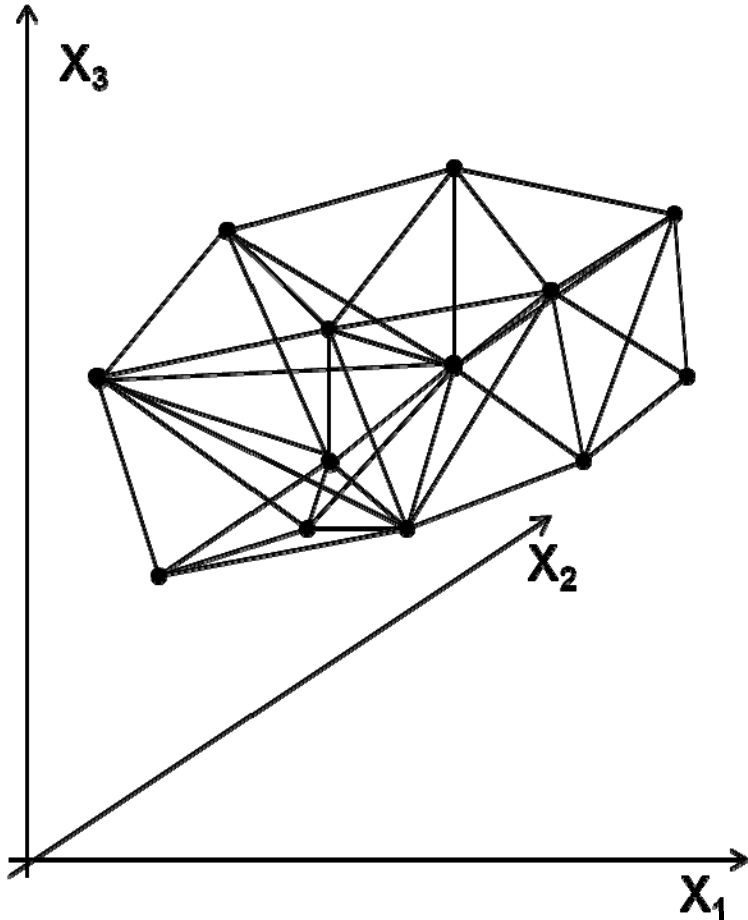


# **Nano-scale phenomena in disordered semiconductors**

**Dimiter Alexandrov**

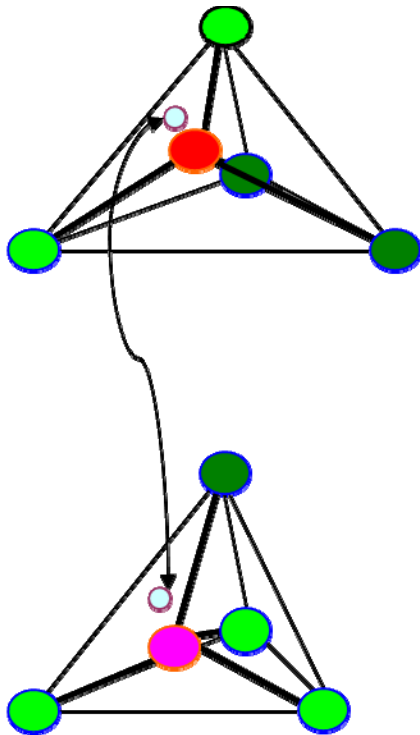
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# Symmetry of the multinary crystal



- Positions of the atoms in the coordinate system of the external observer
- *(the cells of tetrahedral type have edges of different lengths)*

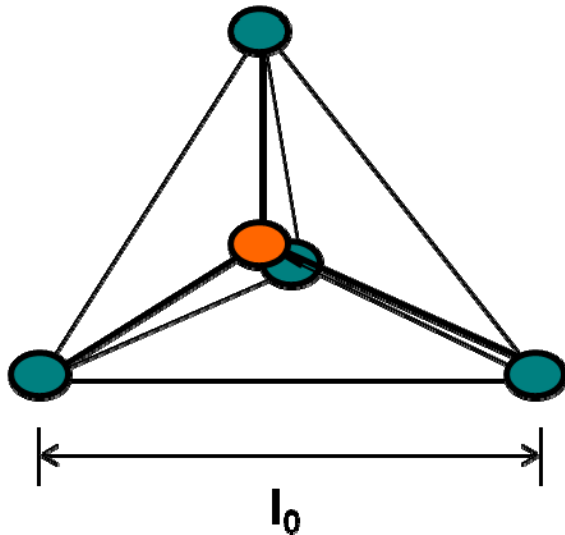
# Energy equivalency in different cells of tetrahedral type



