CMP Lecture 14

School of Physics
The University of Sydney

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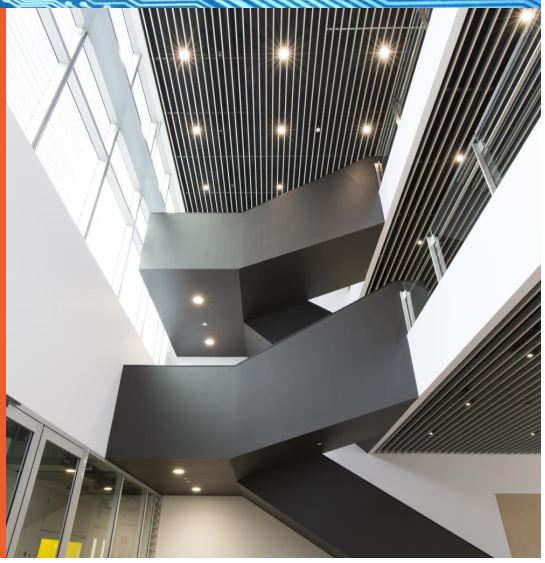

Article

Measuring phonon dispersion at an interface

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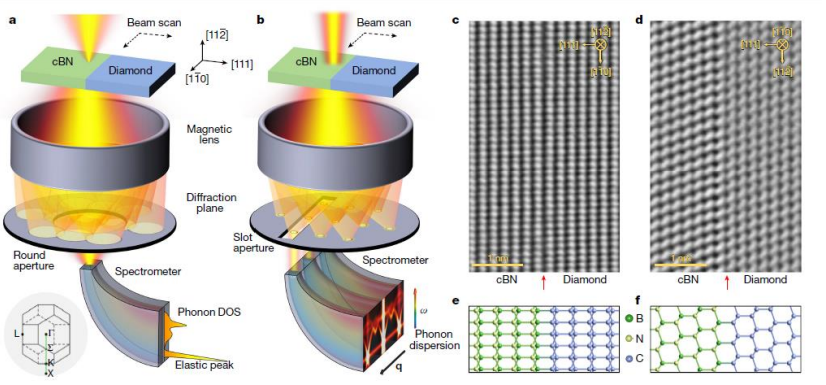
The breakdown of translational symmetry at heterointerfaces leads to the emergence of new phonon modes localized at the interface[1]. These modes have an essential role in thermal and electrical transport properties in devices, especially in miniature ones wherein the interface may dominate the entire response of the device[2]. Although related theoretical work began decades ago[1,3–5], experimental research is totally absent owing to challenges in achieving the combined spatial, momentum and spectral resolutions required to probe localized modes. Here, using the



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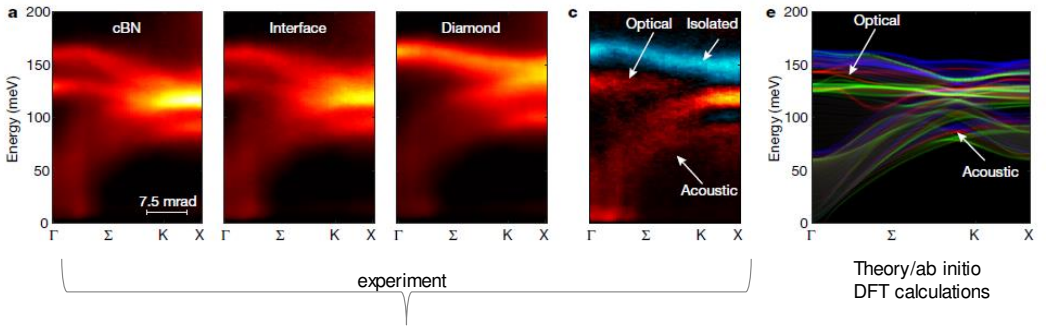
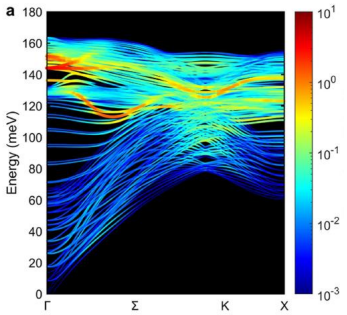


Phonon linewidth due to electron-phonon coupling mapped on the phonon dispersion calculated by density functional perturbation theory.

Compared with bulk modes, the interfacial optical modes couple strongly with electrons because both the interfacial phonon modes and the two-dimensional electron gas are highly confined at the interface.



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Semiconductors

One shouldn't work on semiconductors, that is a filthy mess; who knows whether any semiconductors exist.

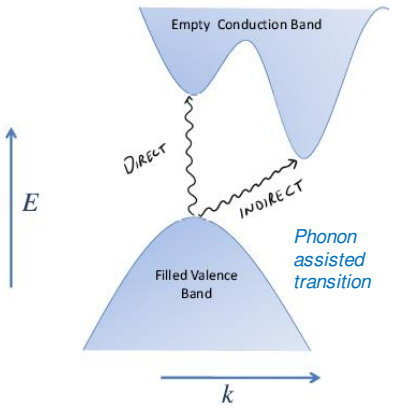
(Über Halbleiter soll man nicht arbeiten, das ist eine Schweinerei; wer weiss, ob es überhaupt Halbleiter gibt.)

