Numerical modelling, an essential tool for **a better understanding** of nano-objects

Numerical modelling is a very useful tool for designing and predicting the physical and chemical properties of nano-objects. Various numerical approaches are available depending on the physical dimensions and time scales being considered. The ambition of physicists working on the numerical modelling of materials is to devise models based on the elementary interactions among atoms. This approach is particularly arduous when the number of atoms is large. However, nanometre-sized objects have a relatively small number of atoms, and so what ordinarily would be extremely difficult to achieve is possible – and has indeed been done – in the nanoworld.

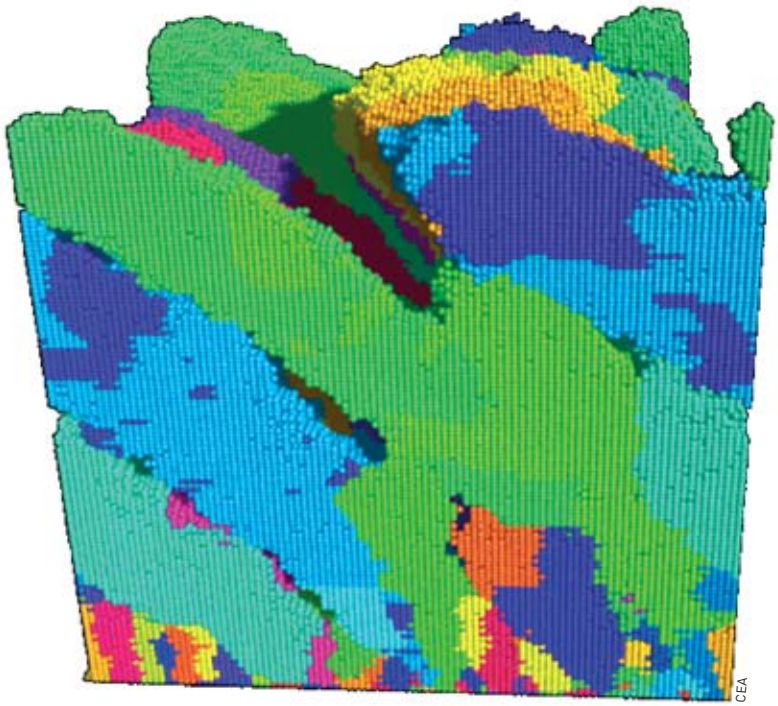
Numerical **modelling** has made great strides in the last decades, mainly thanks to advances in computing power (see box in *From microelectronics to nanoelectronics*) and improvements on **models** and **codes**. Greater data processing capacity is constantly adding to our knowledge of materials and of their processing and time evolution. The industrial design of glasses, steels and **integrated circuits** sometimes calls for an empirical approach. Modelling is necessary both to undertake novel developments and to control current fabrication processes. One approach that is often taken is to describe a material in terms of its constituant **atoms**: this is *atomistic modelling*. Nano-objects, typically ranging from a few atoms (**molecules**) to several tens of thousands of atoms (*e.g.*, **quantum boxes**) can be approached by atomistic modelling. The CEA's Physical Metallurgy Research Unit (Service de recherches de métallurgie physique) has mainly focused on the engineering and structure of nano-objects.

An array of modelling tools

There are various modelling tools for studying nano-objects, each of which has its specific features and its limits. For simplicity they can be split into three categories according to the space and time scales they are designed to explore.

Ab initio models to confirm a growth mechanism

The ***ab initio*** cohesion **models** are designed to determine interactions among atoms directly from the electronic structure of the material, with no adjustable parameters. The solution of approximations to the **Schrödinger equation** will reproduce, and so predict, most of the properties of most materials with accuracy of a few percent. However, the huge amount of computational ressources required limits this approach to systems composed of about a hundred atoms, or at most a thousand in the simplest cases. Very short timescales (~ 10 ps; 1 ps = 10^{-12} s) can also be approached by the methods of ***molecular dynamics*** by solving equations for atomic movement. This method has made it possible, for example, to corroborate a growth mechanism for single-walled **carbon nanotubes** hypothesized from observations of the first growth stages by transmission electron microscopy (see *Conventional electron microscopy: scanning and transmission*). These simulations showed (i) that the **segregation** of the carbon at the surface of a metal particle (the **catalyst**) could lead to the formation of nanotube nuclei, and (ii) that the incorporation of carbon atoms at the tube


CEA

Numerical modelling is an essential tool for gaining deeper knowledge of the growth mechanisms of materials. Here, Monte-Carlo simulation of the columnar growth of thin films of tantalum (scale: width at base 30 nm). The atoms belonging to the same crystal grain are the same colour.