In two different cells of tetrahedral type it is possible to be found two identical points in term of electron propagator  
*(The atomic substitutions in multinary crystal save the valences of the corresponding atoms.)*

# Electron metric system

Basis of the new metric system:  
*the change of the electron energy  
within the primitive cell*



Weyl's metric system:

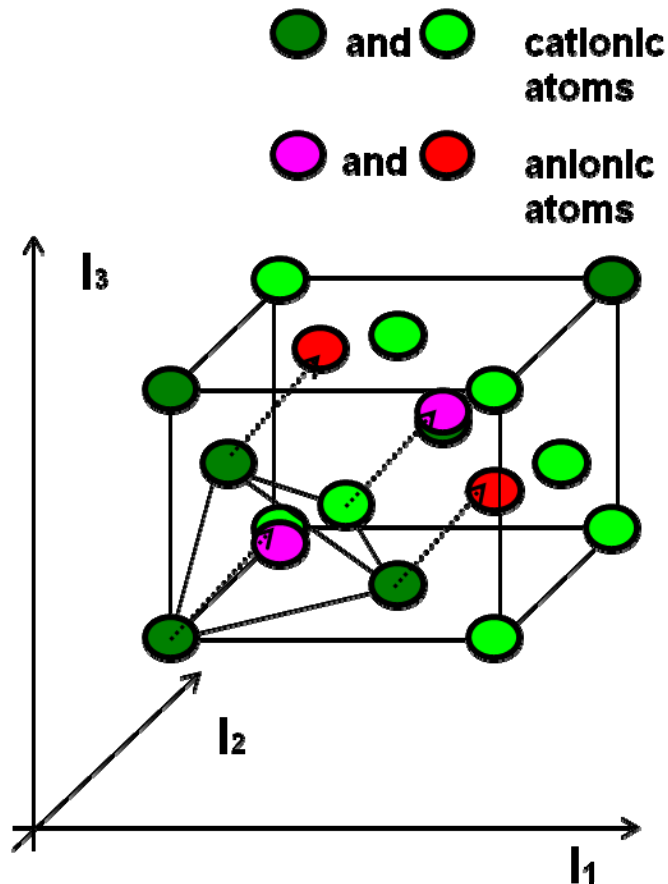
$$l_i = l_0 \exp(\alpha_i \int \Phi_i dx_i)$$

For the tetrahedral cell:

$$l_i = l_0 \exp(\alpha_i \int \mathcal{E}_i dx_i)$$

$i = 1, 2, 3$ , and  $\mathcal{E}_i$  is electrical field strength. The integration between two nodes of the crystal lattice having equal electron charges is equal to zero, i.e.  $l = l_0$ .

# Symmetry of the multinary crystal in the electron metric system



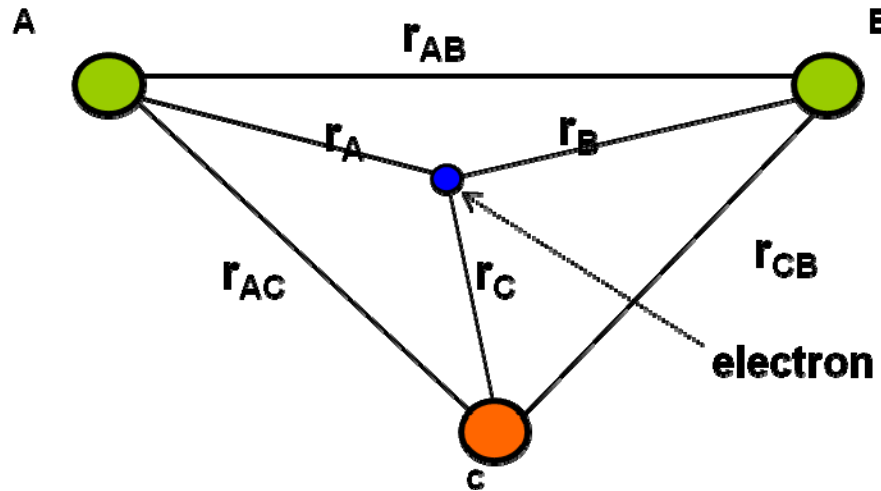
Assumptions:

