 97)	The vibrational modes of adsorbed molecules on a surface are studied by monitoring the absorption or emission of IR radiation from thermally excited modes as a function of energy.	Molecular structure
ISS	Ion scattering spectroscopy (2-4, 8, 98, 99)	Ions are scattered from a surface, and the chemical composition of the surface may be determined by the momentum transfer to surface atoms. The energy range is ≈ 1 keV to 10 MeV, and the lower energies are more surface-sensitive. At higher energies this technique is also known as <i>Rutherford back-scattering</i> (RBS). A compilation of surface structures	Surface structure, composition

		determined with ion scattering summarizing the pre-1988 literature appears in reference [100].	
LEED	Low-energy electron diffraction (2-4, 8, 10-12, 20, 22, 23, 102-104)	Monoenergetic electrons below ≈ 500 eV are elastically back-scattered from a surface and detected as a function of energy and angle. This gives information on the structure of the near surface region. A compilation of surface structures summarizing the pre-1986 literature appears in reference [105].	Surface structure
LEIS	Low-energy ion scattering (3, 4, 11, 106, 107)	Low-energy ions below ≈ 5 eV are scattered from a surface, and the ion "shadowing" gives information on the surface structure. At these low energies the surface-atom ion-scattering cross section is very large, resulting in large surface sensitivity. Accuracy is limited because the low-energy ion-scattering cross sections are not well known.	Surface structure
LEPD	Low-energy positron diffraction (108, 109)	Similar to LEED with positrons as the incident particle. The interaction potential is somewhat different than for electrons, so the form of the structural information is modified.	Surface structure
MEED	Medium-energy electron diffraction (11)	Similar to LEED except the energy range is higher, ≈ 300 -1000 eV.	Surface structure
MEIS	Medium-energy ion scattering (4, 11)	Similar to HEIS, except those incident ion energies are ≈ 50 -500 keV.	Surface structure
	Neutron diffraction (110-112)	Neutron diffraction is not an explicitly surface sensitive technique, but neutron diffraction experiments on large-surface-area sample have provided important structural information on adsorbed molecules and also on surface phase transitions.	Surface structure
NEXAFS	Near-edge X-ray absorption fine structure (71, 72, 113-115)	A core hole is excited as in fine-structure techniques (see EXAFS, SEXAFS, ARPEFS, NPD, APD, EXELFS, SEELFS) except that the fine structure within ≈ 30 eV of the excitation threshold is measured. Multiple scattering is much stronger at low electron energies, so this technique is sensitive to the local three-dimensional geometry, not just the radial separation between the source atom and its neighbors. The excitation cross section may be monitored by detecting the photoemitted electrons or the Auger electrons emitted during the core-hole decay.	Surface structure
NMR	Nuclear magnetic resonance (116, 117)	NMR is not an explicitly surface-sensitive technique, but NMR data on large surface	Chemical state

		<p>area samples ($\geq 1 \text{ m}^2$) have provided useful data on molecular adsorption geometries. The nucleus magnetic moment interacts with an extremely applied magnetic field and provides spectra highly dependent on the nuclear environment of the sample. The signal intensity is directly proportional to the concentration of the active species. This method is limited to the analysis of magnetically active nuclei.</p>	
NPD	Normal photoelectron diffraction (38, 39)	Similar to ARPEFS, but with a somewhat lower energy range.	Surface structure
RBS	Rutherford back-scattering (2, 3, 118, 119)	Similar to ISS, except that the main focus is on depth-profiling and composition. The momentum transfer in back-scattering collisions between nuclei is used to identify the nuclear masses in the sample, and the smaller, gradual momentum loss of the incident nucleus through electron-nucleus interactions provides depth-profile information.	Composition
RHEED	Reflection high-energy electron diffraction (3, 4, 10, 11, 22, 120)	Monoenergetic electrons below $\approx 1\text{-}20 \text{ keV}$ are elastically scattered from a surface at glancing incidence, and detected as a function of energy and angle for small forward-scattering angles. Back-scattering is less important at high energies, and glancing incidence is used to enhance surface sensitivity.	Surface structure, structure of thin films
SEELFS	Surface electron energy loss fine structure (77, 121, 122)	A fine-structure technique similar to EXELFS, except the incident electron is more surface-sensitive because of the lower excitation energy. A compilation of surface structures determined using SEELFS and SEXAFS summarizing the pre-1990 literature appears in reference (123).	Surface structure
SERS	Surface enhanced Raman spectroscopy (59, 124, 125)	Some surface geometries (rough surfaces) concentrate the electric fields of Raman scattering cross section so that it is surface-sensitive. This gives information on surface vibrational modes, and some information on geometry via selection rules.	Surface structure
SEXAFS	Surface extended X-ray absorption fine structure (3, 8, 72, 121, 126-128)	A more surface-sensitive version of EXAFS where the excitation cross-section fine structure is monitored by detecting the photoemitted electrons (PE-SEXAFS), Auger electrons emitted during core-hole decay (Auger-SEXAFS), or ions excited by photoelectrons and desorbed from the surface (PSD-SEXAFS). A compilation of surface structures determined using SEELFS and SEXAFS summarizing the pre-1990 literature appears in reference	Surface structure