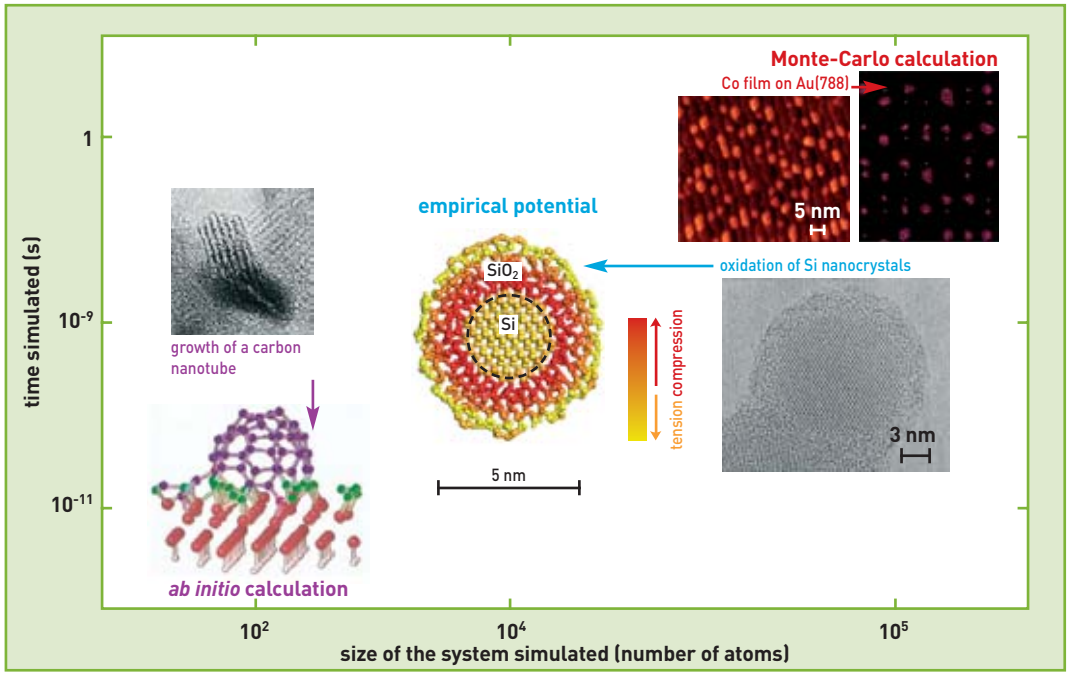


Figure 1. Experimental images of nano-objects and associated numerical simulations. *Ab initio* molecular dynamics calculations show the growth of carbon nanotubes from a metal **nanoparticle** (red spheres) where carbon atoms segregated at the surface (green spheres) are spontaneously incorporated at the base of a nanotube (purple spheres) (Gavillet *et al., Phys. Rev. Lett.*, 87, 275504, 2001). Molecular dynamics calculations with empirical potentials show variations in pressure (colour scale) in a nanocrystal of oxidized silicon (J. Dalla Torre *et al., J. Appl. Phys.*, 92, p. 1084, 2002 and Hofmeister *et al., Eur. Phys. J.*, D 9, p. 137, 1999 for the electron microscopy observations). The Monte-Carlo calculation simulated the heterogeneous growth of a cobalt film on a gold surface, to be compared with the scanning tunnelling microscope image (S. Rohart *et al., Surf. Sc.*, 559, p. 47, 2004).

base in contact with the metal particle was very rapid and took place readily, allowing tube growth by base feeding *via* the catalyst (Figure 1, *ab initio* calculation). *Ab initio* electronic structure calculations also give direct access to electronic properties. It is therefore possible to accurately reproduce the optical absorption spectrum of the nanotubes(1).

Empirical models to elucidate an oxidation mechanism

Empirical potentials make it possible to describe interactions among atoms much more simply than by *ab initio* methods. The **electrons** are not treated explicitly; instead the chemical bond is described by an interatomic potential energy function. However, this approach requires an empirical determination of actual interactions among atoms, and the quality of this determination sets limits on the usefulness of the modelling. This approach is hampered by the large number of parameters that have to be incorporated. The evolution of systems made up of several tens of thousands of atoms is easily reproduced for physical durations of the order of a nanosecond (1 ns = 10^{-9} s). Figure 1 (empirical potential) shows the result of a molecular dynamics simulation of the **oxidation** of nanocrystals of **silicon** (Si) (see *Fluorescent semiconducting nanocrystals show their colours*). When these nanocrystals are heated in an oxygen atmosphere, a shell of silicon oxide (SiO_2) forms on the surface, and the oxidation proceeds no further. This effect, which is not fully understood experimentally, can be analyzed by molecular dynamics. Simulations show that the shell is tension-strained at the surface and compression-strained at the interface. In this configuration, a molecule of oxygen will diffuse preferentially outwards of the shell rather than inwards, and so the oxidation stops through lack of oxygen at the interface.

(1) See, for example, the work conducted at the Irradiated Solids Laboratory of the Solid State, Atoms and Molecules Research Department (CEA/DSM/Drecam/LSI, Drecam: Département de recherche sur l'état condensé, les atomes et les molécules).