*i)* The tetrahedral cell is electro-neutral;

*ii)* The atomic substitutions in multinary crystal save the valences of the corresponding atoms;

*iii)* The electrical charges are of point type and they are concentrated exclusively in the nodes of the crystal lattice;

# Constant $I_0$



$$\{-\hbar^2 \Delta / 2m + e^2 [ |Z|^2 / (4 r_{AB}) - |Z|^2 / (2 r_{AC}) - |Z|^2 / (2 r_{BC})$$
$$- |Z| / (2 r_A) - |Z| / (2 r_B) + |Z| / r_C ] \} \psi = E \psi$$

# Constant $l_0$ (ctn)

$$\{-\hbar^2 \Delta / 2m + e^2 [ |Z|^2 / (4 l_0) - |Z|^2 / (2 l_0 \exp(3\alpha e |Z|/2)) - |Z|^2 / (2 l_0 \exp(3\alpha e |Z|/2)) - |Z| / (2 l_0 \exp(\alpha\beta)) - |Z| / (2 l_0 \exp(-\alpha\beta)) + |Z| / (l_0 \exp(-\alpha\beta) \exp(-3\alpha e |Z|/2)) ]\} \psi = E \psi$$

$$l_0 = e^2 / (E_{\min} - H_0) [ ( |Z|^2 / 4 - |Z|^2 / (2 \exp(-3\alpha e |Z|/2)) - |Z|^2 / (2 \exp(3\alpha e |Z|/2)) - |Z| H_{-\beta} / 2 - |Z| H_{\beta} / 2 + |Z| H_{\beta} / ( \exp(-3\alpha e |Z|/2) ) ]$$

The binary alloys InN, GaN and AlN have values of  $|Z|$  - 1.56, 1.48 and 1.36 respectively. It means that it can be considered that average  $|Z| = 1.47$  for the tetrahedral cells of  $\text{In}_x\text{Ga}_{1-x}\text{N}$ , of  $\text{In}_x\text{Al}_{1-x}\text{N}$  and of  $\text{Ga}_x\text{Al}_{1-x}\text{N}$  with error not greater than 7.5%, and the corresponding tetrahedral edge  $l_0$  in the electron metric system.

# Electron wave vector and electron states in multinary crystal

Assumptions:

- The quasi-elementary tetrahedral cell is electro-neutral;
- The electrons belonging to both the conduction band and the valence band have energies  $E$  greater than the potential energy  $U$  of the nuclei of certain quasi-elementary tetrahedral cell;

# Electron wave vector and electron states in multinary crystal (ctn)

- for the external metric system:

$$(1/\hbar) \int \{2m [E - U(x_i)]\}^{1/2} dx_i = |x_B - x_A| k_{xi} = n \pi$$

$|x_B - x_A|$  is tetrahedral edge

- for the electron metric system:

$$(1/\hbar) \int \{2m [E - U(l)]\}^{1/2} dl = l_0 k_l = n \pi$$

$l_0$  is tetrahedral edge

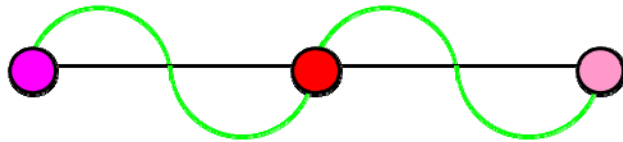
# Electron wave vector and electron states in multinary crystal (ctn)

## Conclusions:

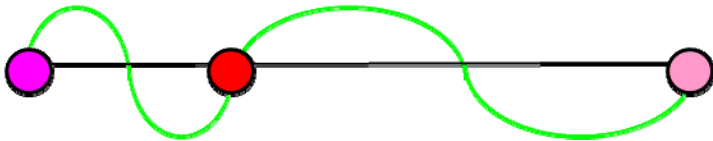
- The electron wave length  $\lambda_l$  in the electron metric system stays unchanged when the electron is moving through different quasi-elementary tetrahedral cells;
- The electron wave length  $\lambda_{x_i}$  in the external metric system changes when the electron is moving through different quasi-elementary tetrahedral cells.
- The Bloch's theorem is satisfied in the electron metric system.
- The number of electron states remains unchanged in different metric systems. (It means one can determine the electron states in the electron metric system and they give the corresponding states in the external metric system.)
- Considering that a sub-lattice of the multinary crystal is built by different sort of atoms one must expect that the electron energy corresponding to certain electron state depends on the quasi-elementary cell, i.e. the following formula is valid.