Wofgang Pauli, 1931

4

Direct and indirect electron transitions

Solid State Basics Ch. 16.5



Band-gap determines minimum energy excitation.
If *k* for valence band maximum same as for conduction band minimum, called "direct band-gap". If not, called "indirect band-gap".

Band insulators cannot absorb photons which have energies less than their band-gap energy. This is because a single such photon does not have the energy to excite an electron from the valence band into the conduction band.
Since the valence band is completely filled, the minimum energy excitation is of the band-gap energy - so a low energy photon creates no excitations at all.
As a result, these low-energy photons do not get absorbed by this material at all, and they pass right through the material.

Direct transitions – strong light absorption
Indirect transitions – weak light absorption

Direct and indirect electron transitions

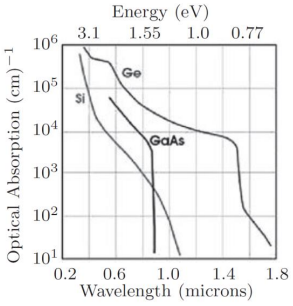


Table 16.1 Colors corresponding to photon energies.

Color	$\hbar\omega$
Infrared	< 1.65 eV
Red	~ 1.8 eV
Orange	~ 2.05 eV
Yellow	~ 2.15 eV
Green	~ 2.3 eV
Blue	~ 2.7 eV
Violet	~ 3.1 eV
Ultraviolet	> 3.2 eV

For an insulator with band-gap > 3.2 eV, it appears transparent since it cannot absorb any wavelength of visible light (see table below), e.g. diamond, quartz (silicon dioxide).

Semiconductors with somewhat smaller band gaps will absorb photons with energies above the band gap but will be transparent to photons below this band gap. E.g., cadmium sulfide (CdS) has a band gap of 2.6 eV, so that violet and blue light are absorbed, but red and green light are transmitted. Thus, the material looks reddish.
Semiconductors with very small band gaps (such as GaAs, Si, Ge) look black, since they absorb all frequencies of visible light.

Why semiconductors?

Semiconductors: they are here, there, and everywhere

- **Computers** Silicon (Si) MOSFETs (metal–oxide–semiconductor field-effect transistor), ICs (integrated circuits), CMOS (Complementary Metal-Oxide-Semiconductor) **laptops, anything "intelligent"**
- **Cell phones, pagers** Si ICs, GaAs FETs, BJTs (Bipolar junction transistors)
- **CD players** AlGaAs and InGaP laser diodes, Si photodiodes
- **TV remotes, mobile terminals** Light emitting diodes (LEDs)
- **Satellite dishes** InGaAs MMICs (Monolithic Microwave ICs)
- **Fiber networks** InGaAsP laser diodes, pin photod
- **Traffic signals, car taillights** GaN LEDs (light emitting diodes) (green, blue) InGaAsP LEDs (red, amber)
- **Air bags** Si MEMs (Microelectromechanical systems), Si ICs
- **...important, especially to Elec. Eng.& Computer Science**

III-Nitrides (AlN, GaN, InN) revolutionary development
-Can now have full spectrum of colour in LEDs!
(for a long time couldn't get blue)

Shuji Nakamura, professor at the Materials Department, University of California, Santa Barbara - regarded as the inventor of the blue LED, a major breakthrough in lighting technology.

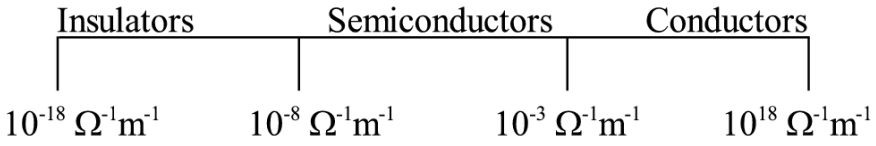
2014 Nobel Prize for Physics "for the invention of efficient blue light-emitting diodes, which has enabled bright and energy-saving white light sources" along with Isamu Akasaki and Hiroshi Amano.

Introduction

Semiconductors are materials whose electrical properties lie between conductors and insulators.

E.g.: Silicon and Germanium

Difference in conductivity



Semiconductor materials

- **Elemental semiconductors:** Si and Ge (column IV of periodic table) – composed of single species of atoms.
- **Compound semiconductors:** combinations of atoms of column III and column V and some combinations from column II and VI (combination of two different atoms results in binary compounds).
- There are also three-element (ternary) compounds (GaAsP) and four-elements (quaternary) compounds such as InGaAsP.

(a)	II	III	IV	V	VI
		B	C		
		Al	Si	P	S
	Zn	Ga	Ge	As	Se
	Cd	In		Sb	Te

(b)	Elemental	IV compounds	Binary III-V compounds	Binary II-VI compounds
	Si	SiC	AlP	ZnS
	Ge	SiGe	AlAs	ZnSe
			AlSb	ZnTe
			GaP	CdS
			GaAs	CdSe
			GaSb	CdTe
			InP	
			InAS	
			InSb	

Can engineer the characteristics of the material by changing the composition, e.g. can change the value of the energy band gap, which is a key property.

Semiconductor materials

- The wide variety of electronic and optical properties of semiconductors provides the device engineer with great flexibility in the design of electronic and opto-electronic functions.
- **Ge** was widely used in the early days of semiconductor development for transistors and diodes.
- **Si** is now used for the majority of transistors and integrated circuits.
- **Compounds** are widely used in high-speed devices and devices requiring the emission or absorption of light.