Computation of Monte-Carlo calculation to elucidate a heterogeneous growth mechanism

The kinetic **Monte-Carlo method** offers a way to approach the evolution of several million atoms over relatively long time spans, of the order of several hours. The model works by reducing the number of atomic events to keep only those events considered significant for macroscopic evolution. A probabilistic treatment ranks the occurrence of the selected events. The formation of a set of nano-objects, their organization and their interactions can be modelled. For example, the heterogeneous growth of a film of cobalt Co on the **vicinal surface** of a crystal of gold Au(111) was observed experimentally by scanning tunnelling electron microscopy (see *Local probe microscopy: contact and manipulation*). Kinetic Monte-Carlo simulations made it possible to elucidate the essential mechanisms involved in the growth of the cobalt dots, including in particular the effect of the insertion of atoms of cobalt in place of some gold atoms located at the intersections of fault lines and steps on the vicinal surface (Figure 1, Monte-Carlo calculation).

Control through understanding

Simulation at the atomic scale is a very useful tool to support experiments, or even as a last resort when experiments are impossible, for the study and control of the properties of nano-objects. Experimental size and time scales are directly accessible by simulation methods. The results of simulations allow a detailed analysis of the elementary mechanisms in play, and isolate the most significant ones. Simulation thus helps to gain an overall and a more thorough understanding of nanoscale phenomena.

> **Jacques Dalla Torre†, Laurent Proville** and **François Willaime**
Nuclear Energy Division
CEA Saclay Centre

A From the macroscopic to the nanoworld, and vice versa...

In order to gain a better idea of the size of microscopic and nanoscopic* objects, it is useful to make comparisons, usually by aligning different scales, *i.e.* matching the natural world, from molecules to man, to engineered or fabricated objects (Figure). Hence, comparing the "artificial" with the "natural" shows that artificially-produced **nanoparticles** are in fact smaller than red blood cells.

Another advantage of juxtaposing the two is that it provides a good illustration of the two main ways of developing nanoscale systems or objects: ***top-down*** and ***bottom-up***. In fact, there are two ways into the nanoworld: molecular manufacturing, involving the control of single **atoms** and the building from the ground up, and extreme miniaturization, generating progressively smaller systems.

Top-down technology is based on the artificial, using macroscopic materials that we chip away using our hands and our tools: for decades now, electronics has been applied using **silicon** as a substrate and what are called "**wafers**" as workpieces. In fact, microelectronics is also where the "top-down" synthesis approach gets its name from. However, we have reached a stage where, over and above simply adapting the miniaturization of silicon, we also have to take on or use certain physical phenomena, particularly from **quantum** physics, that operate when working at the nanoscale.

The bottom-up approach can get around these physical limits and also cut manufacturing costs, which it does by using component **self-assembly**. This is the approach that follows nature by assembling molecules to create **proteins**, which are a series of amino acids that the super-molecules, *i.e.* **nucleic acids** (**DNA**, **RNA**), are able to produce within cells to form functional structures that can reproduce in more complex patterns. Bottom-up synthesis aims at structuring the material using "building blocks", including atoms themselves, as is the case with living objects in nature. Nanoelectronics seeks to follow this assembly approach to make functional structures at lower manufacturing cost.

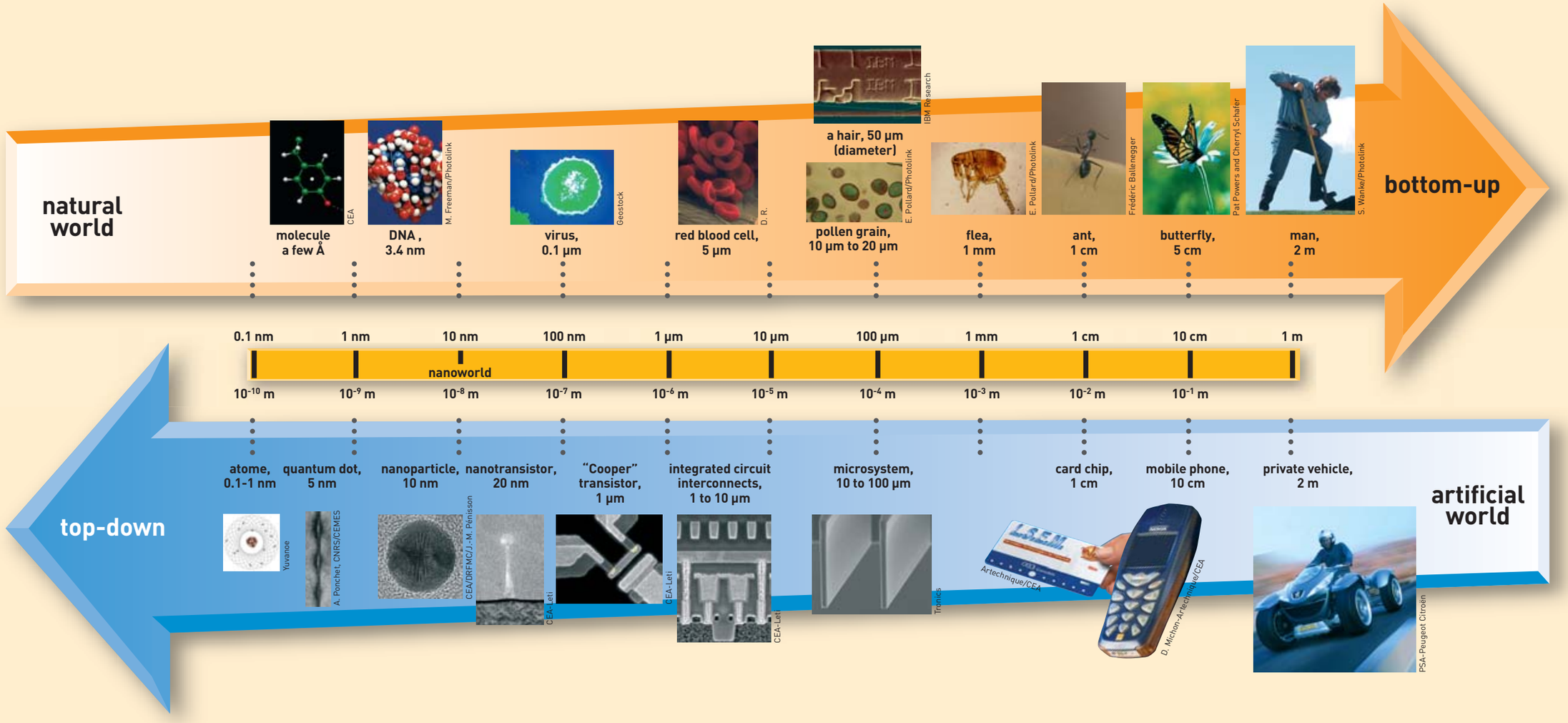
The **nanosciences** can be defined as the body of research into the physical, chemical or biological properties of nano-objects, how to manufacture them, and how they self-assemble by auto-organisazation.