$$E(\mathbf{r}) = \sum_{\mathbf{q}} \delta(\mathbf{r} - \mathbf{R}_{\mathbf{q}}) E(\mathbf{q})$$

# Electron wave length

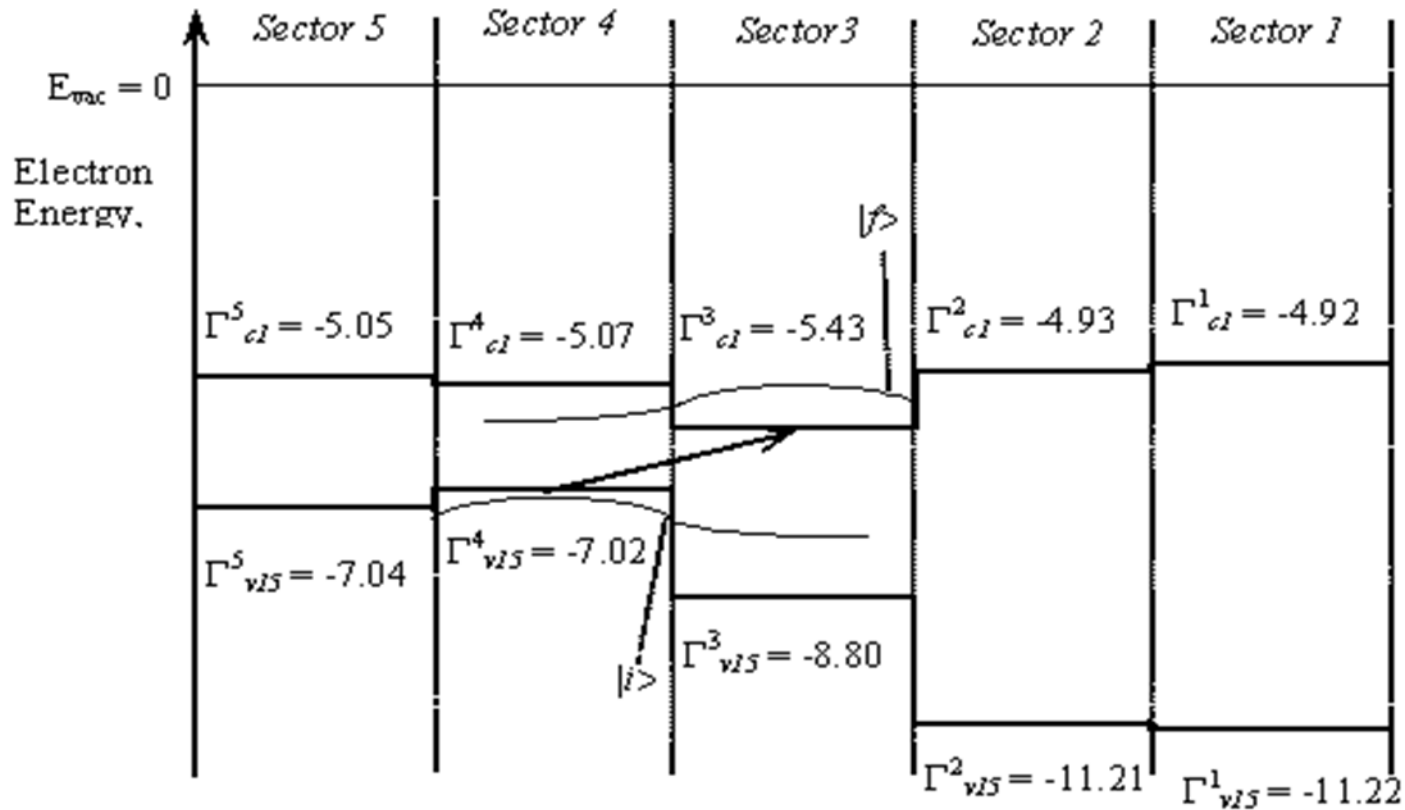


In the electron metric system

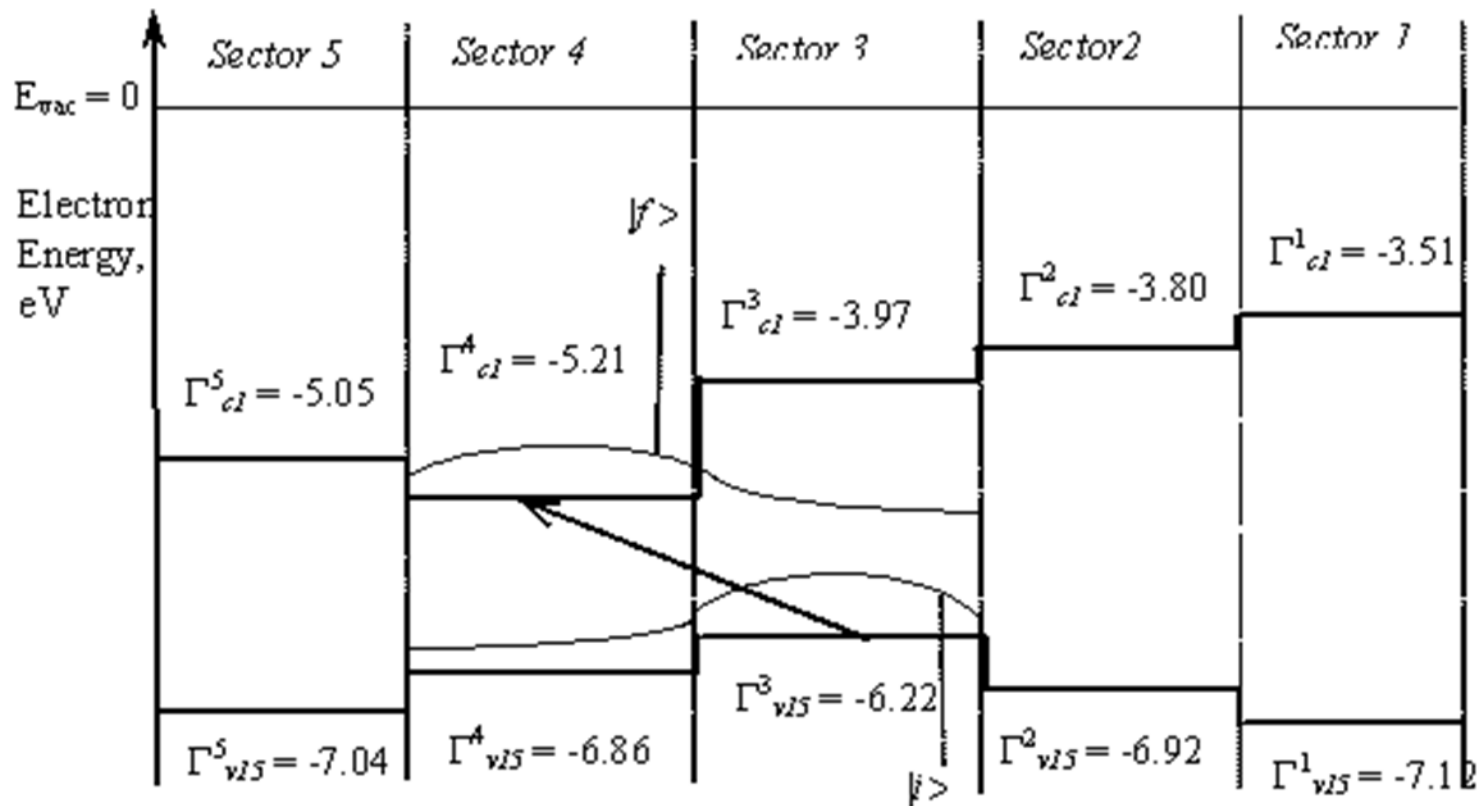


In the external metric system

# Electron band structure of $\text{In}_x\text{Al}_{1-x}\text{N}$

