A

From Abbe's principle to Azbel'–Kaner cyclotron resonance

Abbe's principle states that the smallest distance that can be resolved between two lines by optical instruments is proportional to the wavelength and inversely proportional to the angular distribution of the light observed ($d_{min} = \lambda / n \sin \alpha$). It establishes a prominent physical problem, known as the ''diffraction limit''. That is why it is also called **Abbe's resolution limit**. No matter how perfect an optical instrument is, its resolving capability will always have this diffraction limit. The limits of light microscopy are thus determined by the wavelength of visible light, which is 400–700 nm; the maximum resolving power of the light microscope is limited to about half the wavelength, typically about 300 nm. This value is close to the diameter of a small **bacterium**, and **virus**es, which cannot therefore be visualized. To attain sublight microscopic resolution, a new type of instrument would be needed; as we know today, accelerated electrons, which have a much smaller wavelength, are used in suitable instruments to scrutinize structures down to the 1 nm range.

The diffraction limit of light was first surpassed by the use of **scanning near-field optical microscopes**; by positioning a sharp optical probe only a few nanometers away from the object, the regime of far-field wave physics is circumvented, and the resolution is determined by the probe–sample distance and by the size of the probe which is scanned over the sample.

Also, fluorescence light microscopy based techniques have been developed in order to break the diffraction barrier, as in the case of **fluorescence nanoscopy**.

First described in: E. Abbe, *Beiträge zur Theorie des Mikroskops und der mikroskopischen Wahrnehmung*, Schultzes Archiv für mikroskopische Anatomie **9**, 413–668 (1873).

Abbe's resolution limit → **Abbe's principle**.

More details in: R. Leach, *Fundamental Principles of Engineering Nanometrology* (Elsevier, London, 2010).

aberration – any image defect revealed as distortion or blurring in optics. This deviation from perfect image formation can be produced by optical lenses, mirrors and electron lens systems. Examples are astigmatism, chromatic or lateral aberration, coma, curvature of field, distortion, and spherical aberration.

What is What in the Nanoworld, Third Edition. Victor E. Borisenko and Stefano Ossicini.

In astronomy, it is an apparent angular displacement in the direction of motion of the observer of any celestial object due to the combination of the velocity of light and of the velocity of the observer.

***ab initio* (approach, theory, calculations)** – Latin meaning “from the beginning”. It supposes that primary postulates, also called first principles, form the background of the referred theory, approach or calculations. The primary postulates are not so directly obvious from experiment, but owe their acceptance to the fact that conclusions drawn from them, often by long chains of reasoning, agree with experiment in all of the tests which have been made. For example, calculations based on the **Schrödinger** wave **equation**, as well as on the basis of **Newton equations** of motion or any other fundamental equations, are considered to be *ab initio* calculations.

Abney’s law states that the shift in apparent hue of spectral color that is desaturated by addition of white light is toward the red end of the spectrum if the wavelength is below 570 nm and toward the blue if it is above.

First described in: W. Abney, E. R. Festing, *Colour photometry*, Phil. Trans. Roy. Soc. London **177**, 423–456 (1886).

More details in: W. Abney, *Researches in colour vision* (Longmans & Green, London, 1913).

Abrikosov vortex – a specific arrangement of lines of a magnetic field in a **type II superconductor**.

First described in: A. A. Abrikosov, *An influence of the size on the critical field for type II superconductors,* Doklady Akademii Nauk SSSR **86**(3), 489–492 (1952) – in Russian.

Recognition: in 2003 A. A. Abrikosov, V. L. Ginzburg, A. J. Leggett received the Nobel Prize in Physics for pioneering contributions to the theory of superconductors and superfluids.

See also www.nobel.se/physics/laureates/2003/index.html.

More details in: A. A. Abrikosov, Nobel Lecture: *Type-II superconductors and the vortex lattice,* Rev. Mod. Phys. **76**(3), 975–979 (2004).

absorption – a phenomenon arising when electromagnetic radiation or atomic particles enter matter. In general, two kinds of attenuation accompany the passage of radiation and particles through matter, which are absorption and scattering. Both obey the law $I = I_0\exp(-\alpha x)$, where I_0 is the intensity (flux density) of radiation entering the matter, and I is the intensity depth x. In the absence of scatter, α is the **absorption coefficient**, and in the absence of absorption, α is the scattering coefficient. If both forms of attenuation are present, α is termed the total absorption coefficient → **dielectric function**.

acceptor (atom) – an impurity atom, typically in semiconductors, which accepts electron(s). Acceptor atoms usually form electron energy levels slightly higher than the uppermost field energy band, which is the valence band in semiconductors and dielectrics. An electron from this band is readily excited into the acceptor level. The consequent deficiency in the previously filled band contributes to the hole conduction.

achiral → **chirality**.

acoustic phonon – a quantum of excitation related to an acoustic mode of atomic vibrations in solids → **phonon**.

actinic – pertaining to electromagnetic radiation capable of initiating photochemical reactions, as in photography or the fading of pigments.

actinodielectric – a dielectric exhibiting an increase in electrical conductivity when electromagnetic radiation is incident upon it.

activation energy – an energy in excess over a ground state, which must be added to a system to allow a particular process to take place.

adatom – an atom adsorbed on a solid surface.

adduct – a chemical compound that forms from the addition of two or more substances. The term comes from Latin meaning "drawn toward". An adduct is a product of the direct addition of two or more distinct molecules, resulting in a single reaction product containing all atoms of all components, with formation of two chemical bonds and a net reduction in bond multiplicity in at least one of the reactants. The resultant is considered a distinct molecular species. In general, the term is often used specifically for products of addition reactions.

adiabatic approximation is used to solve the **Schrödinger equation** for electrons in solids. It assumes that a change in the coordinates of a nucleus passes no energy to electrons, that is the electrons respond adiabatically, which then allows the decoupling of the motion of the nuclei and electrons → **Born-Oppenheimer approximation**.

adhesion – the property of a solid to cling to another solid controlled by intermolecular forces at their interface.

adiabatic principle – perturbations produced in a system by altering slowly external conditions resulting, in general, in a change in the energy distribution in it, but leaving the phase integrals unchanged.

adiabatic process – a thermodynamic procedure which take place in a system without an exchange of heat with surroundings.

adjacent charge rule states that it is possible to write formal electronic structures for some molecules where adjacent atoms have formal charges of the same sign. In the Pauling formulation (1939), it states that such structures will not be important owing to instability resulting from the charge distribution.

adjoint operator – an operator **B** such that the inner products ($\mathbf{A}x,y$) and ($x,\mathbf{B}y$) are equal for a given operator **A** and for all elements x and y of the **Hilbert space**. It is also known as **associate operator** and **Hermitian conjugate operator**.

adjoint wave functions – functions in the Dirac electron theory which are formed by applying the **Dirac matrix** to the **adjoint operators** of the original wave functions.

admittance – a measure of how readily alternating current will flow in an electric circuit. It is the reciprocal of **impedance**. The term was introduced by Heaviside (1878).

adsorption – a type of **absorption**, in which only the surface of a matter acts as the absorbing medium. **Physisorption** and **chemisorption** are distinguished as adsorption mechanisms.

Term coined by: H. Kayser *Über die Verdichtung von Gasen an Oberflächen in ihrer Abhängigkeit von Druck und Temperatur*, Ann. Phys. **12**, 526–547 (1880).

AES – an acronym for **Auger electron spectroscopy**.

affinity → **electron affinity**.

AFM – an acronym for **atomic force microscopy**.

Aharonov–Bohm effect – the total amplitude of electron waves at a certain point oscillates periodically with respect to the magnetic flux enclosed by the two paths due to the interference effect. The design of the interferometer appropriate for experimental observation of this effect is shown in Figure A.1. Electron waves come from the waveguide to left terminal, split into two equal amplitudes going around the two halves of the ring, meet each other and interfere in the right part of the ring, and leave it through the right terminal. A small solenoid carrying magnetic flux Φ is positioned entirely inside the ring so that its magnetic field passes through the annulus of the ring. It is preferable to have the waveguide sufficiently small in order to restrict a number of possible coming electron modes to one or a few.

