

# CONDENSED MATTER LABORATORY

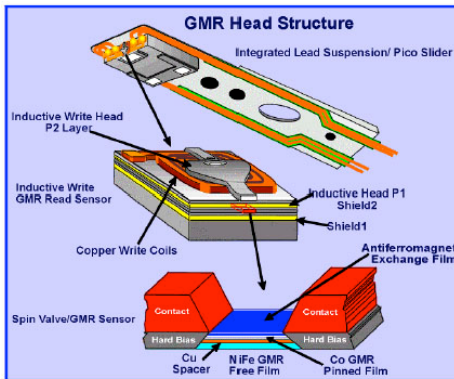
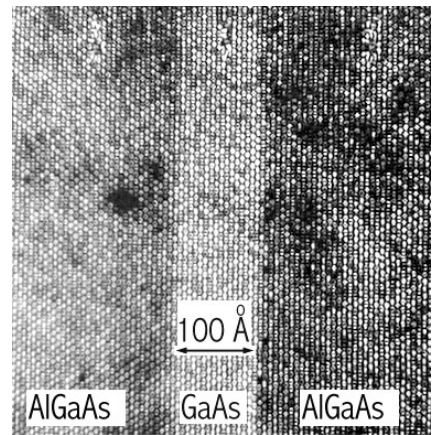
## Introduction

A nanostructure is an object with at least one dimension of the order of 1-100 nm. These dimensions are comparable to the De Broglie wavelength of an electron with energy comparable to  $k_B T$  at room temperature (0.024 eV),

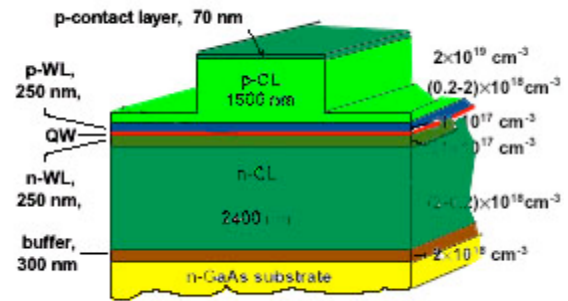
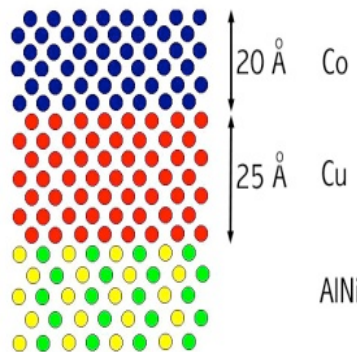
$$\lambda = \frac{2\pi}{k} = \frac{h}{\sqrt{2Em}} \approx 10^{-6} \text{ cm}$$

(1 eV =  $1.6 \times 10^{-12}$  erg,  $h = 6.619 \times 10^{-27}$  erg s,  $m = 9.11 \times 10^{-28}$  g). Therefore in a nanostructure the quantum effects are not negligible, and often they are dominant. Because of the nanometric dimension surface effects may also become important.

Devices containing artificial structures with dimensions of the order of a few nm that exploit quantum effects are already in use, as shown by the following examples. The readers of compact disks contain a laser diode that works because it contains a particular semiconductor layer called quantum well (QW) about 10 nm thick (see figure). If this layer were thicker the diode could not emit coherent light at ambient temperature. The figure at the right is a transmission electron microscopy (TEM) image showing the single atoms in a QW of GaAs in AlGaAs. The figure below is a sketch of a laser diode that shows the position of the QW. The head that reads high-capacity hard disks in your computers can do it because it contains layers of Co and Cu that are about ten atomic layers thick (see figure below). The properties of some optical filters and some stained glasses are caused by nanometer size crystals that they contain.

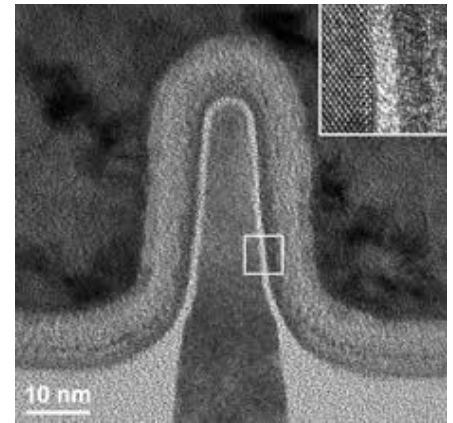


Commercial IBM giant magnetoresistance read head.