Nanotechnologies cover all the methods that can be used to work at molecular scale to reorganize matter into objects and materials, even progressing to the macroscopic scale.

300-mm silicon wafer produced by the Crolles2 Alliance, an illustration of current capabilities using top-down microelectronics.

* From the Greek *nano meaning* "very small", which is also used as a prefix meaning a billionth (10^{-9}) of a unit. In fact, the **nanometre** (1 nm = 10^{-9} metres , or a billionth of a metre), is the master unit for nanosciences and nanotechnologies.

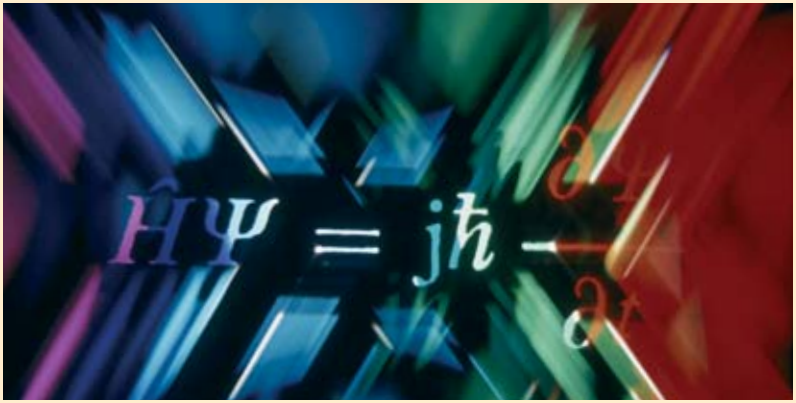
A (next)


natural world
bottom-up
molecule a few Å
CEA
DNA , 3.4 nm
M. Freeman/Photolink
virus, 0.1 µm
Geostock
red blood cell, 5 µm
D. R.
a hair, 50 µm (diameter)
IBM Research
pollen grain, 10 µm to 20 µm
E. Pollard/Photolink
flea, 1 mm
E. Pollard/Photolink
ant, 1 cm
Frédéric Ballenegger
butterfly, 5 cm
Pat Powers and Cheryl Schafer
man, 2 m
S. Wanke/Photolink
0.1 nm
1 nm
10 nm
100 nm
1 µm
10 µm
100 µm
1 mm
1 cm
10 cm
1 m
nanoworld
10-10 m
10-9 m
10-8 m
10-7 m
10-6 m
10-5 m
10-4 m
10-3 m
10-2 m
10-1 m
top-down
artificial world
atome, 0.1-1 nm
Yuvanoe
quantum dot, 5 nm
A. Ponchet, CNRS/CEMES
nanoparticle, 10 nm
CEA/DRFMC/J.-M. Pénisson
nanotransistor, 20 nm
CEA-Leti
"Cooper" transistor, 1 µm
CEA-Leti
integrated circuit interconnects, 1 to 10 µm
CEA-Leti
microsystem, 10 to 100 µm
Tronics
card chip, 1 cm
Artechnique/CEA
mobile phone, 10 cm
D. Michon-Artechnique/CEA
private vehicle, 2 m
PSA-Peugeot Citroën

B A guide to quantum physics

Quantum physics (historically known as quantum mechanics) covers a set of physical laws that apply at microscopic scale. While fundamentally different from the majority of laws that appear to apply at our own scale, the laws of quantum physics nevertheless underpin the general basis of physics at all scales. That said, on the macroscopic scale, quantum physics in action appears to behave particularly strangely, except for a certain number of phenomena that were already curious, such as **superconductivity** or superfluidity, which in fact can only explained by the laws of quantum physics. Furthermore, the transition from the validating the paradoxes of quantum physics to the laws of classical physics, which we find easier to comprehend, can be explained in a very general way, as will be mentioned later.