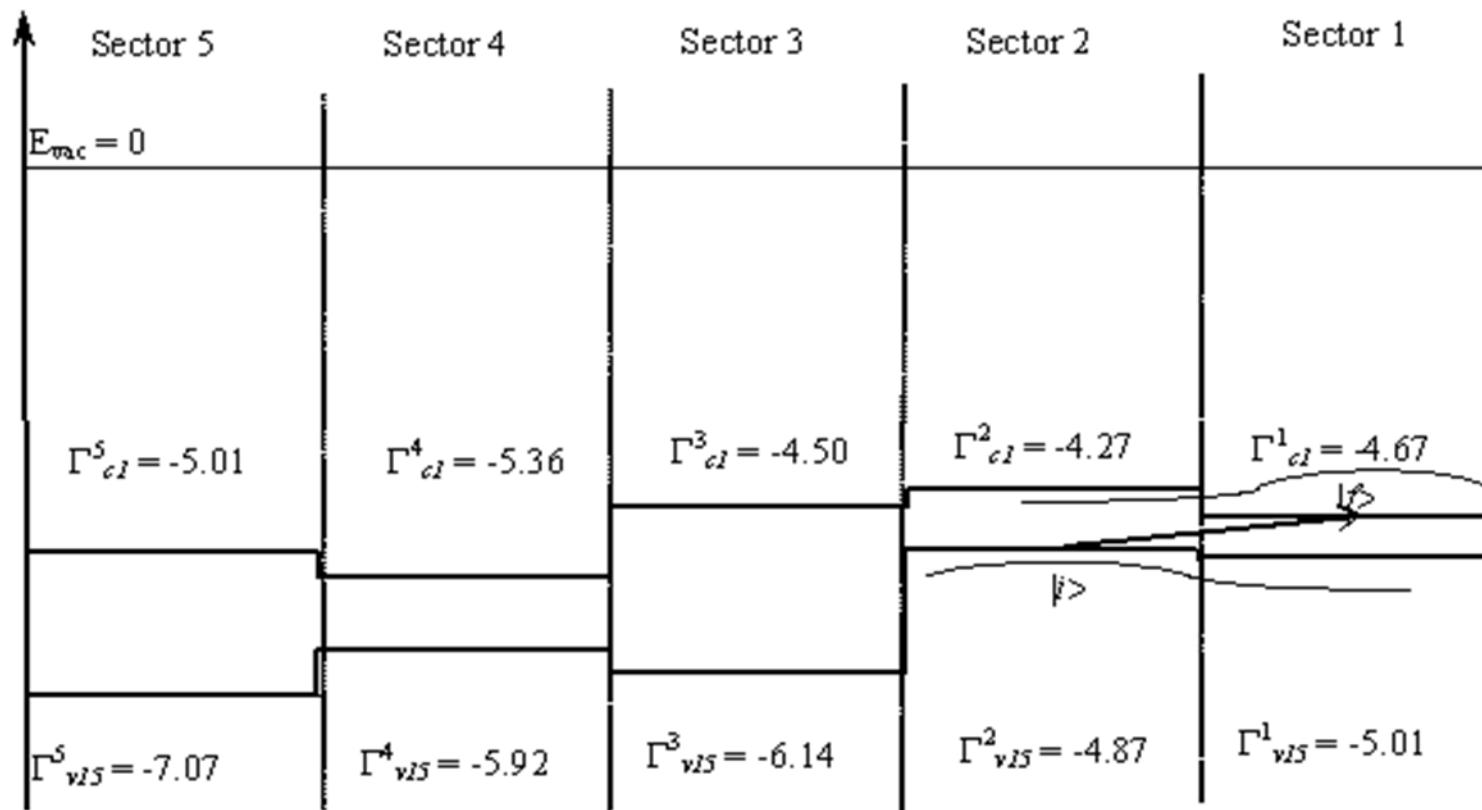


# Electron band structure of $\text{In}_x\text{Ga}_{1-x}\text{N}$

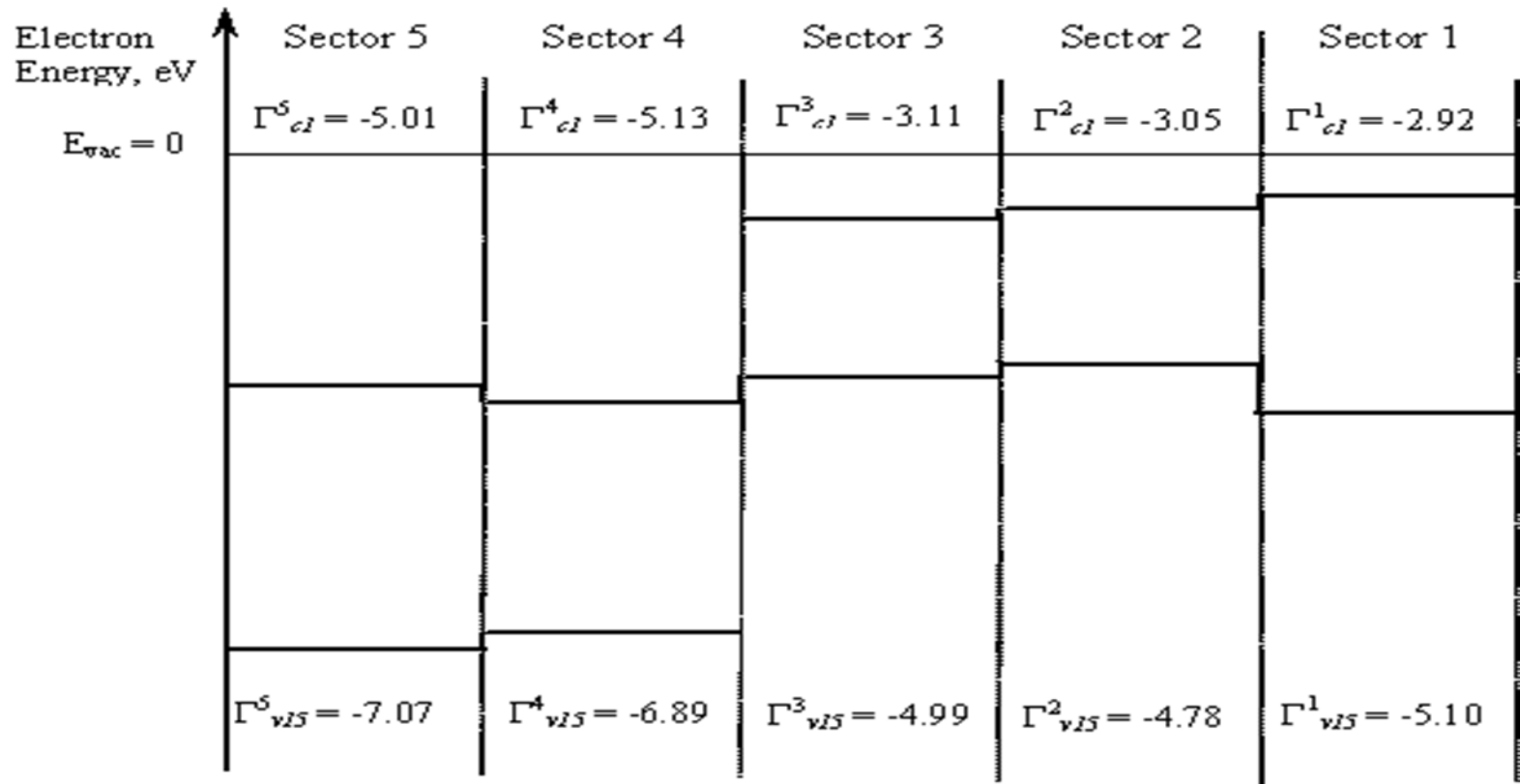


# Electron band structure of non-stoichiometric InN:In

Electron energy, eV



# Electron band structure of non-stoichiometric InN:N



# Optical phenomena