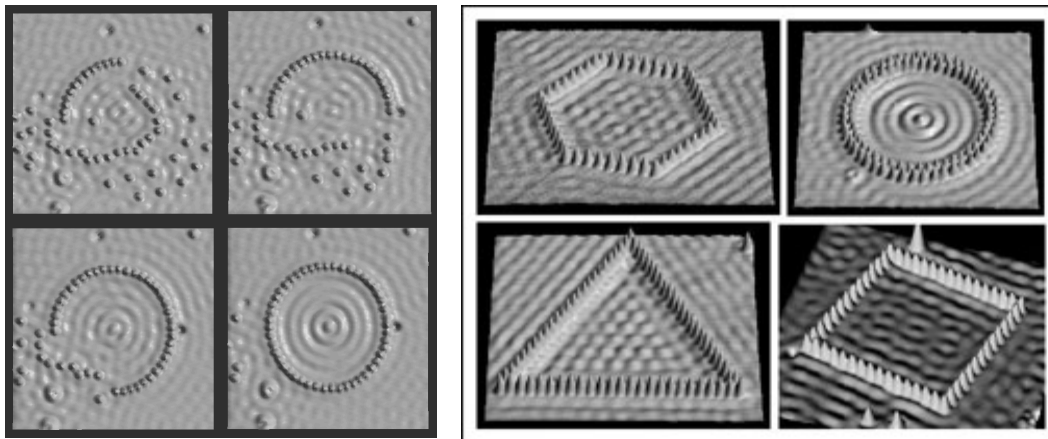
When the electrons in a system are confined at least in a dimension in a region so narrow that quantum effects

become important, the system is told to show quantum confinement. The dimensions of the components of some electronic devices today in use (in processors, in memories,...) are sometimes of the order of a few nm, but in this cases the quantum effects are not dominant. The figure on the right is a cross section of a transistor of one of these devices. The nanostructures and the systems with quantum confinement are also important for the fundamental physics that can be done with them. A list of Nobel prizes for researches in this field is:

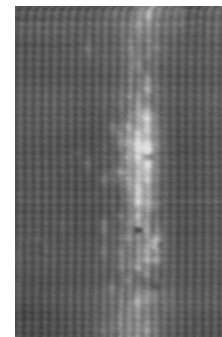


- |   |                                |
|---|--------------------------------|
| 2014 Isamu Akasaki, Hiroshi Amano and Shuji Nakamura      | GaN blue LED                   |
| 2010 Andre Geim, Konstantin Novoselov                     | graphene                       |
| 2007 Albert Fert and Peter Grünberg                       | giant magnetoresistance        |
| 2000 Zhores I. Alferov, Herbert Kroemer, Jack S. Kilby    | Microelectr.,optoelectronics   |
| 1998 Robert B. Laughlin, Horst L. Störmer, Daniel C. Tsui | Fractional quantum Hall effect |
| 1986 Ernst Ruska, Gerd Binnig, Heinrich Rohrer            | STM                            |
| 1985 Klaus von Klitzing                                   | Quantum Hall effect            |

It is now possible to assemble nanostructure atom by atom, for instance with instruments like the scanning tunnelling microscope (STM). The first figure below show the construction of a “quantum corral” formed by 48 Fe atoms with a diameter of 15 nm. The waves inside the circle of the Fe atoms are the oscillation of the square modulus of the wavefunction of the electron trapped inside the corral. The figures have been obtained by using the same STM that has built the structures.

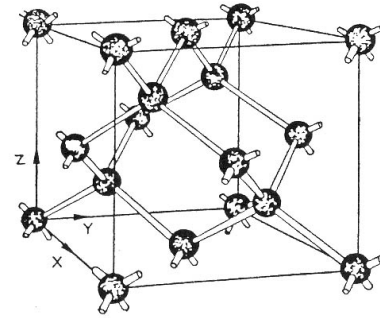


An example of a nanostructure is a quantum dot (QD), an island of a few nanometers of a crystalline semiconductor A inside a crystalline semiconductor B obtained without breaking the periodicity of the lattice sites of the crystal. The QDs could allow the fabrication of quantum computers. The figure shows a cross section of a InAs QD in GaAs. The QD is about 5 nm x 2 nm. The image has been taken by a STM.



Some properties of semiconductors used in devices with quantum confinement.