The overall current through the structure from the left port to the right one depends on the relation between the length of the ring arms and the inelastic mean

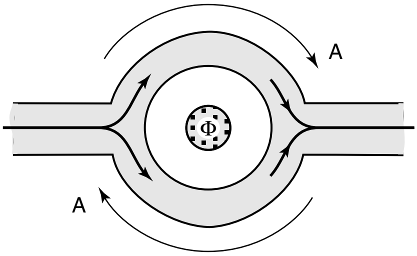

Figure A.1 Schematic layout of the interferometer for observation of the Aharonov–Bohm effect. Small solenoid inside the ring produces the magnetic field of the flux Φ enclosed between the two arms and characterized by the vector potential **A**.

free path of electrons in the ring material. If this relation meets the requirements for quasi-ballistic transport, the current is determined by the phase interference of the electron waves at the exit (right) terminal. The vector potential **A** of the magnetic field passing through the ring annulus is azimuthal. Hence electrons travelling in either arms of the ring move either parallel or antiparallel to the vector potential. As a result, there is a difference in the phases of the electron waves coming to the exit port from different arms. It is defined to be $\Delta\Phi = \mathbf{2}\pi(\Phi/\Phi_0)$, where $\Phi_0 = h/e$ is the quantum of flux. The interference of the electron waves appears to be periodic in the number of flux quanta passing through the ring. It is constructive when Φ is a multiple of Φ_0 and destructive halfway between. It produces a periodic modulation in the transverse conductance (resistance) of the ring by the magnetic field, which is known as the magnetic Aharonov–Bohm effect. It is worthwhile to note here that real devices hardly meet the requirements for observation of ‘‘pure’’ Aharonov–Bohm effect. The point is that the magnetic field penetrates the arms of the interferometer, not just the area enclosed by them. This leads to additional current variations at high magnetic fields, while the enclosed flux dominates at low magnetic fields.

First described in: Y. Aharonov, D. Bohm, *Significance of electromagnetic potentials in the quantum theory*, Phys. Rev. **115**(3), 485–491 (1959).

More details in: A. Batelaan, A. Tonomura, *The Aharonov–Bohm effects: Variations on a subtle theme*. Phys. Today **62**(9), 38–43 (2009).

Aharonov–Casher effect supposes that a beam of neutral particles with magnetic dipole moments passing around opposite sides of a line charge will undergo a relative quantum phase shift. The effect has a ‘‘duality’’ with the **Aharonov–Bohm effect**, where charged particles passing around a magnetic solenoid experience a phase shift despite, it is claimed, experiencing no classical force. It is pointed out that a magnetic dipole particle passing a line charge does indeed experience a classical electromagnetic force in the usual electric-current model for a magnetic dipole. This force will produce a relative lag between dipoles passing on opposite sides of the line charge, and the classical lag then leads to a quantum phase shift. Thus, the effect has a transparent explanation as a classical lag effect.

First described in: Y. Aharonov, A. Casher, *Topological quantum effects for neutral particles*, Phys. Rev. Lett. **53**(4), 319–321 (1984).

More details in: D. Rohrlich, *The Aharonov-Casher effect*, in: *Compendium of Quantum Physics: Concepts, Experiments, History and Philosophy*, edited by F. Weinert, K. Hentschel, D. Greenberger, B. Falkenburg (Springer, Berlin, 2009).

Airy equation – the second order differential equation $d^2y/dx^2 = xy$, also known as the **Stokes equation**. Here x represents the independent variable and y is the value of the function.

First described in: G. B. Airy, Trans. Camb. Phil. Soc. **6**, 379 (1838); G. B. Airy, *An Elementary Treatise on Partial Differential Equations* (1866).

Airy functions – solutions of the **Airy equation**. The equation has two linearly independent solutions, conventionally taken as the Airy integral functions Ai(x) and Bi(x). They are plotted in Figure A.2. There are no simple expressions for them in terms of elementary functions, while for large absolute values of x: $\mathrm{Ai}(x) \sim \pi^{-1/2}x^{-1/4}\exp[-(2/3)x^{3/2}]$, $\mathrm{Ai}(-x) \sim (1/2)\pi^{-1/2}x^{-1/4}\cos[-(2/3)x^{3/2} - \pi/4]$. Airy functions arise in solutions of the **Schrödinger equation** for some particular cases.

First described in: G. B. Airy, *An Elementary Treatise on Partial Differential Equations* (1866).

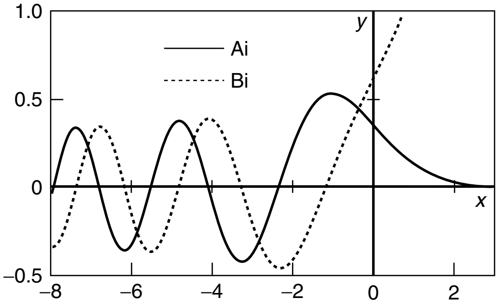

Figure A.2 Airy functions.

Airy spirals – spiral interference patterns formed by quartz cut perpendicularly to the axis in convergent circularly polarized light.

Recognition: in 1831 G. B. Airy received the Copley Medal of the Royal Society for their studies on optical subjects.

ALD –an acronym for **atomic layer deposition**.

aldehydes – organic compounds that have at least one hydrogen atom bonded to the **carbonyl group** (>C=O). These may be RCHO or ArCHO compounds with R representing an **alkyl group** ($–C_nH_{2n+1}$) and Ar representing an **aromatic ring**.

algorithm – a set of well-defined rules for the solution of a problem in a finite number of steps.

aliphatic compound – an organic compound in which carbon atoms are joined together in straight or branched chains. The simplest aliphatic compound is methane (CH_4). Most aliphatic compounds provide exothermic combustion reactions, thus allowing their use as a fuel.

alkanes → **hydrocarbons**.

alkenes → **hydrocarbons**.

alkyl groups → **hydrocarbons**.

allotropy – the property of a chemical element to exist in two or more different structural modifications in the solid state. The term **polymorphism** is used for compounds.

alternating current Josephson effect → **Josephson effects**.

Al'tshuler–Aronov–Spivak effect – occurs when the resistance of the conductor in the shape of a hollow cylinder oscillates as a function of the magnetic flux threading through the hollow with a period of $hc/2e$. This effect was predicted for the diffusive regime of the charge transport where the mean free path of the electrons is much smaller than the sample size. The conductance amplitude of the oscillations is of the order of e^2/h and depends on the phase coherence length over which an electron maintains its phase coherence. Coherent backscattering of an electron when there is interference in a pair of backscattered spatial waves with time-reversal symmetry causes the oscillations.

First described in: B. L. Al'tshuler, A. G. Aronov, B. Z. Spivak, *Aharonov–Bohm effect in non-ordered conductors*, Pis'ma Zh. Eksp. Teor. Fiz. **33**(2), 101–103 (1981) – in Russian.

More details in: K. Nakamura, T. Harayama, *Quantum Chaos and Quantum Dots* (Oxford University Press, Oxford, 2004).

amides – organic compounds that are nitrogen derivates of **carboxylic acids**. The carbon atom of a carbonyl group ($>C=O$) is bonded directly to a nitrogen atom of an $-NH_2$, $-NHR$ or $-NR_2$ group, where R represents an **alkyl group** ($-C_nH_{2n+1}$). The general formula of amides is $RCONH_2$.

amines – organic compounds that are ammonia molecules with hydrogen substituted by **alkyl groups** ($-C_nH_{2n+1}$) or **aromatic rings**. These can be RNH_2, R_2NH, or R_3N, where R is an alkyl or aromatic group.

amino acid – an organic compound containing an amino group (NH_2), a carboxylic acid group (COOH), and any of various side groups that are linked together by **peptide bonds**. The basic formula is $NH_2CHRCOOH$. Amino acids are building blocks of **proteins**.

There are twenty standard amino acids used in protein biosynthesis. These are presented in Figure A.3.

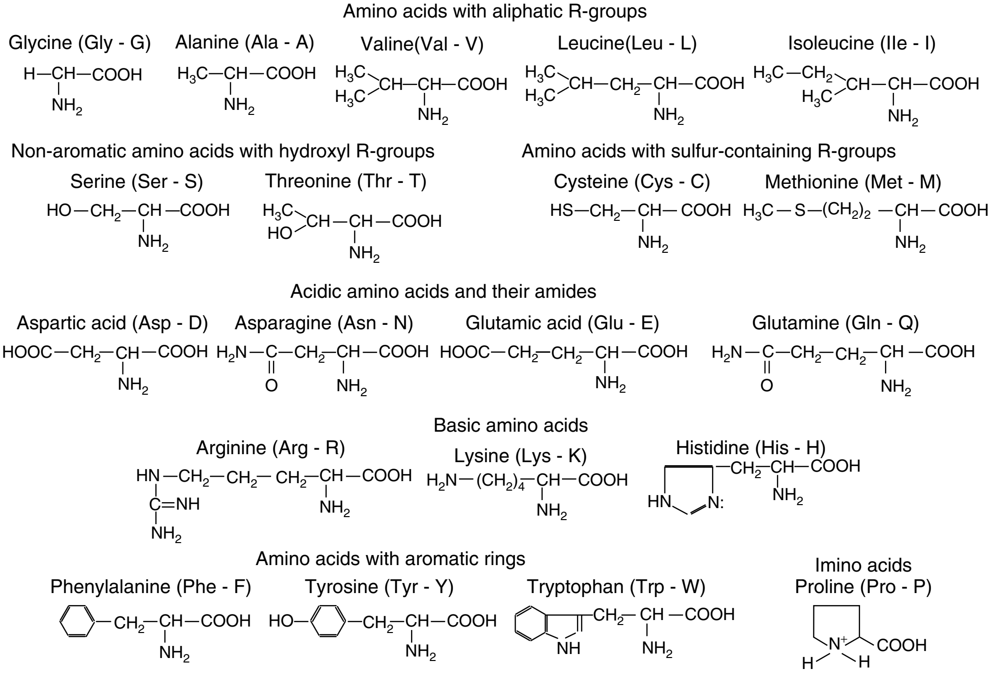

Figure A.3 Amino acids found in proteins. Their symbols are shown in parentheses.