Quantum physics gets its name from the fundamental characteristics of quantum objects: characteristics such as the angular momentum (**spin**) of **discrete** or discontinuous particles called **quanta**, which can only take values multiplied by an elementary *quantum*. There is also a **quantum of action** (product of a unit of energy multiplied by time) called **Planck's constant** (symbolized as h) which has a value of 6.626 x 10^{-34} joule·second.



D. Sarraute/CEA

An "artist's impression" of the Schrödinger equation.

While classical physics separates *waves* from *particles*, quantum physics somehow covers both these concepts in a third group, which goes beyond the simple wave-particle duality that Louis de Broglie imagined. When we attempt to comprehend it, it sometimes seems closer to waves, and sometimes to particles. A quantum object cannot be separated from how it is observed, and has no fixed attributes. This applies equally to a particle - which in no way can be likened to a tiny little bead following some kind of trajectory - of light (**photon**) or matter (**electron**, **proton**, **neutron**, **atom**, etc.).

This is the underlying feature behind the **Heisenberg uncertainty principle**, which is another cornerstone of quantum physics. According to this principle (which is more *indeterminacy* than *uncertainty*), the position and the velocity of a particle cannot be measured *simultaneously* at a given point in time. Measurement remains possible, but can never be more accurate than *h*, Planck's constant. Given that these approximations have no intrinsically real value outside the observation process, this simultaneous determination of both position and velocity becomes simply impossible.

B (next)

At any moment in time, the quantum object presents the characteristic of *superposing* several states, in the same way that one wave can be the *sum* of several others. In quantum theory, the amplitude of a wave (like the peak, for example) is equal to a **probability amplitude** (or probability wave), a complex number-valued function associated with each of the possible sates of a system thus described as quantum. Mathematically speaking, a physical state in this kind of system is represented by a **state vector**, a function that can be added to others *via* superposition. In other words, the sum of two possible state vectors of a system is *also* a possible state vector of that system. Also, the product of two vector spaces is also the sum of the vector products, which indicates **entanglement**: as a state vector is generally spread through space, the notion of local objects no longer holds true. For a pair of entangled particles, *i.e.* particles created together or having already interacted, that is, described by the *product* and not the *sum* of the two individual state vectors, the fate of each particle is linked - entangled - with the other, regardless of the distance between the two. This characteristic, also called *quantum state entanglement*, has staggering consequences, even before considering the potential applications, such as quantum cryptography or - why not? - teleportation. From this point on, the ability to predict the behaviour of a quantum system is reduced to probabilistic or statistical predictability. It is as if the quantum object is some kind of "juxtaposition of possibilities". Until it has been measured, the measurable size that supposedly quantifies the physical property under study is not strictly defined. Yet as soon as this measurement process is launched, it destroys the **quantum superposition** through the "collapse of the wave-packet" described by Werner Heisenberg in 1927. All the properties of a quantum system can be deduced from the equation that Erwin Schrödinger put forward the previous year. Solving the **Schrödinger equation** made it possible to determine the energy of a system as well as the **wave function**, a notion that tends to be replaced by the probability amplitude.

According to another cornerstone principle of quantum physics, the **Pauli exclusion principle**, two identical half-spin ions (**fermions**, particularly electrons) cannot simultaneously share the same position, spin and velocity (within the limits imposed by the uncertainty principle), *i.e.* share the same *quantum state*. **Bosons** (especially photons) do not follow this principle, and can exist in the same quantum state.

The coexistence of **superposition states** is what lends **coherence** to a quantum system. This means that the theory of **quantum decoherence** is able to explain why macroscopic objects, atoms and other particles, present "classical" behaviour whereas microscopic objects show quantum behaviour. Far more influence is exerted by the "environment" (air, background radiation, etc.) than an advanced measurement device, as the environment radically removes all *superposition of states* at this scale. The larger the system considered, the more it is coupled to a large number of degrees of freedom in the environment, which means the less "chance" (to stick with a probabilistic logic) it has of maintaining any degree of quantum coherence.

TO FIND OUT MORE:

Étienne Klein, *Petit voyage dans le monde des quanta*, Champs, Flammarion, 2004.

C Molecular beam epitaxy

Quantum wells are grown using Molecular Beam Epitaxy (from the Greek *taxi*, meaning order, and *epi*, meaning over), or MBE. The principle of this physical deposition technique, which was first developed for growing III-V **semiconductor crystals**, is based on the evaporation of ultra-pure elements of the component to be grown, in a furnace under ultra-high vacuum (where the pressure can be as low as $5 \cdot 10^{-11}$ mbar) in order to create a pure, pollution-free surface. One or more thermal beams of **atoms** or **molecules** react on the surface of a single-crystal wafer placed on a substrate kept at high temperature (several hundred °C), which serves as a lattice for the formation of a film called epitaxial film. It thus becomes possible to stack ultra-thin layers that measure a millionth of a millimetre each, *i.e.* composed of only a few atom planes.