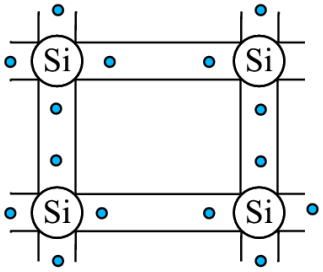
- The electronic and optical properties of semiconductors are strongly affected by impurities, which may be added in precisely controlled amounts (e.g. an impurity concentration of one part per million can change a sample of Si from a poor conductor to a good conductor of electric current). This process is called doping.

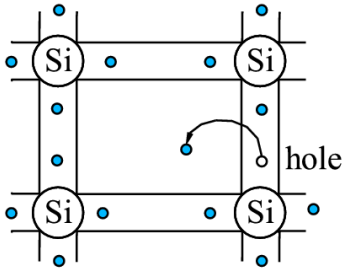
Intrinsic semiconductors

- Pure, i.e. not doped, semiconductors are called intrinsic.
- For the electronic properties of a semiconductor, “pure” means pure within 1 part per million to 1 part per billion.
- It is almost impossible to make really pure samples.

Intrinsic semiconductors: electrons and holes

e.g. Si and Ge are **tetravalent** elements – each atom of Si (Ge) has 4 valence electrons in crystal matrix.



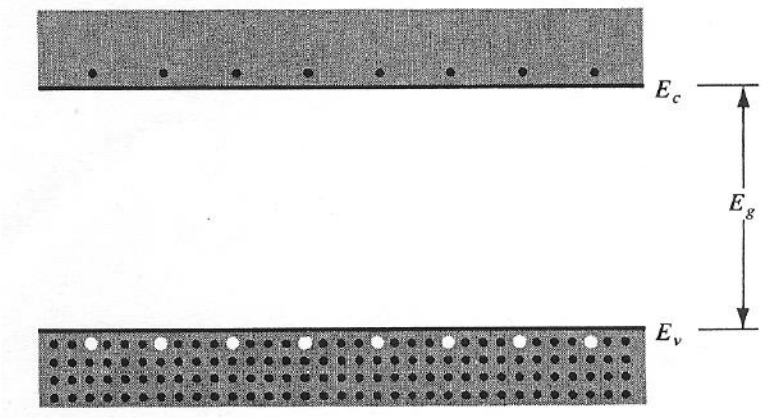


T=0 all electrons are bound in covalent bonds;
no carriers available for conduction.

For T> 0 thermal fluctuations can break electrons binding, creating free electron-hole pairs (EHP).
EHP's are the only charge carriers in intrinsic materials. Both can move throughout the lattice and therefore conduct current.

Since electron and holes are created in pairs – the electron concentration in the conduction band, n (electron/cm^3) is equal to the concentration of holes in the valence band, p (holes/cm^3).

Intrinsic semiconductors: electrons and holes



For T>0

there would be some electrons in an otherwise empty conduction band and some unoccupied states in an otherwise filled valence band.

Electron-hole pairs in a semiconductor. The bottom of the conduction band denoted as E_c and the top of the valence band denoted as E_v.

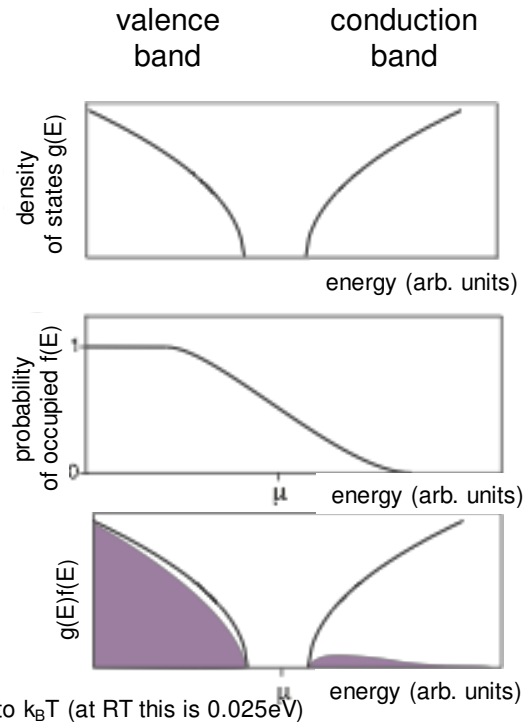
Doped semiconductors

- A **very small** amount of impurities can have a big influence on the conductivity of a semiconductor.
- Controlled addition of impurities is called doping.
- There are two types of doping: ***n* doping** (impurities increasing #electrons) and ***p* doping** (impurities increasing #holes).
- Typical doping levels are in the order of 10^{19} to 10^{23} impurity atoms per m^3. Remember: Si has a concentration of $5x10^{28}$ atoms per m^3 and an intrinsic carrier concentration of 10^{16} electrons/holes per m^3 at room temperature.

  (note, sometimes we will use per cm^3 and sometimes per m^3)

Can a material with μ in a band gap conduct?