		123.	
SFA	Surface force apparatus (129-132)	Two bent mica sheets with atomically smooth surfaces are brought together with distance of separation in the nanometer range. The forces acting on molecular layers between the mica plates perpendicular and parallel to the plate surfaces can be measured.	Forces acting on molecules squeezed between mica plates are measured.
SFG	Sum frequency generation (133-135)	Similar to SHG. One of the lasers has a tunable frequency that permits variation of the second harmonic signal. In this way the vibrational excitation of the adsorbed molecules is achieved.	Surface structure
SHG	Second harmonic generation (133, 136, 137)	A surface is illuminated with a high-intensity laser, and photons are generated at the second harmonic frequency through nonlinear optical processes. For many materials, only the surface region has the appropriate symmetry to produce the SHG signal. The nonlinear polarizability tensor depends on the nature and geometry of adsorbed atoms and molecules.	Electronic structure, molecular orientation
SIMS	Secondary ion mass spectrometry (2-4, 99, 138-144)	Ions and ionized clusters ejected from a surface during ion bombardment are detected with a mass spectrometer. Surface chemical composition and some information on bonding can be extracted from SIMS ion fragment distributions.	Surface composition
SPI	Surface penning ionization (2, 23)	Natural atoms, usually He, in electronically excited states collide with a surface at thermal energies. A surface electron may tunnel into an occupied electronic level of the incoming gas atom, causing the incident atom to ionize and eject an electron, which is then detected. This technique measures the density of states near the Fermi level of the substrate and is highly surface-sensitive.	Electronic structure
SPLEED	Spin-polarized low-energy electron diffraction (24, 145)	Similar to LEED, except the incident electron beam is spin-polarized. This is particularly useful for the study of surface magnetism and magnetic ordering.	Magnetic structure
STM	Scanning tunneling microscopy (2, 35, 146-152)	The topography of a surface is measured by mechanically scanning of a probe over a surface. The distance from the probe to the surface is measured by the probe-surface tunneling current. Angstrom resolution of surface features is routinely obtained.	Surface structure
SXAPS	Soft X-ray appearance potential spectroscopy	Another name for APXPS	
TEM	Transmission electron microscopy (11, 12, 153, 154)	TEM can provide surface information for carefully prepared and oriented bulk samples. Real images have been formed of the edges of crystals where surface planes	Surface structure

		and surface diffusions have been observed. Diffraction patterns of reconstructed surfaces, superimposed on the bulk diffraction pattern, have also provided surface structural information.	
TDS	Thermal desorption spectroscopy (3, 155-159)	An adsorbate-covered surface is heated, usually at a linear rate, and the desorbing atoms or molecules are detected with a mass spectrometer. This gives information on the nature of adsorbate species and some information on adsorption energies and the surface structure.	Composition, heat of adsorption, surface structure
TDP	Temperature programmed desorption (3, 157-159)	Similar to TDS, except the surface may be heated at a nonuniform rate to obtain more selective information on adsorption energies.	Composition, heat of adsorption, surface structure
UPS	Ultraviolet photoemission spectroscopy (2-4, 20, 22, 23, 42, 89, 160, 161) Work function measurements (3, 20, 22, 162, 163)	Electrons photoemitted from the valence and conduction bands are detected as a function of energy to measure the electronic density of states near the surface. This gives information on the bonding of adsorbates to the surface (see ARUPS). Changes in substrate's work function during the adsorption of atoms and molecules provide information about charge transfer between the adsorbate and the substrate and also about chemical bonding.	Valance band structure Electronic structure
XANES	X-ray absorption near-edge structure	Another name for NEXAFS.	
XPS	X-ray photoemission spectroscopy (2-4, 16, 22, 61-63, 164, 165)	Electrons photoemitted from atomic core levels are detected as a function of energy. The shifts of core-level energies give information on the chemical environment of the atoms (see ARXPS, ARXPD).	Composition, oxidation state
XRD	X-ray diffraction (166-168)	X-ray has been carried out at extreme glancing angles of incidence where total reflection ensures surface sensitivity. This provides structural information that can be interpreted by well-known methods. An extremely high X-ray flux is required to obtain useful data from single-crystal surfaces. Bulk X-ray diffraction is used to determine the structure of organometallic clusters, which provide comparisons to molecules adsorbed on surfaces.	Surface structure

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