The elements are evaporated or sublimated from an ultra-pure source placed in an **effusion cell** (or Knudsen cell; an enclosure where a molecular flux moves from a region with a given pressure to another region of lower pressure) heated by the **Joule effect**. A range of structural and analytical probes can monitor film growth *in situ* in real time, particularly using surface quality analysis and grazing angle phase transitions by LEED (*Low energy electron diffraction*) or RHEED (*Reflection high-energy electron diffraction*). Various **spectroscopic** methods are also used, including Auger **electron** spectroscopy, secondary **ion** mass spectrometry (SIMS), **X-ray** photoelectron spectrometry (XPS) or **ultraviolet** photoelectron spectrometry (UPS).

As *ultra-high-vacuum* technology has progressed, molecular beam epitaxy has branched out to be applied beyond III-V semiconductors to embrace metals and insulators. In fact, the vacuum in the growth chamber, whose design changes depending on the properties of the matter intended to be deposited, has to be better than 10^{-11} mbar in order to grow an ultra-pure film of exceptional crystal quality at relatively low substrate temperatures. This value corresponds to the vacuum quality when the growth chamber is at rest. Arsenides, for example, grow at a residual vacuum of around 10^{-8} mbar as soon as the arsenic cell has reached its set growth temperature.

The pumping necessary to achieve these performance levels draws on several techniques using ion pumps, cryopumping, titanium sublimation pumping, diffusion pumps or turbomolecular pumps. The main impurities (H_2, H_2O, CO and CO_2) can present partial pressures of lower than 10^{-13} mbar.

D The transistor, fundamental component of integrated circuits

The first transistor was made in germanium by John Bardeen and Walter H. Brattain, in December 1947. The year after, along with William B. Shockley at **Bell Laboratories**, they developed the bipolar transistor and the associated theory. During the 1950s, transistors were made with **silicon** (Si), which to this day remains the most widely-used **semiconductor** due to the exceptional quality of the interface created by silicon and silicon oxide (SiO_2), which serves as an insulator. In 1958, Jack Kilby invented the **integrated circuit** by manufacturing 5 components on the same **substrate**. The 1970s saw the advent of the first microprocessor, produced by Intel and incorporating 2,250 transistors, and the first memory. The complexity of integrated circuits has grown exponentially (doubling every 2 to 3 years according to "Moore's law") as transistors continue to become increasingly miniaturized.

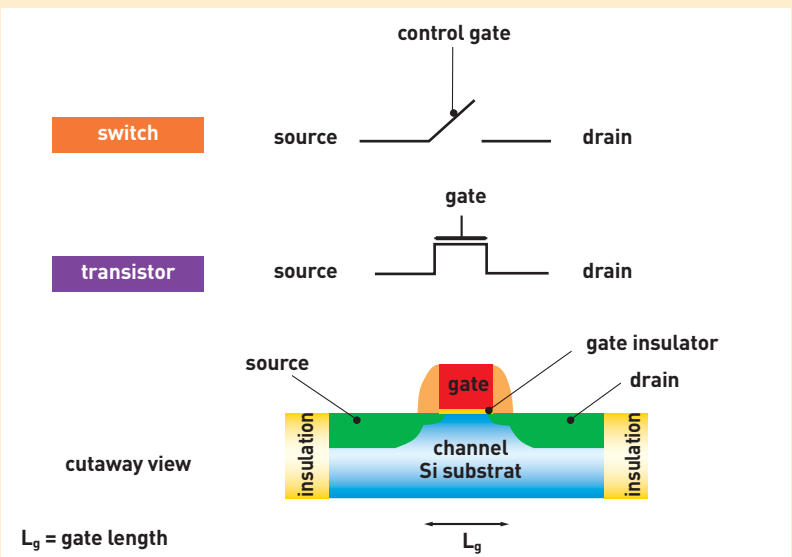


Figure.
A MOS transistor is a switching device for controlling the passage of an electric current from the source (S) to the drain (D) via a gate (G) that is electrically insulated from the conducting channel. The silicon substrate is marked B for Bulk.

The transistor, a name derived from *trans*fer and res*istor*, is a fundamental component of microelectronic integrated circuits, and is set to remain so with the necessary changes at the nanoelectronics scale: also well-suited to amplification, among other functions, it performs one essential basic function which is to open or close a current as required, like a switching device (Figure). Its basic working principle therefore applies directly to processing binary code (0, the current is blocked, 1 it goes through) in logic circuits (inverters, gates, adders, and memory cells).