Just as the letters of the alphabet can be combined to form an almost endless variety of words, amino acids can be linked in varying sequences to form a huge variety of proteins.

More details in: //en.wikipedia.org/wiki/Amino_acid.

Amontons' law currently supposes the statement that the friction force between two bodies is directly proportional to the applied load (normal), with a constant of proportionality that is the friction coefficient. This force is constant and independent of the contact area, the surface roughness and the sliding velocity.

In fact, this statement is a combination of a few laws: the law of Euler and Amontons stating that friction is proportional to the loading force, the law of Coulomb → **Coulomb law (mechanics)** stating that friction is independent of the velocity, and the law of Leonardo da Vinci stating that friction is independent of the area of contact. In particular, Leonardo da Vinci arrived (1500) at the result that on an inclined plane a slider would move if the ratio between the tangential and normal components of the gravitational force exceeded one-fourth.

First described in: G. Amontons, *De la résistance causée dans les machines,* Mem. Acad. Roy. Sci. A, 206–222 (1699).

More details in: R. Schnurmann, *Amontons' law, "traces" of frictional contact, and experiments on adhesion*, J. Appl. Phys. **13**(4), 235 (1942).

amorphous solid – a solid with no long-range atomic order.

Ampère currents – molecular-ring currents postulated to explain the phenomenon of magnetism as well as the apparent nonexistence of isolated magnetic poles.

Ampère's law, as amended by Maxwell, states that magnetomotive force round any closed curve equals the electric current flowing through any closed surface bounded by the curve. The force appears clockwise to an observer looking in the direction of the current. It means that $\int \mathbf{Hdl} = I$, where $\mathbf{H}$ is the magnetic field strength, I is the current enclosed. The linear integral is taken round any closed path. If the current is flowing in a conducting medium, $I = \int \mathbf{Jds}$, where $\mathbf{J}$ is the current density. Finally, it may be shown that $\nabla x\mathbf{H} = \mathbf{J}$, which is a statement of Ampère's law at a point in a conducting medium.

First described in: A. M. Ampère, *Mémoire sur les effets du courant électrique,* Annales de chimie et de physique **15**, 59–118 (1820).

More details in: André-Marie Ampère, *Exposé méthodique des phénomènes électrodynamiques et des lois de ces phénomènes* (Plasson, Paris, 1822).

Ampère's rule states that the direction of the magnetic field surrounding a conductor will be clockwise when viewed from the conductor if the direction of current flow is away from the observer.

First described in: A. M. Ampère, *Mémoire sur les effets du courant électrique,* Annales de chimie et de physique **15**, 59–118 (1820).

More details in: André-Marie Ampère, *Exposé méthodique des phénomènes électrodynamiques et des lois de ces phénomènes* (Plasson, Paris, 1822).

Ampère's theorem states that an electric current flowing in a circuit produces a magnetic field at external points equivalent to that due to a magnetic shell whose bounding edge is the the conductor and whose strength is equal to the strength of the current.

First described in: A. M. Ampère, *Mémoire sur les effets du courant électrique,* Annales de chimie et de physique **15**, 59–118 (1820).

More details in: André-Marie Ampère, *Exposé méthodique des phénomènes électrodynamiques et des lois de ces phénomènes* (Plasson, Paris, 1822).

amphichiral → **chirality**.

AND operator → **logic operator**.

Anderson insulator – a solid state material with insulating properties defined by the interaction of electrons with impurities and other lattice imperfections. The material is characterized by a robust energy gap, which is a gap for charge excitations between the **Fermi energy** and spatially extended states. Any related metal-to-insulator transition is a type of quantum phase transitions in which the energy gap is formed.

More details in: F. Gebhard, *The Mott Metal-Insulator Transition: Models and Methods* (Springer, Heidelberg, 2010).

Andersen-Nose algorithm – a method used in **molecular dynamics simulation** for numerical integration of ordinary differential equation systems based on a quadratic presentation of time-dependent atom displacement.

First described in: S. Nose, F. Yonezawa, *Isothermal–isobaric computer simulations of melting and crystallization of a Lennard–Jones system*, J. Chem. Phys. **84**(3), 1803–1812 (1986).

Anderson localization means that electron wave function becomes spatially localized and the conductivity vanishes at zero temperature when the mean free path of electrons is short comparable to the Fermi wavelength ($\lambda_F = 2\pi/k_F$); multiple scattering becomes important. Metal-insulator transition takes place due to disorders. In the localized states, the wave function decays exponentially away from the localization center, that is $\psi(r) \sim \exp(-r/\xi)$, where ξ is called the localization length. Anderson localization depends strongly on dimensionality.

First described in: P. W. Anderson, *Absence of diffusion in certain random lattices*, Phys. Rev. **109**(5), 1492–1505 (1958).

Recognition: in 1977 P. W. Anderson, N. F. Mott and J. H. van Vleck received the Nobel Prize in Physics for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems.

See also www.nobel.se/physics/laureates/1977/index.html.

Anderson rule, which is also called the **electron affinity rule**, states that vacuum levels of two materials forming a **heterojunction** should be lined up. It is used for construction of energy band diagrams of **heterojunctions** and **quantum wells**.

The **electron affinity** χ of the materials is used for the lining up procedure. This material parameter is nearly independent of the position of the Fermi level, unlike the **work function**, which is measured from the Fermi level and therefore depends strongly on doping.

Figure A.4 shows the band alignment at the interface between small band gap material A with the electron affinity χ_A and large band gap material B with the electron affinity χ_B supposing $\chi_A > \chi_B$. According to the rule the offset of the conduction band $\Delta E_c = \Delta E_{cB} - \Delta E_{cA} = \chi_A - \chi_B$. Correspondingly, the offset of the valence band ΔE_v can be predicted from the above diagram accounting for both electron affinities and band gaps of the materials. At a temperature above absolute zero the

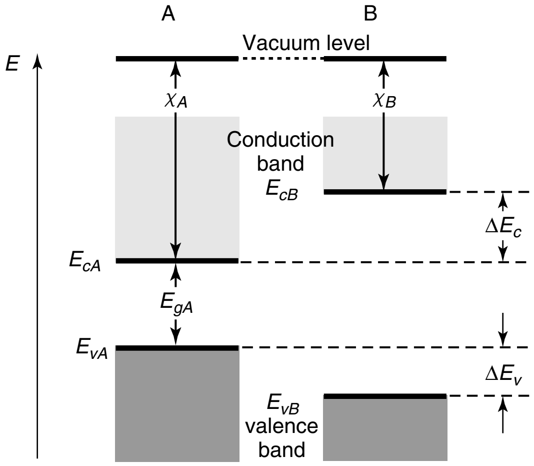

Figure A.4 Alignment of the bands at a heterojunction according to Anderson's rule.

misalignment of the Fermi levels, if there is any, is eliminated by redistribution of free charge carriers at the interface between the barrier and well regions.

The validity of the rule was discussed by H. Kroemer in his paper *Problems in the theory heterojunction discontinuities* CRC Crit. Rev. Solid State Sci. **5**(4), 555–564 (1975). The hidden assumption about the relation between the properties of the interface between two semiconductors and those of the much more drastic vacuum-to-semiconductor interface is a weak point of the rule.

First described in: R. L. Anderson, *Germanium-gallium arsenide heterojunction*, IBM J. Res. Dev. **4**(3), 283–287 (1960).

Andreev process – reflection of a **quasiparticle** from the potential barrier formed by normal **conductor** and **superconductor** when the barrier height is less than the particle energy. It results in the temperature leap at the barrier if a heat flow takes place there. The conductor part of the structure can be made of a metal, **semimetal** or degenerate **semiconductor**.

The basic concept of the process is schematically illustrated in Figure A.5 for an electron crossing the interface between a conductor and superconductor.

There is a superconducting energy gap opened up for a single electron on the superconductor side. Thus, an electron approaching the barrier from the metal side with the energy above the **Fermi level**, but still within the gap, cannot be accommodated in the superconductor as a single particle. It can only form a **Cooper pair** there that needs an additional electron from the metal side with the energy below the Fermi level to come. This removed electron leaves behind a hole in the Fermi sea. If the incident electron had a momentum $\hbar k$, the generated hole has the momentum $-\hbar k$. It traces the same path as the electron, but in the opposite direction. Describing the phenomenon one says that the incident electron is reflected as a hole.