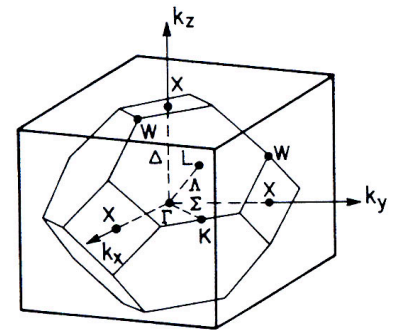
Silicon, germanium and diamond. The silicon atom has filled 1s, 2s and 2p levels, and 4 electrons in the 3s and 3p levels. The silicon crystal has the face-centered cubic (fcc) lattice and a base formed by a pair of Si atoms spaced by 2.37 Å. Each Si atom is bound to 4 Si atoms at the vertices of a tetrahedron. All the Si-Si bonds have the same length, 2.37 Å. Diamond, germanium and grey tin have the same crystal structure, but different cell size. C, Si and Ge are tetravalent.



Perspective view of diamond structure.

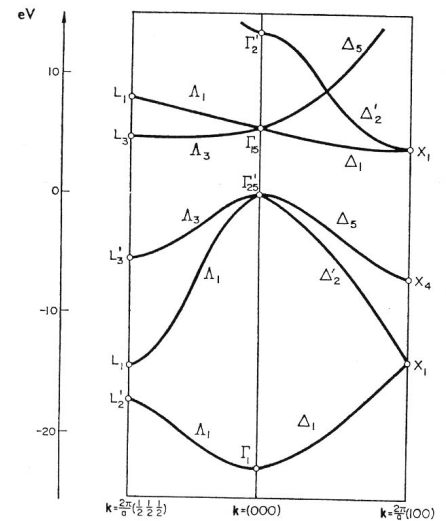
Bond length [Å]    size of the conventional cell [Å]

Diamond	1.4	3.57
Silicon	2.37	5.43
Germanium	2.45	5.55



Brillouin zone for diamond and zincblende lattices

The Brillouin zone (BZ) of the diamond structure is shown in the figure. Some high-symmetry points of the BZ are also indicated. Let us consider diamond. The two 1s electrons of each carbon atom form core levels with a binding energy of about 290 eV and are therefore not relevant for the energy scale of everyday life. The four 2s and 2p electrons fill the three lower energy bands shown at the right. Between the filled bands at the bottom and the empty bands at the top there is an energy gap of about 5 eV. In a Si crystal the 1s, 2s and 2p electrons form core levels about 1500 eV, 150 eV and 100 eV below the vacuum level, the four 3s and 3p electrons fill the valence bands shown in the lower part of the figure, that are very similar to those of diamond.



1 Energy bands for diamond. (From Bassani and Yoshimine, ref. [2].) The zero of energy has been taken to lie at the top of the valence band.

The energy gap between the filled valence bands and the empty conduction bands in the upper part of the figure is about 1.3 eV. The electronic structure of a Ge crystal is again very similar, with the valence bands filled by the four 4s and 4p electrons and an energy gap of about 0.7 eV.

Diamond, Si and Ge are group IV semiconductors.

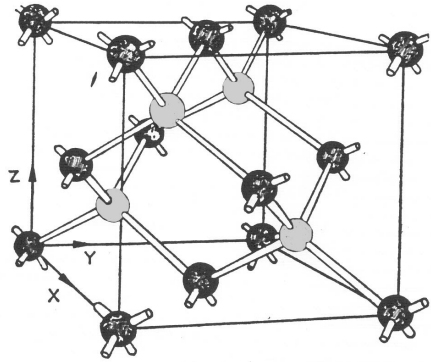
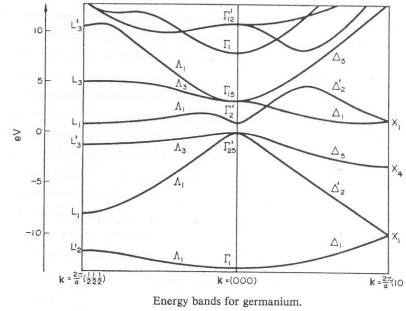
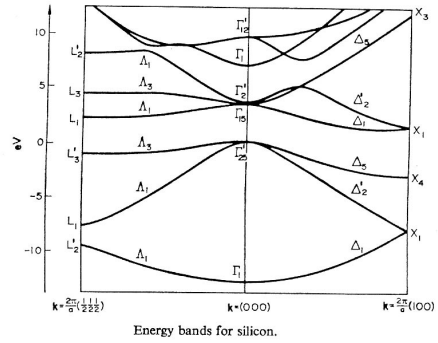
The diamond, Si and Ge crystals are formed a base made by a pair of C, Si or Ge atoms in a fcc Bravais lattice. Let us consider for instance the Ge crystal, and replace all the Ge-Ge pairs by Ga-As pairs. Ga and As are at the left and at the right of Ge in the periodic

table. One is trivalent, the other is pentavalent, while Ge is tetravalent. On the average, the potential felt by an electron after this substitution is not changed appreciably. The new crystal is a gallium arsenide crystal (GaAs), has the same fcc structure of the Ge crystal, but now each Ga atom is bound to four As atoms and each As is bound to four Ga atoms in a structure called zincblende structure (see figure at right, black atoms are Ga, grey atoms are As).