The transistor, which is based on the transport of **electrons** in a solid and not in a vacuum, as in the electron tubes of the old **triodes**, comprises three **electrodes** (*anode, cathode* and *gate*), two of which serve as an electron *reservoir*: the **source**, which acts as the emitter filament of an electron tube, the **drain**, which acts as the collector plate, with the gate as "controller". These elements work differently in the two main types of transistor used today: *bipolar junction transistors*, which came first, and *field effect transistors* (**FET**).

Bipolar transistors use two types of **charge carriers**, electrons (negative charge) and **holes** (positive charge), and are comprised of identically **doped** (p or n) semiconductor substrate parts

D (next)

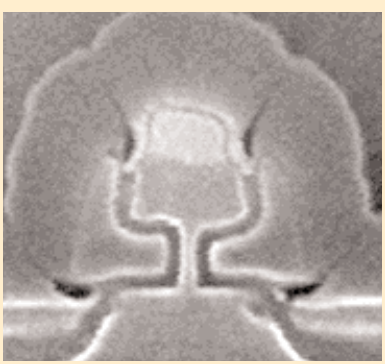
separated by a thin layer of inversely-doped semiconductor. By assembling two semiconductors of opposite types (a p-n junction), the current can be made to pass through in only one direction. Bipolar transistors, whether n-p-n type or p-n-p type, are all basically current amplifier controlled by a gate current[1]: thus, in an n-p-n transistor, the voltage applied to the p part controls the flow of current between the two n regions. Logic circuits that use bipolar transistors, which are called TTL (for transistor-transistor logic), consume more energy than field effect transistors which present a zero gate current in off-state and are voltage-controlled.

Field effect transistors, most commonly of **MOS** (metal oxide semiconductor) type, are used in the majority of today's **CMOS** (C for complementary) logic circuits[2]. Two n-type regions are created on a p-type silicon crystal by doping the surface. These two regions, also called drain and source, are thus separated by a very narrow p-type space called the **channel**. The effect of a positive current on the control electrode, naturally called the **gate**, positioned over the semiconductor forces the holes to the surface, where they attract the few mobile electrons of the semiconductor. This forms a conducting channel between source and drain (Figure). When a negative voltage is applied to the gate, which is electrically insulated by an oxide layer, the electrons are forced out of the channel. As the positive voltage increases, the channel resistance decreases, letting progressively more current through.

In an integrated circuit, transistors together with the other components (**diodes**, condensers, resistances) are initially incorporated into a "chip" with more or less complex functions. The circuit is built by "sandwiching" layer upon layer of conducting materials and insulators formed by **lithography** (Box E, ***Lithography, the key to miniaturization***). By far the most classic application of this is the microprocessor at the heart of our computers, which contains several hundred million transistors (whose size has been reduced 10,000-fold since the 1960s), soon a billion. This has led to industrial manufacturers splitting the core of the processors into several subunits working in parallel!

Lucent Technologies Inc./Bell Labs

The very first transistor.



STMicroelectronics

8 nanometre transistor developed by the Crolles2 Alliance bringing together STMicroelectronics, Philips and Freescale Semiconductor.

(1) This category includes **Schottky transistors** or **Schottky barrier transistors** which are field effect transistors with a metal/semiconductor control gate that, while more complex, gives improved charge-carrier mobility and response times.

(2) Giving **MOSFET** transistor (for Metal Oxide Semiconductor Field Effect Transistor).

E Lithography, the key to miniaturization

Optical lithography (photolithography) is a major application in the particle-matter interaction, and constitutes the classical process for fabricating integrated circuits. It is a key step in defining circuit patterns, and remains a barrier to any future development. Since resolution, at the outset, appears to be directly proportional to wavelength, feature-size first progressed by a step-wise shortening of the wavelength λ of the radiation used.

Artechnique

Photolithography section in ultra-clean facilities at the STMicroelectronics unit in Crolles (Isère).

The operation works via a reduction lens system, by the *exposure* of a photoresist film to energy particles, from the ultraviolet (UV) photons currently used through to X photons, ions, and finally electrons, all through a mask template carrying a pattern of the desired circuit. The aim of all this is to transfer this pattern onto a stack of insulating or conducting layers that make up the mask. These layers will have been deposited previously (the *layering* stage) on a wafer of semiconductor material, generally silicon. After this process, the resin dissolves under exposure to the air (*development*). The exposed parts of the initial layer can then be etched selectively, then the resin is lifted away chemically before deposition of the following layer. This lithography step can take place over twenty times during the fabrication of an integrated circuit (Figure).

In the 1980s, the microelectronics industry used mercury lamps delivering near-UV (g, h and i lines) through quartz optics, with an emission line of 436 nanometres (nm). This system was able to etch structures to a feature-size of 3 microns (μm). This system was used through to the mid-90s, when it was replaced by excimer lasers emitting **far-UV** light (KrF, krypton fluoride at 248 nm, then ArF, argon fluoride at 193 nm, with the photons thus created generating several electronvolts) that were able to reach a resolution of 110 nm, pushed to under 90 nm with new processes.

In the 1980s, the CEA's Electronics and Information Technology Laboratory (Leti) pioneered the application of lasers in lithography and the fabrication of integrated circuits using excimer lasers, and even the most advanced integrated circuit production still uses these sources.