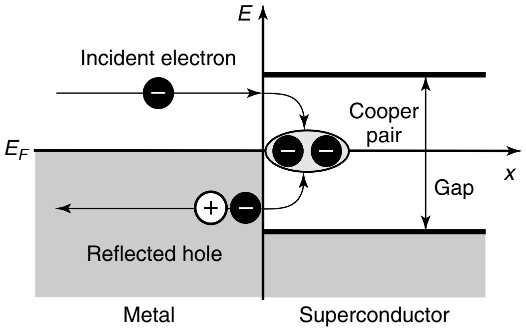

Figure A.5 Andreev reflection process.

First described in: A. F. Andreev, *Thermal conductivity of the intermediate state of superconductors,* Zh. Exp. Teor. Fiz. **46**(5), 1823–1928 (1964) – in Russian.

More details in: C. W. J. Beenakker, *Colloquium: Andreev reflection and Klein tunneling in graphene,* Rev. Mod. Phys. **80**(4), 1337–1354 (2008).

Ångstrom – a metric unit of length measurements that corresponds to 10^{-10} m. The atomic diameters are in the range of 1–2 Å. It is named in honor of the nineteenth-century physicist Anders Jonas Ångstrom, one of the founders of modern spectroscopy.

angular momentum – the energy of a rotating particle. It is quantized for quantum particles as $L^2 = l(l+1)\hbar^2$, where $l = 0, 1, 2, n-1$, where n is the principal quantum number. In an atom electrons with $l = 0$ are termed s states, $l = 1$ (p states), $l = 2$ (d states), $l = 3$ (f states), $l = 4$ (g states). The letters s, p, d were first used to describe characteristic features of spectroscopic lines and stand for ''sharp'', ''principal'', and ''diffuse''. After d the letters run alphabetically.

anisodesmic structure – a structure of an ionic crystal in which bound groups of ions tend to be formed → **mesodesmic** and **isodesmic structures**.

anisotropy (of matter) – different physical properties of a medium in different directions. The alternative is **isotropy**.

anisotropic magnetic resistance – the difference in **magnetoresistance** when the resistance of a **conductor** is measured by the current passing either parallel or perpendicular to the material → **giant magnetoresistance effect**.

First described in: W. Thomson (Lord Kelvin), *On the electro-dynamic qualities of metals: effects of magnetization on the electric conductivity of nickel and of iron,* Proc. R. Soc. London **8**, 546–550 (1856).

anodizing = anodic oxidation, is the formation of an adherent oxide film on the surface of a metal or semiconductor when it is anodically polarized in a suitable electrolyte or plasma of an electric discharge in a gas.

anomalous Hall effect – an additional voltage proportional to the magnetization arising in **Hall effect** measurements in **ferromagnetic** materials. Unlike the ordinary **Hall effect**, this contribution is strongly temperature dependent.

The related transverse resistivity ρ_{xy} in ferromagnetics contains the contribution due to the magnetization M in addition to the usual **Hall effect**: $\rho_{xy} = R_0 B + 4\pi R_a M$, where B is the magnetic field induction, R_0 is the usual Hall coefficient, and R_a is the anomalous Hall coefficient. This expression can be used as an experimental tool to measure the magnetization as a function of temperature.

In general, the anomalous Hall effect occurs in solids with broken time- reversal symmetry, typically in a ferromagnetic phase, as a consequence of **spin–orbit coupling**.

First described in: E. H. Hall, *On the new action of magnetism on a permanet electric current*, Philos. Mag. **10**, 301–329 (1880); E. H. Hall, *On the possibility of transverse currents in ferromagnets*, Philos. Mag. **12**, 157–160 (1881).

More details in: N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, N. P. Ong, *Anomalous Hall effect*, Rev. Mod. Phys. **82**(2), 1539–1592 (2010).

See also www.lakeshore.com/pdf-files/systems/Hall-Data-Sheets/Anomalous-Hall1.pdf.

anomalous Zeeman effect → **Zeeman effect**.

antibody – an inducible immunoglobulin **protein** produced by B lymphocytes of the immune system, in humans and other higher animals, which recognizes and binds to a specific **antigen** molecule of a foreign substance introduced into the organism. When antibodies bind to corresponding antigens they set in motion a process to eliminate the antigens.

antibonding orbital – the orbital which, if occupied, raises the energy of a molecule relative to the separated atoms. The corresponding wave function is orthogonal to that of the bonding state → **bonding orbital**.

antiferroelectric – a dielectric of high permittivity, which undergoes a change in crystal structure at a certain transition temperature, usually called the antiferroelectric **Curie temperature**. The antiferroelectric state in contrast to a **ferroelectric** state possesses no net spontaneous polarization below the Curie temperature. No hysteresis effects are therefore exhibited by this type of materials. Examples: $BaTiO_3$, $PbZrO_3$, $NaNbO_3$.

antiferromagnetic → **magnetism**.

antigen – any foreign substance, such as virus, bacterium, or **protein**, which, after introduction into an organism (humans and higher animals), elicits an immune response by stimulating the production of specific **antibodies**. It also can be any large molecule, which binds specifically to an antibody.

anti-Stokes line → **Raman effect**.

anti-dot – a **quantum dot** made of wider band gap semiconductor in/on a smaller band gap semiconductor, for example Si dot in/on Ge substrate. It repels charge carriers rather than attracting them.

anti-wires – the **quantum wires** made of wider band gap semiconductor in/on a smaller band gap semiconductor. They repel charge carriers rather than attracting them.

APCVD – an acronym for **atmospheric pressure chemical vapor deposition**.

APFIM – an acronym for **atom probe field ion microscopy**.

a priori – Latin meaning ''before the day''. It usually indicates some postulates or facts known logically prior to the referred proposition. It pertains to deductive reasoning from assumed axioms or self-evident principles.

approximate self-consistent molecular orbital method – the **Hartree-Fock theory** as it stands is too time consuming for use in large systems. However, it can be used in a parametrized form, and this is the basis of many of the semi-empirical codes used like **Complete Neglect of Differential Overlap (CNDO)** and **Intermediate Neglect of Differential Overlap (INDO)**.

In the **CNDO** method all integrals involving different atomic orbitals are ignored. Thus, the overlap matrix becomes the unit matrix. Moreover, all the two-center electron integrals between a pair of atoms are set equal and the resonance integrals are set proportional to the overlap matrix. A minimum basis set of valence orbital is chosen using **Slater type orbitals**. These approximations strongly simplify the Fock equation.

In the **INDO** method the constraint present in CNDO that the monocentric two-electron integrals are set equal is removed. Since INDO and CNDO execute on a computer at about the same speed and INDO contains some important integrals neglected in CNDO, INDO performs much better than CNDO especially in prediction of molecular spectral properties.

It is interesting to note that the first papers dealing with the CNDO method appear in a supplementary issue of the Journal of Chemical Physics that contains the proceedings of the International Symposium on Atomic and Molecular Quantum theory dedicated to R. S. Mulliken → **Hund–Mulliken theory**, held in USA on 18–23 January 1965.

First described in: J. A. Pople, D. P. Santry, G. A. Segal, *Approximate self-consistent molecular orbital theory. I. Invariant procedures*, J. Chem. Phys. **43**(10), S129–S135 (1965); J. A. Pople, D. P. Santry, G. A. Segal, *Approximate self-consistent molecular orbital theory. II. Calculations with complete neglect of differential overlap*, J. Chem. Phys. 43(10), S136–S151 (1965); J. A. Pople, D. P. Santry, G. A. Segal, *Approximate self consistent molecular orbital theory. III. CNDO results for AB_2 and AB_3 systems*, J. Chem. Phys. **44**(9), 3289–3296 (1965).

More details in: J. A. Pople, *Quantum chemical models*, Rev. Mod. Phys., **71** (5), 1267–1274 (1999).

Recognition: in 1998 J. A. Pople shared with W. Kohn the Nobel Prize in Chemistry for his development of computational methods in quantum chemistry.

See also www.nobel.se/chemistry/laureates/1998/index.html.

APW – an acronym for an **augmented plane wave**.

archaea – are single-celled organisms thriving in a variety of habitats. Most of the archaea prefer extreme environments. Archaea form together with bacteria and eucarya the three domains in life.

argon laser – a type of **ion laser** with ionized argon as the active medium. It generates light in the blue and green visible light spectrum, with two energy peaks: at 488 and 514 nm.

armchair structure → **carbon nanotube**.

aromatic compounds → **hydrocarbons**.

aromatic ring → **hydrocarbons**.

Arrhenius equation – the equation in the form $V = V_0 \exp(-E_a/k_B T)$, which is often used to describe temperature dependence of a process or reaction rate V, where V_0 is the temperature independent pre-exponential factor, E_a is the activation energy of the process or reaction, and T is the absolute temperature. The plot representing $\log(V/V_0)$ as a function of $1/k_B T$ or $1/T$ is called the **Arrhenius plot**. It is used to extract the activation energy E_a as the slope of a linear part of the curve.

First described by J. H. van't Hoff in 1884; in 1889, S. Arrhenius provided a justification and interpretation for it. See S. A. Arrhenius, *Über die Reaktiongeschwindigkeit der Inversion vor Rohrzucker durch Säuren*, Z. Phys. Chem. **4**, 226 (1889).