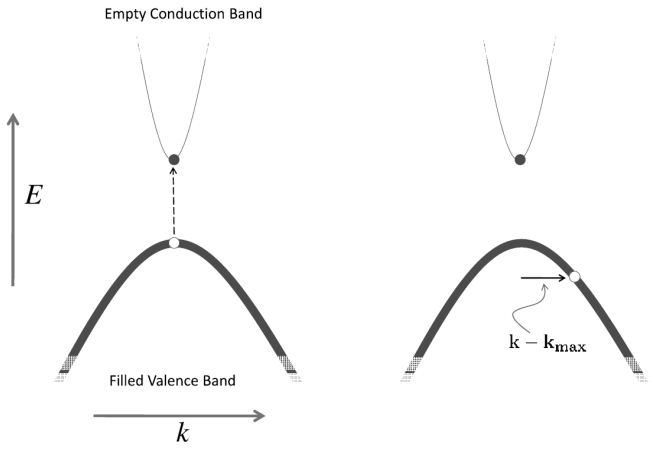
	gap size (eV)
InSb	0.18
InAs	0.36
Ge	0.67
Si	1.11
GaAs	1.43
SiC	2.3
diamond	5.5
MgF_2	11



If the gap is sufficiently small compared to k_BT (at RT this is 0.025eV) a material would not be a metal according to our definition but it would conduct!

Holes

Excite electron from valence band to conduction band, e.g., absorbing a photon or thermal excitation.
Absence of electron in valence band called a "hole" – treat holes as elementary particles.



To conserve charge, if the electron is negative, the hole is positively charged.

Electron can fall back into the hole, releasing energy and emitting photon, annihilating the electron and hole.
Moving the hole to a ***k*** away from the top of the valence band costs energy.
Energy of the system on right Is greater (less favourable) than that on left by

$$E = \hbar^2|\mathbf{k} - \mathbf{k_{max}}|^2/(2m^*)$$

Effective mass of electrons

As before, describe curvature at bottom of band in terms of effective mass.
Near bottom of conduction band, where **k**=**k** $_{min}$

$$E_{\text{elect}} = \frac{\hbar^2|\mathbf{k} - \mathbf{k_{min}}|^2}{2m^*_{\text{elect}}}$$

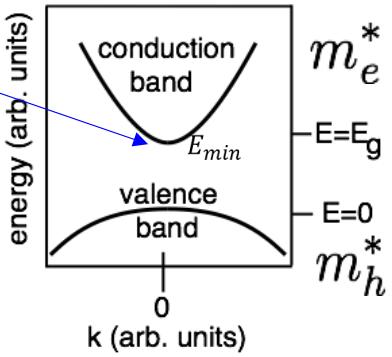
$$E = E_{min} + \alpha|\mathbf{k} - \mathbf{k_{min}}|^2 + \ldots$$

The effective mass is defined as,

$$\frac{\hbar^2}{m^*} = \frac{\partial^2 E}{\partial k^2} = 2\alpha$$

And the corresponding group velocity is

$$\mathbf{v} = \nabla_{\mathbf{k}} E/\hbar = \hbar(\mathbf{k} - \mathbf{k_{min}})/m^*$$



Chosen in analogy with free electron behaviour

$$E = \frac{\hbar^2|\mathbf{k}|^2}{2m}$$

$$\mathbf{v} = \nabla_{\mathbf{k}} E/\hbar = \hbar\mathbf{k}/m$$

Recall, for free electron

Effective mass of holes

For the top of the valence band, can write:

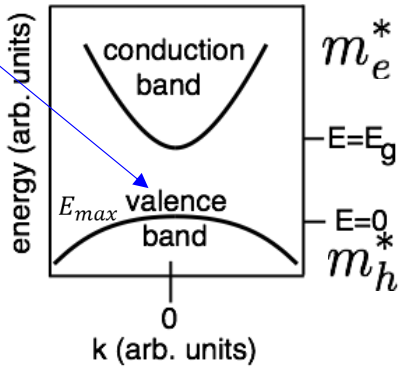
$$E = E_{\max} - \alpha|\mathbf{k} - \mathbf{k_{max}}|^2 + \ldots$$

And define effective mass for holes,

$$\frac{\hbar^2}{m^*_{\text{hole}}} = -\frac{\partial^2 E}{\partial k^2} = 2\alpha$$

Energy to move hole away from top of band is positive (thus makes sense to take effective mass as positive):

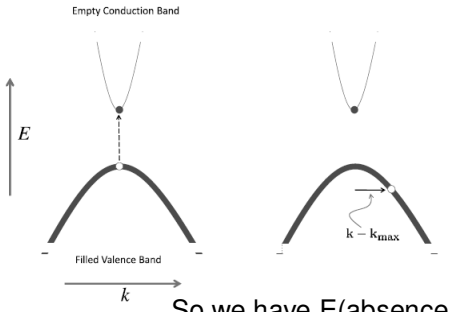
$$E_{\text{hole}} = \frac{\hbar^2|\mathbf{k} - \mathbf{k_{max}}|^2}{2m^*_{\text{hole}}} + constant$$



And corresponding hole group velocity is:

$$\mathbf{v}_{\text{hole}} = \nabla_{\mathbf{k}} E_{\text{hole}}/\hbar = \hbar(\mathbf{k} - \mathbf{k_{max}})/m^*_{\text{hole}}$$

The momentum and velocity of a hole



We see that moving a hole away from the top of the valence band costs positive energy. This can be viewed as pushing a balloon under water.

The lowest energy configuration of having a hole in the valence band is with the electrons at the lowest energy possible and the hole at the highest energy possible.

So we have E(absence of electron in state **k**) = −E(electron in state **k**).