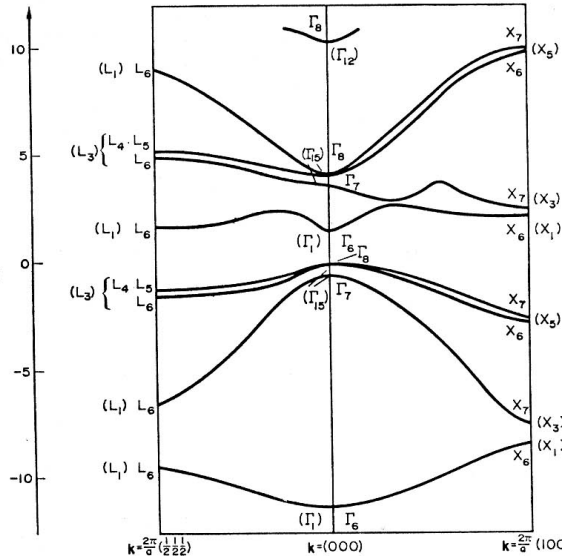
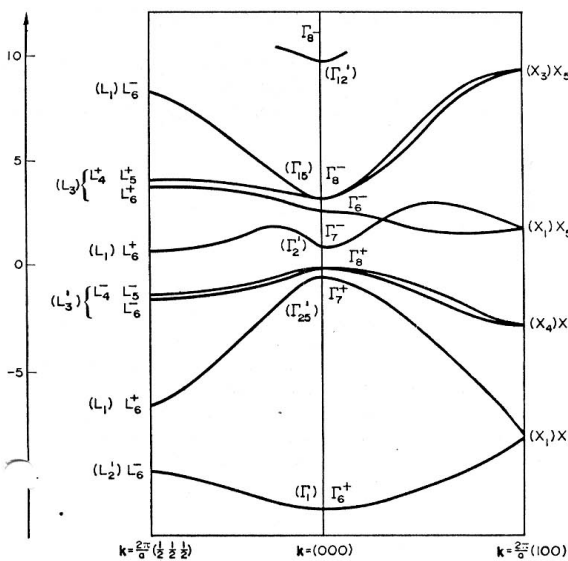
Also the electronic structure of GaAs is similar to that of Ge, the 4s and 4p electrons of Ga and As fill the conduction bands and the energy gap between the conduction and the valence bands is about 1.5 eV.

Crystals formed by atoms of the third column (Al, Ga, In) and of the fifth column of the periodic table (N, P, As, Sb), such as AlAs, GaP, InSb, InP....., called III-V semiconductors, have the same structure of GaAs and similar energy bands. The differences are in the lattice parameters and in the energy gaps that are wider in crystals formed by light atoms and narrower in those formed by heavy atoms.

For instance AlAs has a gap wider than that of GaAs, 2.3 eV vs 1.5 eV. The lattice parameter of the two crystals differ by about 1%. Let us take a GaAs crystal and substitute some Ga atoms with Al atoms at random positions, forming  $\text{Al}_{1-x}\text{Ga}_x\text{As}$ , with  $0 < x < 1$ . The system is now no more periodic, but since the potential felt by a valence electron on a Al atom is similar to that felt on a



Perspective view of zincblende structure



Energy bands for germanium with the inclusion of spin-orbit interaction. In brackets we provide the irreducible representations for the states of the simple group. (From ref. [15].)

Energy bands for GaAs with the inclusion of spin-orbit interaction. The irreducible representations for the states of the simple group are supplied in brackets. (From ref. [15].)