Recognition: in 1901 J. H. van't Hoff received the Nobel Prize in Chemistry in recognition of the extraordinary services he has rendered by the discovery of the laws of chemical dynamics and osmotic pressure in solutions. In 1903 S. Arrhenius received the Nobel Prize in Chemistry in recognition of the extraordinary services he had rendered to the advancement of chemistry by his electrolytic theory of dissociation.

See also www.nobel.se/chemistry/laureates/1901/index.html.

See also www.nobel.se/chemistry/laureates/1903/index.html.

artificial atom(s) → **quantum confinement**.

Asaro–Tiller–Grinfeld instability arises in a growing stressed film, that is, the surface of the stressed film is unstable against perturbations with wavelengths longer than the critical wavelength,

$$\lambda_{cr} = \frac{\pi\gamma}{\varepsilon^2}\frac{(1-\nu)}{2G(1+\nu)^2},$$

where γ is the surface tension, ε is the misfit strain of the growing layer with respect to the substrate, ν is the **Poisson ratio** of the material, and G is its shear modulus.

First described in: R. J. Asaro, W. A. Tiller, *Surface morphology development during stress corrosion cracking: Part I: via surface diffusion*, Metall. Trans. **3**, 1789–1796 (1972); M. A. Grinfeld, *Instability of the separation boundary between a nonhydrostatically stressed elastic body and a melt*, Sov. Phys. Dokl. **31**, 831–835 (1986).

More details in: M. A. Grinfeld, *Thermodynamic Methods in the Theory of Heterogeneous Systems* (Longman, New York, 1991).

associate operator → **adjoint operator**.

atmospheric pressure chemical vapor deposition (APCVD) → **chemical vapor deposition**.

atomic engineering – a set of techniques used to built atomic-size structures. Atoms and molecules may be manipulated in a variety of ways by using the interaction present in the tunnel junction of **scanning tunneling microscope (STM)**. In a sense, there is a possibility to use the proximal probe in order to extend our touch to a realm where our hands are simply too big.

Two formal classes of atomic manipulation processes are distinguished: parallel processes and perpendicular processes. In the class of parallel processes an adsorbed atom or molecule is forced to move along the substrate surface. In the class of perpendicular processes the atom or molecular is transferred from the surface to the STM tip or vice versa. In both processes the goal is the purposeful rearrangement of matter on the atomic scale. One may view the act of rearrangement as a series of steps that results in the selective modification or breaking of chemical bonds between atoms and subsequent creation of new ones. It is equivalent to a procedure that causes a configuration of atoms to evolve along some time-dependent potential energy hyper-surface from an initial to a final configuration. Both points of view are useful in understanding physical mechanisms by which atoms may be manipulated with a proximal probe.

In the class of parallel processes, the bond between the manipulated atom and the underlying surface is never broken. This means that the adsorbate always lies within the absorption potential well. The relevant energy scale for these processes is the energy of the barrier to diffusion across the surface. This energy is typically in the range of 1/10 to 1/3 of the adsorption energy and thus varies from about 0.01 eV for weakly bound physisorbed atoms on a close-packed metal surface to 1 eV for strongly bound chemisorbed atoms. There are two parallel processes tested for atomic manipulation: field-assisted diffusion and sliding process.

The field-assisted diffusion is initiated by interaction of the spatially inhomogeneous electric field of an STM tip with the dipole moment of an adsorbed atom. The inhomogeneous electric field leads to a potential energy gradient at the surface resulting in a field-assisted directional diffusion motion of the adatom. In terms of the potential energy the process can be presented as follows.

An atom in an electric field $E(r)$ is polarized with a dipole moment $p = \mu + \overleftrightarrow{\alpha} E(r) + \cdots$, where μ is the static dipole moment, $\overleftrightarrow{\alpha} E(r)$ the induced dipole moment, and $\overleftrightarrow{\alpha}$ the polarizability tensor. The related spatially dependent energy of the atom is given by $U(r) = -\mu E(r) - 1/2 \overleftrightarrow{\alpha}(r) E(r) E(r) + \cdots$. This potential energy is added to the periodic potential at the substrate surface. Weak periodic corrugation of the energy occurs. The resulting potential reliefs are shown in Figure A.6. A broad or sharp potential well is formed under the STM tip depending on the particular interaction between the tip, adatom and substrate atoms. The interaction of the electric field with the adsorbate dipole moment gives rise to a broad potential well. The potential energy gradient causes the adatom to diffuse toward the potential minimum under the tip. When there is a strong attraction of the adsorbate to the tip by chemical binding, it leads to a rather steep potential well located directly below the tip apex. The adsorbate remains trapped in the well as the tip is moved laterally.

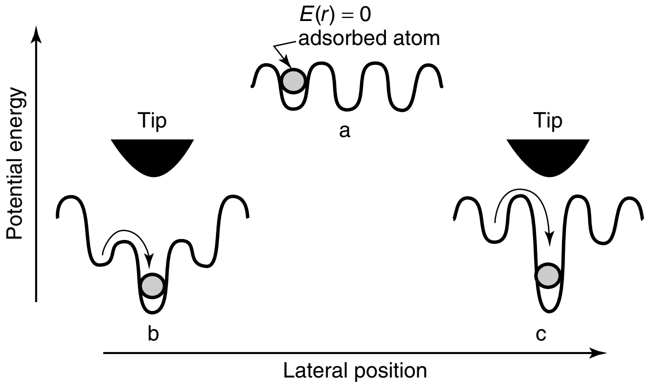

Figure A.6 Schematic of the potential energy of an adsorbed atom as a function of its lateral position on a surface above which there is located the STM tip.

Realization of field-assisted diffusion needs the substrate to be positively biased. At a negative substrate polarity the static and induced dipole terms being opposite in sign compensate each other. In this case no potential well and related stimulating energy gradient for diffusion are produced.

The sliding process supposes pulling of an adsorbate across the surface by the tip of a proximal probe. The tip always exerts a force on an adsorbate bound to the surface. One component of this force is due to the interatomic potential, that is, the chemical binding force, between the adsorbate and the outermost tip atoms. By adjusting the position of the tip one may tune the magnitude and the direction of the force exerted on the adsorbate, thus forcing it to move across the surface.

The main steps of atomic manipulation via the sliding process are depicted in Figure A.7. The adsorbate to be moved is first located with the STM in its imaging mode and then the tip is placed near the adsorbate (position "*a*"). The tip–adsorbate interaction is subsequently increased by lowering the tip toward the adsorbate (position "*b*"). This is achieved by changing the required tunnel current to a higher value and letting the feedback loop move the tip to a height which yields the higher demanded current. The adsorbate–tip attractive force must be sufficient to keep the adsorbate located beneath the tip. The tip is then moved laterally across the surface under constant current conditions (path "*c*") to the desired destination (position "*d*"), pulling the adsorbate along with it. The process is terminated by reverting to the imaging mode (position "*e*"), which leaves the adsorbate bound to the surface at the desired location.

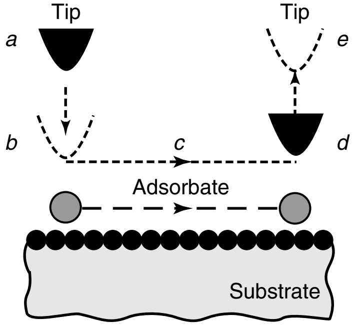

Figure A.7 Schematic of the sliding process: *a* and *e*–imaging, *b*–connecting, *c*–sliding, *d*–disconnecting.

In order for the adsorbate to follow the lateral motion of the tip, the tip must exert enough force on the adsorbate to overcome the lateral forces between the adsorbate and the surface. Roughly speaking, the force necessary to move an adsorbate from site to site across the surface is given by the ratio of the corrugation energy to the separation between atoms of the underlying surface. However, the presence of the tip may also cause the adsorbate to be displayed normal to the surface relative to its unperturbed position. The displaced adsorbate would have an altered in-plane interaction with the underlying surface. If the tip pulls the adsorbate away from the surface causing a reduction of this in-plane interaction, then we would expect our estimate to be an upper bound for the force necessary to move the adsorbate across the surface.

The manipulation of an adsorbate with the sliding process may be characterized by a threshold tip height. Above this height the adsorbate-tip interaction is too weak to allow manipulation. At the threshold this interaction is just strong enough to allow the tip to pull the adatom along the surface. The absolute height of the STM tip above the surface is not directly measured. But resistance of the tunnel junction strongly correlated to the tip–surface separation is accurately controlled. An increasing resistance corresponds to greater tip–surface separation, and hence to their weaker interaction. The threshold resistance to slide an adsorbate depends on the particular arrangement of atoms at the apex of the tip. But for that reason it can vary by not more than a factor of 4. The resistance is more sensitive to the chemical nature of the adatom and surface atoms ranging from tens kΩ to a few MΩ. The ordering of the threshold resistances is consistent with the simple notion that the corrugation energy scales with the binding energy and thus greater force must be applied to move adatoms that are more strongly bound to the surface.