The next step for high-volume production was expected to be the F_2 laser (λ = 157 nm), but this lithography technology has to all intents and purposes been abandoned due to complications involved in producing optics in CaF_2, which is transparent at this wavelength. While the shortening of wavelengths in exposure tools has been the driving factor behind the strong resolution gain already achieved, two other factors have nevertheless played key roles. The first was the development of polymer-lattice photoresists with low absorbance at the wavelengths used, implementing progressively more innovative input energy reflection/emission systems. The second was enhanced optics reducing diffraction interference (better surface quality, increase in numerical aperture).

Over the years, the increasing complexity of the optical systems has led to resolutions actually *below* the source wavelength. This development could not continue without a major technological breakthrough, a huge step forward in wavelength. For generations of integrated circuits with a lowest resolution of between 80 and 50 nm (the next "node" being at 65 nm), various different approaches are competing to offer particle projection at ever-shorter wavelengths. They use either "soft" X-rays at extreme ultraviolet wavelength (around 10 nm), "hard" X-rays at wavelengths below 1 nm, ions or electrons.

The step crossing below the 50 nm barrier will lead towards low-electron-energy (10 eV)-enabled nanolithography with technology solutions such as the scanning tunnelling microscope and molecular beam epitaxy (Box C) for producing "superlattices".

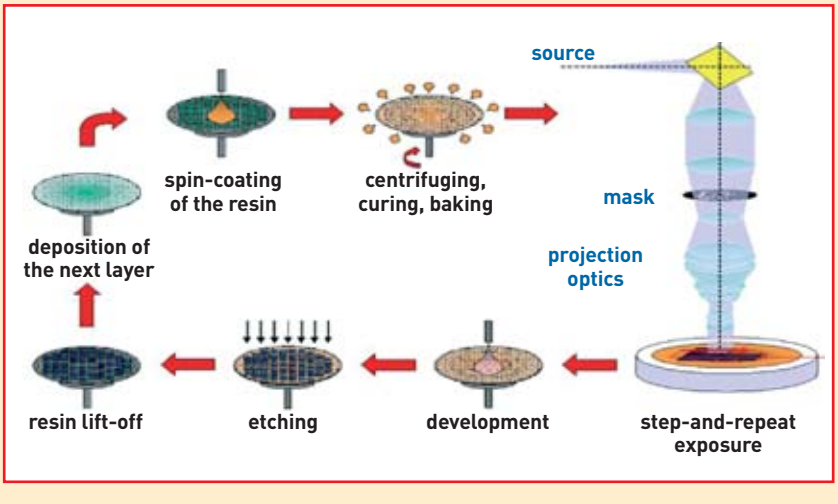


Figure. The various phases in the lithography process are designed to carve features out of the layers of conducting or insulating materials making up an integrated circuit. The sequences of the operation are laying of a photoresist, then projecting the pattern on a mask using a reduction optics system, which is followed by dissolution of the resin that is exposed to the light beam (development). The exposed parts of the initial layer can then be etched selectively, then the resin is lifted away before deposition of the following layer.

G The tunnel effect, a quantum phenomenon

Quantum physics predicts unexpected behaviour that defies ordinary intuition. The tunnel effect is an example. Take the case of a marble that rolls over a bump. Classical physics predicts that unless the marble has enough kinetic energy it will not reach the top of the bump, and will roll back towards its starting point. In quantum physics, a particle (proton, electron) can get past the bump even if its initial energy is insufficient, by "tunnelling" through. The tunnel effect makes it possible for two protons to overcome their mutual electrical repulsion at lower relative velocities than those predicted by classical calculations.

Tunnel effect microscopy is based on the fact that there is a finite probability that a particle with energy lower than the height of a potential barrier (the bump) can still jump over it. The particles are electrons travelling through the space between two electrodes. These electrodes are a fine metal tip terminating in a single atom, and the metal or semiconductor surface of the sample. In classical physics a solid surface is considered as a well-defined boundary with electrons confined inside the solid. By contrast, in quantum physics each electron has wave properties that make its location uncertain. It can be visualized as an electron cloud located close to the surface. The density of this cloud falls off exponentially with increasing distance from the solid surface. There is thus a certain probability that an electron will be located "outside" the solid at a given time. When the fine metal tip is brought near the surface at a distance of less than a nanometre, the wave function associated with the electron is non-null on the other side of the potential barrier and so electrons can travel from the surface to the tip, and *vice versa*, by the tunnel effect. The potential barrier crossed by the electron is called the tunnel barrier. When a low potential is applied between the tip and the surface, a tunnel current can be detected. The tip and the surface being studied together form a local tunnel junction. The tunnel effect is also at work in Josephson junctions where a direct current can flow through a narrow discontinuity between two superconductors.

In a transistor, an unwanted tunnel effect can appear when the insulator or grid is very thin (nanometre scale). Conversely, the effect is put to use in novel devices such as Schottky barrier tunnel transistors and carbon nanotube assemblies.