Momentum

If an electron is added to a band in a state **k** then the crystal momentum increases by ħ**k**. Likewise, if an electron in state **k** is removed from an otherwise filled band, then the crystal momentum in the band must decrease by ħ**k**. Thus, the absence of an electron in state **k** corresponds to a hole whose crystal momentum is −ħ**k**, and thus $\mathbf{k}_{\text{hole}} = -\mathbf{k}_{\text{electron}}$

Group velocity

Analogous to the electron can write for the hole,

$\mathbf{v}_{\text{hole}} = \nabla_{\mathbf{k}} E_{\text{hole}}/\hbar = \hbar(\mathbf{k} - \mathbf{k_{max}})/m^*_{\text{hole}}$

Comparing to that of a (missing) electron at the same **k**, we have $\mathbf{v}_{\text{electron-missing}} = \mathbf{v}_{\text{hole}}$ since m_e^* is negative due to the curvature and $\mathbf{k}_{\text{hole}} = -\mathbf{k}_{\text{electron}}$

Means the time evolution of a state is independent of whether it is occupied or not

The effective mass

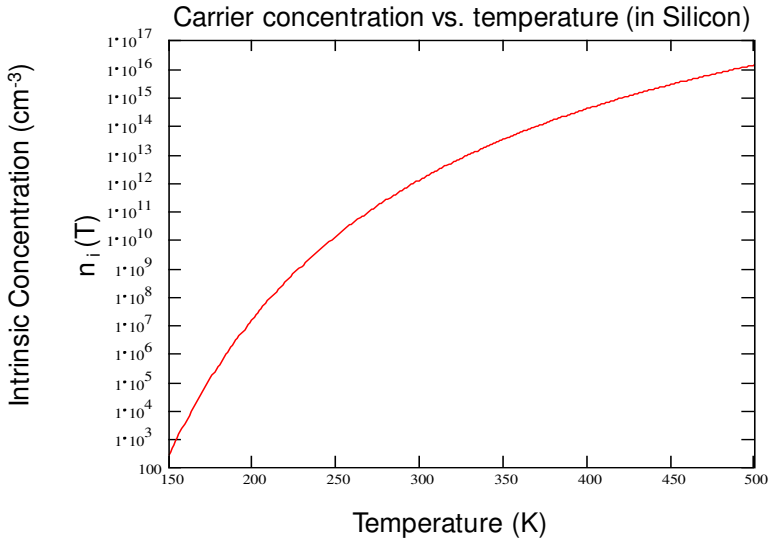
	m_e^*/m_e	m_h^*/m_e
InSb	0.014	0.4
InAs	0.022	0.4
Ge	0.6	0.28
Si	0.43	0.54
GaAs	0.065	0.5
Na	1.2	
Cu	0.99	
Sb	0.85	

m_e is the mass of the electron

$$m^* = \hbar^2 \left(\frac{d^2 E(k)}{dk^2} \right)^{-1}$$

Increasing conductivity by temperature

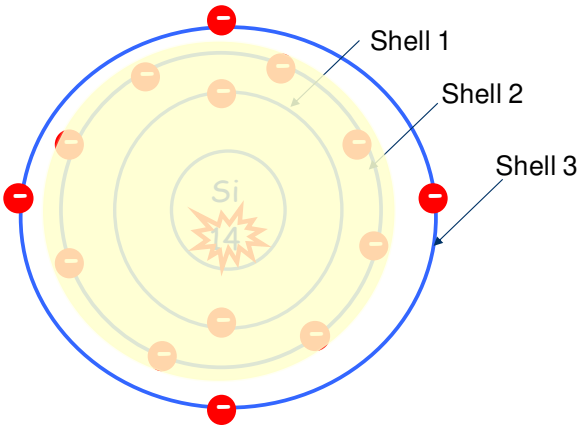
As temperature increases, the number of free electrons and holes created increases exponentially.



Therefore, the conductivity of a semiconductor is influenced by temperature

The silicon atomic structure

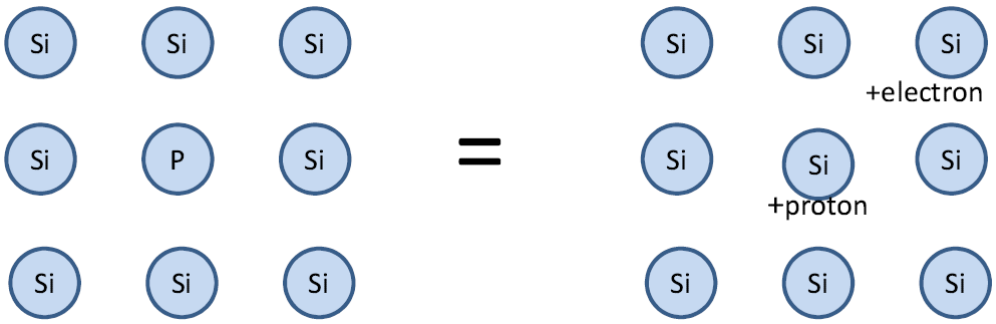
Si: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$



Silicon: our primary example and focus
Atomic no. 14
14 electrons in three shells: 2) 8) 4
i.e., 4 electrons in the outer "bonding" shell
Silicon forms strong covalent bonds with 4 neighbors.

However, like all other elements it would prefer to have 8 electrons in its outer shell.