In perpendicular processes an atom, molecule or group of atoms is transferred from the tip to the surface or initially from the surface to the tip and then back to a new site on the surface. In order to illustrate the main regularities of these processes we discuss transferring an adsorbed atom from the surface to the tip. The relevant energy for such process is the height of the potential barrier that the adsorbate should come through to go from the tip to the surface. The height of this barrier depends on the separation of the tip from the surface. It approaches the adsorption energy in the limit of large tip–surface separation and goes to zero when the tip is located close enough to the adsorbate. By adjusting the height of the tip one may tune the magnitude of this barrier. Electrical biasing of the tip with respect to the substrate, as it is usually performed in STM, controls the transfer process. Three approaches distinguished by the physical mechanisms employed have been proposed for perpendicular manipulations of atoms. These are transfer on- or near-contact, field evaporation and electromigration.

The transfer on- or near-contact is conceptually the simplest among the atomic manipulation processes. It supposes the tip to be moved toward the adsorbate until the adsorption well on the tip and surface sides of the junction coalesce. That is, the energy barrier separating the two wells is gone and the adsorbate can be considered simultaneously bound to the tip and the surface. The tip is then withdrawn, carrying the adsorbate with it. For the process to be successful the adsorbate's bond to the surface must be broken when the tip is moved out. One might expect that the adsorbate would ''choose'' to remain bound to the side of the junction on which it has the greatest binding energy. However, the ''moment of choice'' comes when the adsorbate has strong interactions with both tip and surface, so the binding energy argument may be too simple. It does not account for the simultaneous interaction of the adsorbate with the tip and the surface.

At a slightly increased separation between the tip and sample surface, the adsorption well of the tip and surface atom are close enough to significantly reduce the intermediate barrier but have it still remain finite, such that thermal activation is sufficient for atom transfer. It is called transfer-near-contact. This process has a rate proportional to $\nu\exp(-E_a/k_BT)$, where ν is the frequency factor, and E_a the reduced energy barrier between the tip and the sample. The transfer rate exhibits an anisotropy if the depth of the adsorption well is not the same on each side of the barrier. It is important to distinguish this transfer-near-contact mechanism from field evaporation, which requires an intermediate ionic state.

In its simplest form, the transfer on- or near-contact process occurs in the complete absence of any electric field, potential difference, or flow of current between the tip and the sample. Nevertheless, in some circumstances it should be possible to set the direction of transfer by biasing the junction during contact.

The field evaporation uses the ability of ions to drift in the electric field produced by an STM probe. It is a thermally activated process in which atoms at the tip or at the sample surface are ionized by the electric field and thermally evaporated. Drifting in this field they come more easily through the potential Schottky-type barrier separating the tip and the surface because this barrier appears to be decreased by the electric field applied. Such favorable conditions are simply realized for positively charged ions by the use of a pulse voltage applied to the tip separated from a sample surface by about 0.4 nm or smaller. Field evaporation of negative ions meets difficulties associated with the competing effect of field electron emission, which would melt the tip or surface at the fields necessary for negative ion formation.

The electromigration in the gap separating an STM tip and sample has much in common with the electromigration process in solids. There are two components of the force driving electromigration. The first is determined by the electrostatic interaction of the charged adsorbates with the electric field driving the electron current through the gap. The second, which is called the ''wind'' force, is induced by direct scattering of electrons at the atomic particles. These forces are most strongly felt by the atoms in the immediate vicinity of the tunnel junction formed by the tip of a proximal probe and sample surface. The highest electric field and current density are here. Within the electromigration mechanism the manipulated atoms always move in the same direction as the tunneling electrons. Moreover, ''heating'' of adsorbates by tunnel current stimulates electromigration as soon as a ''hot'' particle may more easily jump to a neighboring site. Atomic electromigration is a reversible process.

Summarizing the above-presented physical mechanisms used for manipulation of individual atoms with proximal probes one should remember that there is no universal approach among them. Applicability of each particular mechanism is mainly determined by the physical and chemical nature of the atoms supposed to be manipulated, by the substrate and to some extent by the probe material. An appropriate choice of the adsorbate/substrate systems still remains a state-of-art point.

More details in: *Handbook of Nanotechnology*, edited by B. Bhushan (Springer Verlag, Berlin Heidelberg, 2004).

atomic force microscope – an apparatus used for **atomic force microscopy**.

atomic force microscopy (AFM) originated from **scanning tunneling microscopy (STM)**. Atomic and molecular forces, rather than a tunneling current, are monitored and used for the surface characterization at the atomic scale. The forces are detected by a probe tip mounted on a flexible cantilever, as shown in Figure A.8. Deflection of the cantilever, to a good approximation, is directly proportional to the acting force. It is optically or electronically monitored with high precision. The deflection signal is used to modulate the tip–sample separation in the way it is done in STM with the tunneling current. While scanning, one can obtain a profile of atomic and molecular forces over the sample surface. The sensitivity of AFM to the electronic structure of the sample surface, inherent in STM, is largely absent. Therefore it allows characterization of nonconducting materials.

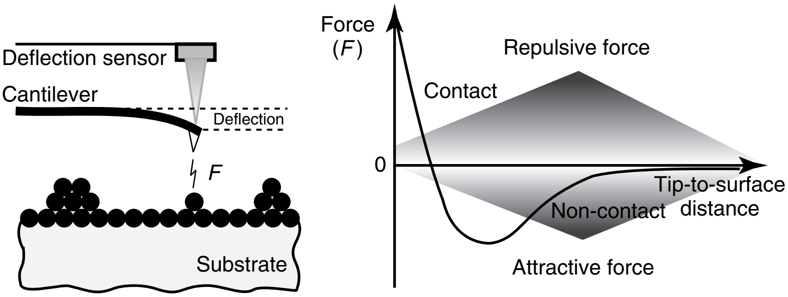

Figure A.8 Tip–sample geometry and registered effect in atomic force microscopy.

There are three principle types of imaging modes of the sample surface in AFM: contact, tapping, and non-contact modes. In the contact mode, the probing tip is always in contact with the sample surface, and surface structure is obtained from the deflection of the cantilever. The force on the tip is repulsive with a mean value of about 10^{-9} N. This force is set by pushing the cantilever against the sample surface with a piezoelectric positioning element. In the tapping mode, the probe tip is periodically in contact with the sample surface, and surface structure is obtained from the change in the vibration amplitude or phase of the oscillating cantilever. In the non-contact mode, the probe tip is not in contact with the sample surface, and surface structure is obtained from the change in the the vibration amplitude or resonant frequency of the oscillating cantilever.

In the contact mode, there is a high possibility that the strong repulsive force acting between the sample surface and the probe tip will destroy the sample surface and/or the tip apex. So, the tapping and non contact modes are widely used because these modes are more gentle than the contact mode.

In the tapping mode, the cantilever is driven at a fixed frequency near resonance with large vibration amplitude. When the probe tip is far from the surface, the vibration amplitude of the oscillating cantilever is held constant. When the probe tip is close to the surface, the probe tip is periodically in contact with the sample surface, and the vibration amplitude of the oscillating cantilever decreases because of cyclic repulsive contact between tip and surface with loss of the energy stored in the oscillating cantilever. The surface structure is obtained by maintaining the vibration amplitude at a constant level using the feedback circuit. The loading force acting between the probe tip and the sample surface can be greatly reduced in the tapping mode.

The atomic force microscopy technique has also been developed to detect electrostatic and magnetic forces as well as friction forces at atomic scale → **electrostatic force microscopy**, **magnetic force microscopy**, **friction force microscopy**.

First described in: G. Binning, C. F. Quate, Ch. Gerber, *Atomic force microscope*, Phys. Rev. Lett. **56**(9), 930–933 (1986).

More details in: W. R. Bowen, N. Hilal, *Atomic Force Microscopy in Process Engineering: An Introduction to AFM for Improved Processes and Products* (Elsevier, Oxford, 2009).

atomic layer deposition (ALD) - a nanotechnological method whereby the film growth involves chemisorption and a sequential set of repeating self-limiting surface reactions. Within this method a substrate with an appropriately processed surface is mounted at a heated holder in a reaction chamber equipped with at least two independent gas or vapor sources and pumping out system. The deposition consists of repeating the following steps: (i) exposure of the substrate to first precursor, (ii) purge or evacuation of the reaction chamber to remove the nonreacted precursors and the gaseous reaction by-products, (iii) exposure of the substrate to the second precursor or another treatment to activate the surface again for the reaction of the first precursor, and (iv) purge or evacuation of the reaction chamber. Each reaction cycle adds a given amount of material to the surface, referred to as the *growth per cycle*. The cycles are repeated as many as required for the desired film thickness (Figure A.9).