Ga atom – they are both trivalent- the disorder do not affect appreciably the electronic structure. A description in terms of band structure, even if the system is no more periodic, is a good approximation. The figure below shows how the energy gap of  $\text{Al}_{1-x}\text{Ga}_x\text{As}$  changes as a function of  $x$ . By choosing the right  $x$  it is possible to obtain the crystal with the

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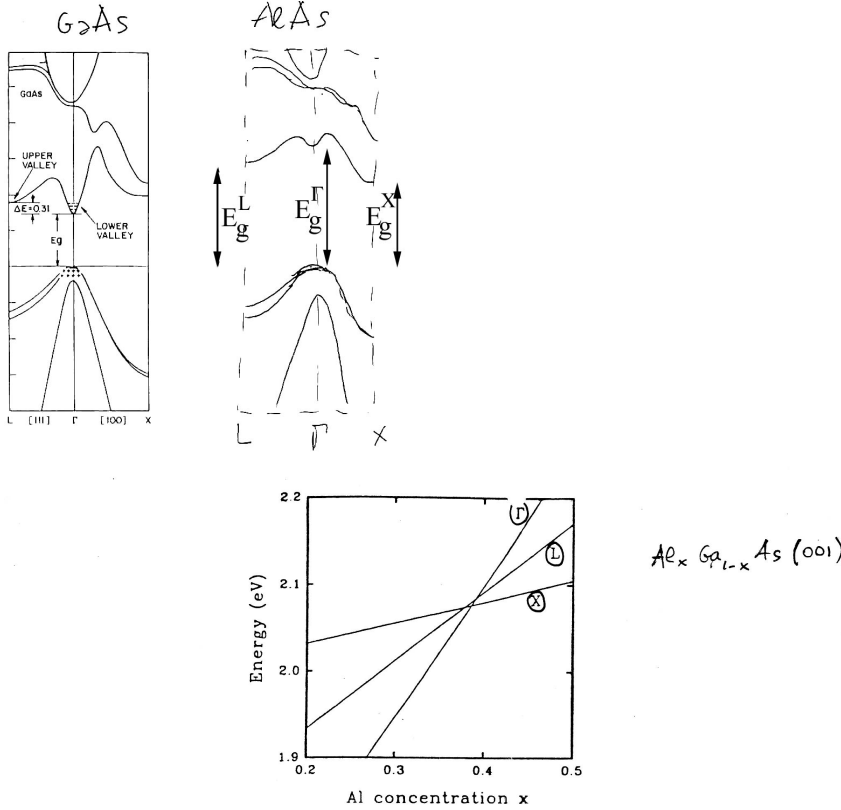


FIG. 5. The energy of the  $\Gamma$ , X, and L energy gaps vs Al concentration  $x$  at low temperature as given by the equations reported in Table III.

TABLE III. Low temperature energy gaps (in eV) for GaAs, AlAs and  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ .

	GaAs	AlAs	$\text{Al}_x\text{Ga}_{1-x}\text{As}$	
$E_g^\Gamma$	$1.5192 \pm 0.0002^a$	$3.14^b$	$1.5194 + (1.36 \pm 0.03)x + (0.22 \pm 0.06)x^2$	$0 < x < 1^c$
$E_g^X$	$1.981 \pm 0.006^d$	$2.250 \pm 0.001^e$	$1.5194 + 1.48x$ $(1.988 \pm 0.003) + (0.207 \pm 0.011)x + (0.055 \pm 0.008)x^2$	$x < 0.8^f$ $0 < x < 1^g$
$E_g^L$	$1.815^d$	-	$(1.974 \pm 0.002) + (0.263 \pm 0.003)x$ $1.775 + 0.792x$	$x < 0.8^f$ $0.2 < x < 0.55$

required gap, within the 1.5 and 2.3 eV. It is also possible to have an energy gap that change from place to place in a crystal by changing  $x$  locally.

The maximum of the valence band in the group IV semiconductors and in the III-V semiconductors is always at  $\Gamma$ , the center of the Brillouin zone,  $k=0$ . The minimum of the conduction band can be at  $\Gamma$ , like in GaAs, or at another point of the Brillouin zone, like in diamond, Si, Ge, AlAs... We will see that the interactions between the photons and the electrons in a crystal depend on the relative position of the maxima and minima in the Brillouin zone. By varying  $x$  is also possible to go from a direct gap semiconductor (i. e. minimum of the conduction band at the same  $k$  of the maximum of the valence band) to an indirect gap semiconductor (extrema at different  $k$ ) keeping the same structure and

lattice parameter.

In all the group IV semiconductors and the III-V semiconductors the lowest valence band is formed by s states mainly, while the upper valence bands derive from p states. These p valence bands have threefold degeneracy at  $\Gamma$ , if relativistic effects (spin-orbit) are neglected.