Adding electrons or holes with impurities: doping

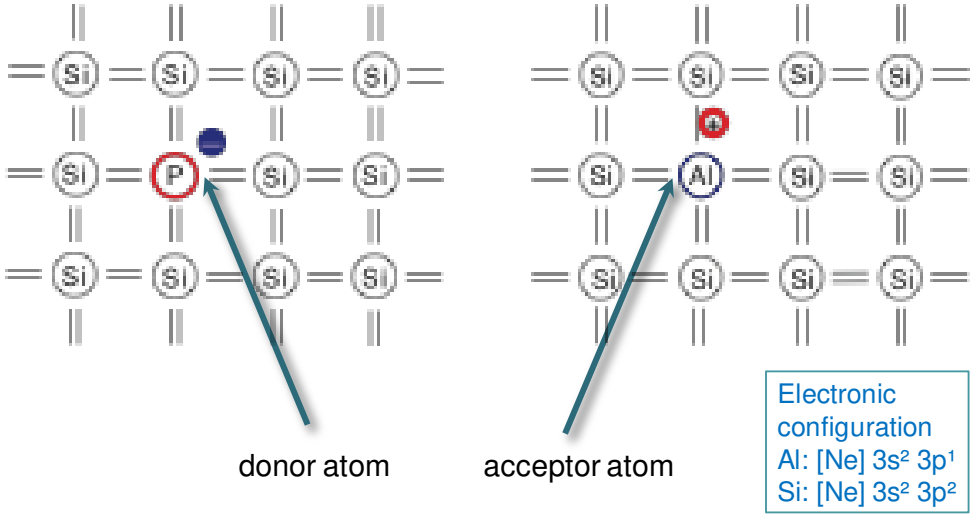


A phosphorous atom P replaces a silicon atom. The P atom is like an Si atom plus an extra electron.
Extra electron goes in conduction band
P is an electron donor in silicon – also called an n-type dopant (*n* is symbol for electron density).

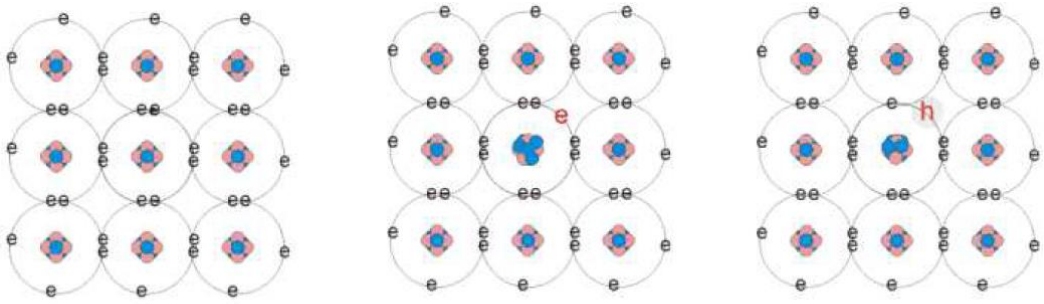
Electronic configuration
P: [Ne] $3s^2\ 3p^3$
Si: [Ne] $3s^2\ 3p^2$

n- and *p*-doping

Analogously, an Al replacing a silicon atom. The Al atom has one fewer electrons than Si. Gives rise to a hole. Al is an electron acceptor in silicon – also called a p-type dopant. p is symbol for hole density.



Adding electrons or holes with impurities: doping



intrinsic

All electrons in covalent bond with 2 electrons

n-doped

Extra electron

p-doped

Extra hole

Adding electrons or holes with impurities: doping

Solid State Basics, Ch. 17

Consider n-type dopant, e.g. P in Si: extra electron in conduction band acts like a free electron with mass *m** but also have positive charge in nucleus of P. Forms a bound state like a H atom – attract each other with potential:

$$V = \frac{e^2}{4\pi\epsilon_r\epsilon_0 r}$$

Energy eigenstates of H atom given by (where *n=1* is the ground state)

$$E_n^{H-atom} = -\mathrm{Ry}/n^2$$

Rydberg constant

$$\mathrm{Ry} = \frac{me^4}{8\epsilon_0^2 h^2} \approx 13.6\mathrm{eV}$$

ionization energy is 13.6 eV

m mass of electron

Radius of wave function $r_n \approx n^2 a_0$

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \approx 0.529\text{x } 10^{-10}\mathrm{m}$$

Bohr radius

Bohr model

Analogously, for a hydrogenic impurity state we have:

$$\mathrm{Ry}^{\mathrm{eff}} = \mathrm{Ry}\left(\frac{m_e^*}{m}\frac{1}{\epsilon_r^2}\right)$$

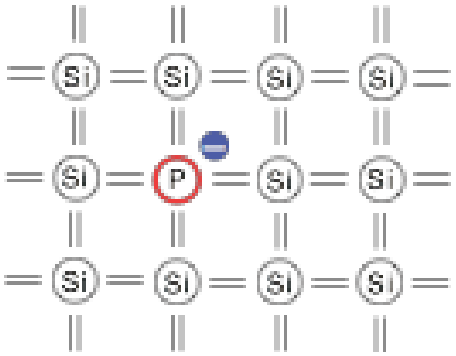
$$\epsilon_0 \longrightarrow \epsilon_0\epsilon_r \qquad m \longrightarrow m_e^*$$

dielectric constant (or relative permittivity)

$$a_0^{\mathrm{eff}} = a_0\left(\epsilon_r\frac{m}{m_e^*}\right)$$

n-doping

Phosphorus penta-valent, adds one electron to the material



The radius of this is quite big, 30 times Bohr radius

Estimate binding energy with Bohr model:

$$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2}\frac{1}{n^2}$$

using the modifications

$$m_e \rightarrow m^* \approx 0.43 m_e$$

$$\epsilon_0 \rightarrow \epsilon_0\epsilon_r \approx 11.7\,\epsilon_0$$

dielectric constant (or relative permittivity)