The precursor gases are designed so that they can fully react with the surface at the deposition conditions (pressure, substrate temperature), but do not react at all with themselves. The precursors are injected into the chamber and react with a surface one-at-a-time in a sequential manner. Separation of the precursors is accomplished by pulsing a purge gas (typically nitrogen or argon) after each precursor pulse to remove excess precursor from the process chamber. A thermodynamic equilibrium of the surface is approached at the end of each reaction step. As a result, the reaction is self-terminating. After a monolayer (monoatomic or monomolecular layer) is adsorbed, the growth stops. The deposition is typically carried out between 100 and 500°C, depending on the precursor, and takes from 0.5 s to a few seconds. The monolayer deposition repeats necessary times in order to fabricate the desired film. A large variety of compounds (oxides, nitrides, A(III)B(V), A(II)B(VI), etc.) are possible to deposit by this method. The application of the ALD method to fabricate Al_2O_3 films on a silicon substrate is illustrated by Figure A.1. Water vapor (H_2O) and trimethylaluminum ($Al(CH_3)_3$) are used as sources of oxygen and aluminum, respectively.

Owing to the self-regulating nature of the ALD process, the film composition and its thickness are controlled in a very accurate manner. Moreover, the films appeared to be extremely conformal and uniform in thickness. ALD is, indeed, useful when there is a need to fabricate films of few monolayer thickness.

First described in: T. Suntola, J. Antson, *Method for producing compound thin films*, US Patent 4 058 430 (1977) and then in the paper M. Ahonen, M. Pessa, T. Suntola,

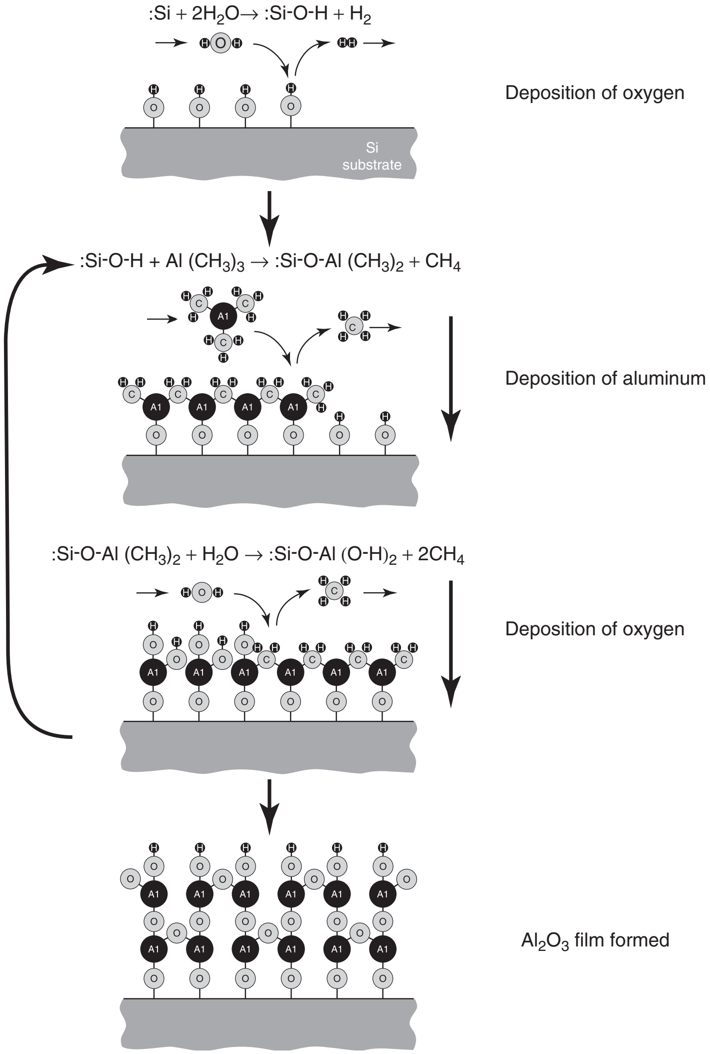

Figure A.9 Atomic layer deposition of Al_2O_3. The symbol ":" denotes compounds formed on the substrate.

A study of ZnTe films grown on glass substrates using an atomic layer evaporation method, Thin Solid Films **65**, 301–307 (1980).

atomic number – the number of protons in the atomic nucleus, and hence the nuclear charge.

atomic orbital – a wave function of a hydrogenic (hydrogen-like) atom. This term expresses something less definite than "orbit" of classical mechanics. When an electron is described by one of the wave functions, one says that it occupies that orbital. It defines the spatial behavior of an electron of a given energy level in a particular atom. An overlap of orbitals in solids produces bands.

In an atom all orbitals of a given value of principal quantum number n form a single shell. It is common to refer to successive shells by the letters: K($n = 1$), L($n = 2$), M($n = 3$), N($n = 4$). The number of orbitals in a shell of principal number n is n^2. In a hydrogenic atom each shell is n^2-fold **degenerate**.

The orbitals with the same value of n but different **angular momentum**, which corresponds to different values of l, form the subshell of a given shell. The subshells are referred to by the letters: s($l = 0$), p($l = 1$), d($l = 2$), f($l = 3$). Thus, the subshell with $l = 1$ of the shell with $n = 3$ is called the 3p subshell. Electrons occupying these orbitals are called 3p electrons. The number of orbitals for different n and l is listed in the Table A.1.

Table A.1 Number of orbitals as a function of the quantum numbers n and l.

$l \rightarrow$ $n \downarrow$	0 s	1 p	2 d	3 f	Total number of orbitals
1	1				1
2	1	3			4
3	1	3	5		9
4	1	3	5	7	16

s orbitals are independent of angle (the angular momentum is zero), so they are spherically symmetrical. The first s orbitals are schematically shown in Figure A.10.

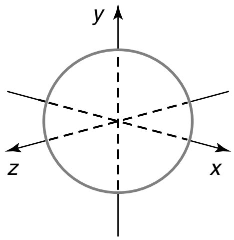

Figure A.10 The form of hydrogenic atomic s orbitals.

p orbitals are formed by electrons with the angular momentum $L^2 = 2\hbar^2$. These orbitals have zero amplitude at $r = 0$. This can be understood in terms of the centrifugal effect of the angular momentum, which flings the electron away from the nucleus. The same effect appears in all orbitals with $l > 0$.

The three 2p orbitals are distinguished by the three different values that m_l can take when $l = 1$, where m_l represents the angular momentum around an axis. They are presented in Figure A.11. Different values of m_l denote orbitals in which the electron has different angular momenta around an arbitrary axis, for instance the

z-axis, but the same magnitude of momentum because l is the same for all three. In this case the orbital with $m_l = 0$ has zero angular momentum around the z-axis. It has the form $f(r) cos\theta$. The electron density, which is proportional to $cos^2\theta$, has its maximum on either side of the nucleus along the z-axis (for $\theta = 0^\circ$ and $\theta = 180^\circ$). For this reason, the orbital is also called a p_z orbital. The orbital amplitude is zero when $\theta = 90^\circ$, so the xy-plane is a nodal plane of the orbital. On this plane the probability of finding an electron occupying this orbital is zero.

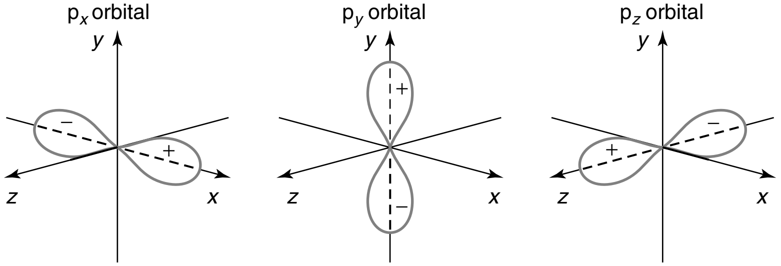

Figure A.11 Three hydrogenic atomic p orbitals, each directed along a different axis.

The orbitals with $m_l = \pm 1$, which are the p_x and p_y orbitals, do have angular momentum about the z-axis. These two orbitals are different in the direction of the electron motion, which are opposite to each other. Nevertheless, they both have zero amplitude at $\theta = 0^\circ$ and $\theta = 90^\circ$ (along the z-axis) and maximum amplitude where $\theta = 90^\circ$, which is in the xy-plane. The p_x and p_y orbitals have the same shape as the p_z orbital, but are directed along x- and y-axis, respectively. Their combinations are standing waves with no net angular momentum around the z-axis, since they are composed of equal but opposite values of m_l.

d orbitals appear when $n = 3$. There are five orbitals in this case with $m_l = 0, \pm 1, \pm 2$, which correspond to five different angular momenta around the z-axis but with the same magnitude of the momentum. The orbitals with opposite values of m_l (and hence opposite senses of motion around the z-axis) may combine in pairs to produce standing waves. An important feature of d orbitals is that they are concentrated much more closely at the nucleus than s and p orbitals are. An example of the d orbital is depicted in Figure A.12.

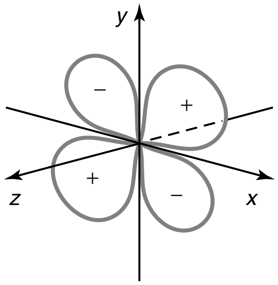

Figure A.12 The d orbital of the xy/r^2 form.

d orbitals are more strongly concentrated near the nucleus and isolated from neighboring atoms than others. They are important in studying properties of **rare-earth** metals.

For the definitions of σ and π orbitals → **molecular orbital**.

atom probe field ion microscopy (APFIM) – the technique originated from field ion microscopy. The analyzed sample is prepared in the form of a sharp tip. A voltage pulse is applied to the tip causing atoms on the surface of the tip to be ejected. The atoms travel down a drift tube where their time of arrival can be measured. The time taken for the atom to arrive at the detector is a measure of the mass of that atom. Thus, compositional analysis of the sample can be carried out on a layer by layer basis.

The technique enables one to determine the chemical identity along with the position of surface atoms with atomic structural resolution. It has no elemental mass limitations, making it unique among analytical instruments.

First described in: E. W. Müller, J. A. Panitz, S. B. McLane, *The atom probe microscope*, Rev. Sci. Instrum. **39**(1), 83–86 (1968).

More details in: T. T. Tsong, *Atom-Probe Field Ion Microscopy: Field Ion Emission, and Surfaces and Interfaces at Atomic Resolution* (Cambridge University Press, Cambridge, 1990).

atto- – a decimal prefix representing 10^{-18}, abbreviated a.

aufbau principle – states that in any atom the lowest energy orbitals fill first. In conjunction with the **Pauli exclusion principle** and the **Hund rules**, it gives the correct electron configuration for an atom or ground state ion.

First described in: N. Bohr, *Der Bau der Atome und die physikalischen und chemischen Eigenschaften der Elemente*, Z. Phys. **9**, 1–67 (1922); E. C. Stoner, *The distribution of electrons among atomic levels*, Phil. Mag. **48**, 719–736 (1924).

Auger effect – formation of non-radiative re-arrangement of atomic electrons after the atom has been ionized in one of its inner shells.

Classically, if an atom is ionized in its S shell, the radiative mode of de-excitation is that in which a transition occurs involving an electron falling from a less tightly bound shell T to S with emission of a quantum of radiation with the energy $E_S - E_T$, which is the difference between the binding energies of the S and T shells, respectively. In the Auger transition, an electron, called the **Auger electron**, is emitted with kinetic energy $E = E_S - E_T - E_U$, with U being the same shell as T or another one less tightly bound than S. For the transition to be energetically possible, of course $E_S - E_T - E_U = 0$. The process can be interpreted as the T electron falling into the S shell, the energy released being used to eject the U electron. The binding energy of the U electron is dashed because when it is ejected the atom is already ionized.

Most observable Auger transitions originate either by primary ionization in the K or L shells of an atom, because transitions due to ionization in the higher shells cause the emission of electrons with energies too low to be detected. The emitted electrons are called Auger electrons. Their energy spectrum is a fingerprint of the chemical nature of the atom. It is widely used for analysis of chemical compositions of matter by **Auger electron spectroscopy**.

First described in: P. Auger, *Sur les rayons* β *secondaires produits dans un gaz par des rayons*, C. R. **177**, 169–171 (1923).

Auger electron – an electron that is expelled from an atom in the **Auger effect**.

Auger electron spectroscopy (AES) – a technique of nondestructive elemental analysis of matter by examining energy distributions of secondary electrons emitted by the **Auger effect**. If a material is bombarded by electrons with an energy sufficient to ionize inner orbits of the atoms, the energy released when the ionized atom rearranges itself to fill the ionized level is characteristic of the atom. This energy may appear as an X-ray photon or may instead go to an outer orbit electron, ejecting it by the radiationless Auger process. Thus, the energy distribution of secondary Auger electrons contains peaks localized at energies which serve to identify the atoms producing them. The depth at which this information can be obtained is 0.5–2 nm for metals, 1.5–4 nm for oxides, and 4–10 nm for polymers.

More details in: M. De Crescenzi, M. N. Piancastelli, *Electron Scattering and Related Spectroscopies* (World Scientific Publishing, Singapore, 1996).

Auger recombination – a transition of an electron from the conduction band to the valence band by transfer of the energy to another free electron or hole. No electromagnetic radiation is emitted during such process.

Auger scattering – one of the interacting charge carriers gives up its potential energy to another and hence relaxes down its energy level.

augmented plane wave (APW) – piecewise defined function consisting of the solution to the **Schrödinger equation** for an isolated atom within a sphere of given radius and a **plane wave** outside this region.

augmented-plane-wave method supposes solving the **Schrödinger equation** for electrons in an atom in terms of a set of fabricated functions that combine the oscillations inside the core with plane waves elsewhere. The potential is assumed to be spherically symmetrical within spheres centered at each atomic nucleus and constant in the interstitial region. Wave functions in the form of augmented plane waves are constructed by matching solutions of the **Schrödinger equation** within each sphere with plane-wave solutions in the interstitial region. Linear combinations of these wave functions are then determined by the **variational method**.

First described in: J. C. Slater, *Wave functions in a periodic potential,* Phys. Rev. **51**(10), 846–851 (1937).

More details in: D. J. Singh, L. Nordström, *Planewaves, pseudopotentials, and the LAPW method* (Springer, New York, 2006).

autocorrelation function – the measure of the dependence of time series values at one time on the values at another time. The term autocorrelation means self-correlation. However, instead of correlation between two different variables, the correlation between two values of the same variable at times x_n and x_{n+k} is analyzed. For a time series $x(n), n = 1, 2, \ldots N$, the autocorrelation function is defined as: $R(k) = \frac{1}{(N-k)} \sum_{n=1}^{N-k} x(n)x(n+k)$, where k is the correlation distance and N is the length of the series. The argument of the autocorrelation function is the correlation distance k, and the function value at k expresses the average correlation between numbers separated by the distance k in the series.

The autocorrelation function is used to detect non-randomness in data and to identify an appropriate time series model if the data are not random. It is a powerful tool to find weak periodic signals in noisy data.

First described in: G. E. P. Box and G. Jenkins, *Time Series Analysis: Forecasting and Control* (Holden-Day, 1976).

autoelectronic emission – an emission of electrons from the surface of a conductor by application of an external electric field in the temperature range where conventional thermo-stimulated electron emission is rather small.

Aviram–Ratner model – a model for unimolecular electrical rectification employing a molecule with electrically isolated electron donor and acceptor groups.

The molecule is postulated to be initially in an electronically neutral state and placed between two metal electrodes. The current flow is proposed to be a three-step process, upon application of a bias. First, an electron passes from the cathode to the acceptor. The Fermi level of the anode is sufficiently lowered under the bias to allow the second step of the process, electron tunneling from the donor to the anode, to occur. Finally, the electron inelastically tunnels from the **acceptor** to the **donor**.

A demonstration **molecular rectifier** consists of a donor π system (tetrathiafulvalene) and an acceptor π system (tetracyanoquinodimethane), separated by a σ bonded (methylene) tunneling bridge.

First described in: A. Aviram, M. A. Ratner, *Molecular rectifiers,* Chem. Phys. Lett. **29**(2), 277–283 (1974).

More details in: G. Cuniberti, G. Fagas, K. Richter, *Introducing Molecular Electronics, Lecture Notes in Physics* **680** (Springer, Berlin, 2005).

Azbel'–Kaner cyclotron resonance – the method used to measure **cyclotron frequencies** in metals and thus useful in **Fermi surfaces** studies. In a large static magnetic field, a semiconductor permeated by a radiofrequency electromagnetic field produces sharp peaks in the radiofrequency energy absorption when the frequency coincides with the cyclotron resonance frequency ω_c. In metals this is impeded by the **skin-depth effect** that prevents the radiofrequency field penetration. In the Azbel'–Kaner method one accepts the limitation that the radiofrequency field can accelerate the electrons only within a very thin surface layer and arranges the geometry of the experiment such that the electrons return to this layer frequently. In order to obtain this the static magnetic field is oriented parallel to the surface of the sample. Thus, any electron at its general helical orbit around the magnetic field lines approaches the surface within the same distance on each cycle. If the radiofrequency coincides with the cyclotron frequency, the electron can resonantly absorb energy from the field. Here the condition for the resonance is $\omega = n\omega_c$ $(n = 1, 2, 3, \ldots)$.

First described in: M. Ya. Azbel', E. A. Kaner, *Cyclotron resonance in metals,* J. Phys. Chem. Solids **6** (2–3), 113–135 (1958); M. Ya. Azbel', E. A. Kaner, Zh. Eksp. Teor. Fiz. **30**, 811 (1956) and **32**, 896 (1957) – in Russian.

More details in: L. M. Falicov, *Fermi surface studies,* in: *Electrons in Crystalline Solids* (IAEA, Vienna, 1973), pp. 207–280.