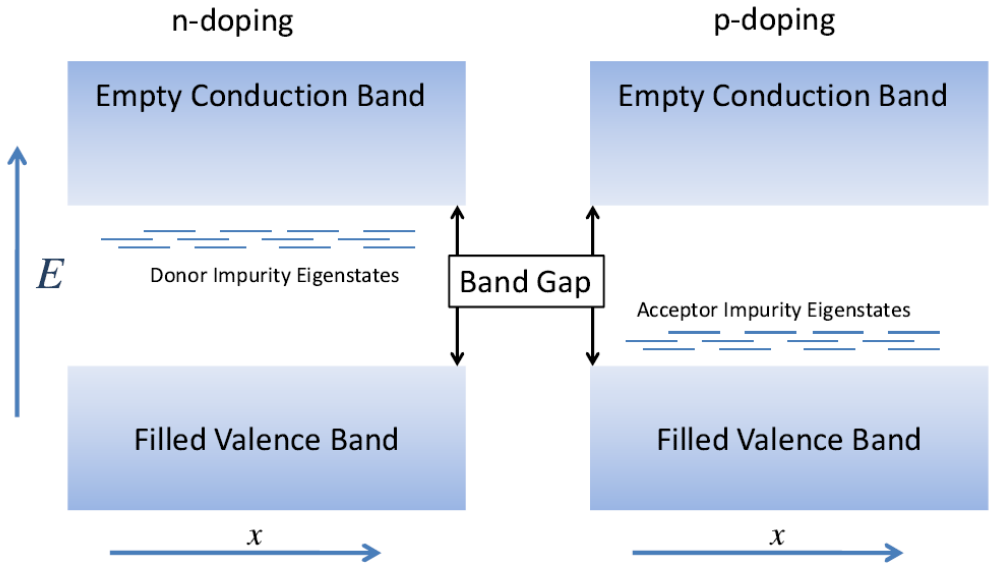
order of magnitude

$$E_1 = -30\ \mathrm{meV}$$

$$a_0^{\mathrm{eff}} = a_0\left(\epsilon_r\frac{m}{m_e^*}\right)$$

This donor impurity forms an energy eigenstate with energy just below the bottom of the conduction band (30 meV below the band bottom only).

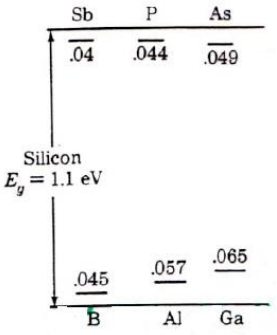
Adding electrons or holes with impurities: doping



Many localized hydrogen-atom-like eigenstates – not exactly the same since each impurity atom is perturbed by other impurity atoms in its environment. If density of impurities high enough, electrons (or holes) can hop from one impurity to the next, forming an *impurity band.*

Extrinsic material

By doping, a crystal can be altered so that it has a predominance of either electrons or holes. Thus, there are two types of doped semiconductors, n-type (mostly electrons) and p-type (mostly holes). When a crystal is doped such that the equilibrium carrier concentrations n and p are different from the intrinsic carrier concentration n_i, the material is said to be *extrinsic.*



The valence and conduction bands of silicon with additional impurity energy levels within the energy gap.

Donor impurities (elements of group V): P, Sb, As
Acceptor elements (group III): B, Al, Ga, In

When impurities or lattice defects are introduced, additional levels are created in the energy band structure, usually within the band gap.

Total number of electrons

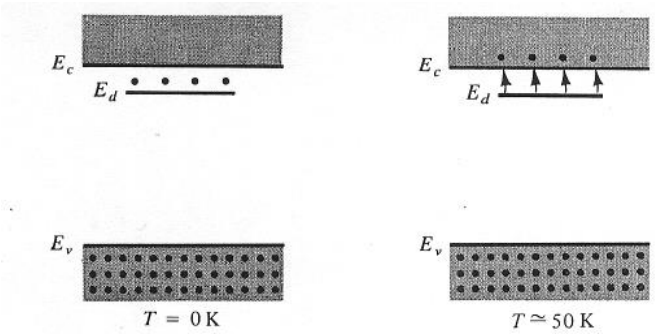
III – Al – 13

IV – Si – 14

V - P - 15

Extrinsic material – donation of electrons

n-type material



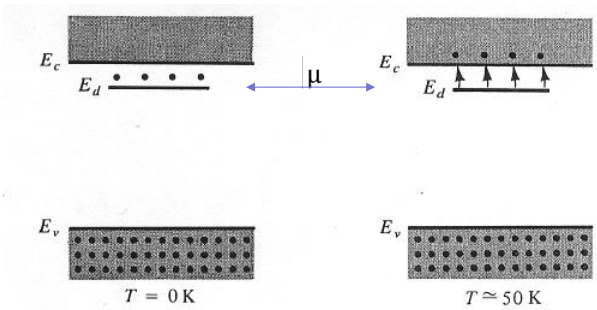
Donation of electrons from a donor level to the conduction band.

An impurity from column V introduces an energy level very near the conduction band in Ge or Si. This level is filled with electrons at 0 K, and very little thermal energy is required to excite these electrons to the conduction band.

Thus, at about 50-100 K nearly all of the electrons in the impurity level are "donated" to the conduction band. Such an impurity level is called a ***donor*** level, and the column V impurities in Ge or Si are called donor impurities.

Extrinsic material – donation of electrons

n-type material



Donation of electrons from a donor level to the conduction band.

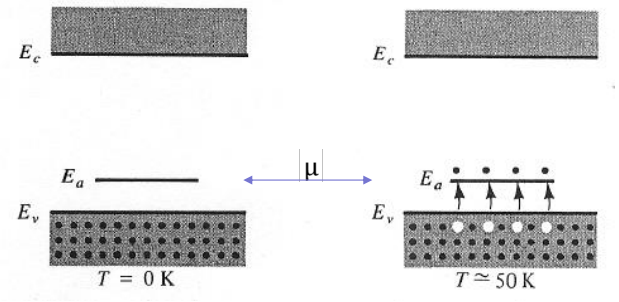
The material doped with donor impurities can have a considerable concentration of electrons in the conduction band, even when the temperature is too low for the intrinsic EHP concentration to be appreciable.

Thus, semiconductors doped with a significant number of donor atoms will have $n_0 >> (n_i, p_0)$ at room temperature. *This is **n-type** material.*

Electronic configuration
P: [Ne] $3s^2\,3p^3$
Si: [Ne] $3s^2\,3p^2$

Extrinsic material – acceptance of electrons

p-type material



Acceptance of valence band electrons by an acceptor level, and the resulting creation of holes.

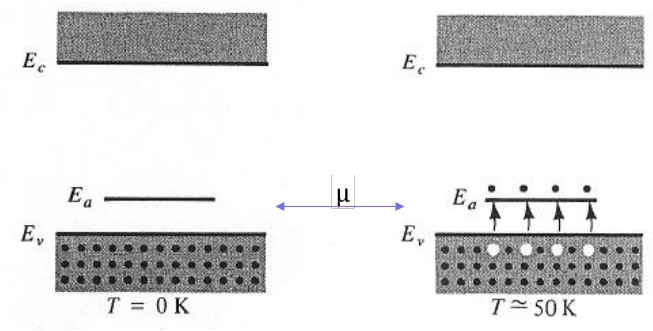
Atoms from column III (B, Al, Ga, and In) introduce impurity levels in Ge or Si near the valence band. These levels are empty of electrons at 0 K.

At low temperatures, enough thermal energy is available to excite electrons from the valence band into the impurity level, leaving behind holes in the valence band.

Electronic configuration
Al: [Ne] $3s^2\ 3p^1$
Si: [Ne] $3s^2\ 3p^2$

Extrinsic material – acceptance of electrons

p-type material

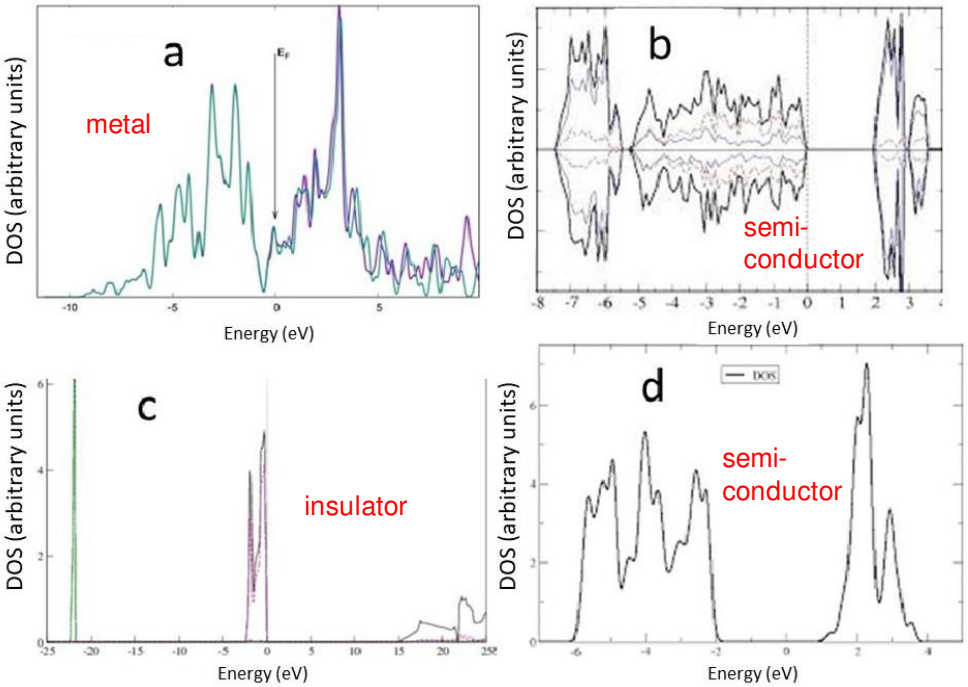


Acceptance of valence band electrons by an acceptor level, and the resulting creation of holes.

Since this type of impurity level "accepts" electrons from the valence band, it is called an *acceptor* level, and the column III impurities are acceptor impurities in Ge and Si.

As figure indicates, doping with acceptor impurities can create a semiconductor with a hole concentration p_0 much greater than the conduction band electron concentration n_0 (***this is p-type material***).

Schematic band diagrams



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