in InN and related alloys

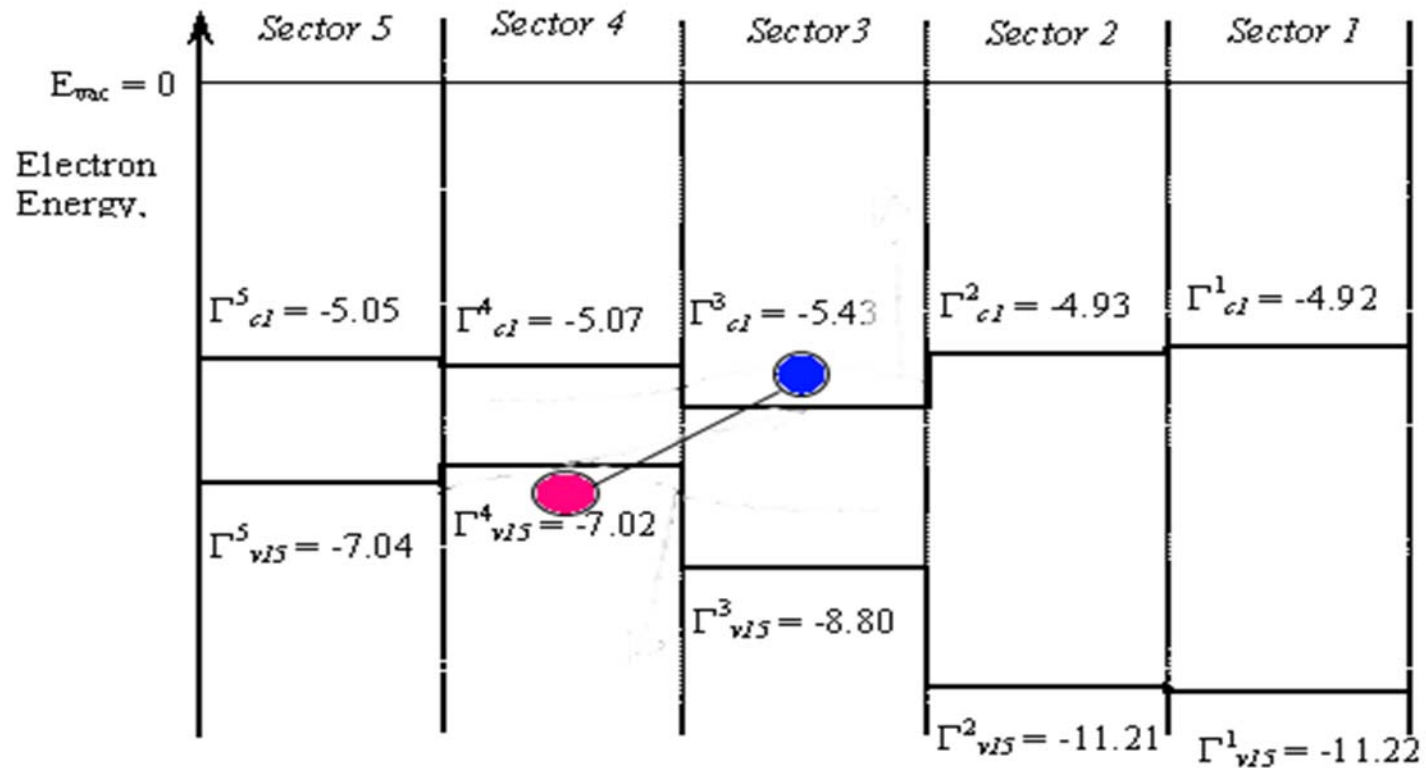
## 1. Tunnel optical absorptions

- for  $\text{InO}_y\text{N}_{1-y} \leftrightarrow \sim 1.19 \text{ eV}$
- for  $\text{In}_x\text{Al}_{1-x}\text{N} \leftrightarrow 1.58 - 1.62 \text{ eV}$
- for  $\text{In}_x\text{Ga}_{1-x}\text{N} \leftrightarrow 1.40 - 1.56 \text{ eV}$
- for non-stoichiometric  $\text{InN:In} \leftrightarrow \sim 0.2 \text{ eV}$

# Optical phenomena...(ctn)

## 2. Excitons of the structure

(the example is on basis of the electron band structure of  $\text{In}_x\text{Al}_{1-x}\text{N}$ )



# Optical phenomena .... (ctn)

## 3. Excitons of the structure and PL spectra

Annihilation between both the electron and the hole belonging to exciton of the structure determines the PL spectrum:

- for  $\text{InO}_y\text{N}_{1-y}$   $\leftrightarrow$  0.84 – 1.01 eV
- for  $\text{In}_x\text{Al}_{1-x}\text{N}$   $\leftrightarrow$  0.765 – 0.778 eV
- for  $\text{In}_x\text{Ga}_{1-x}\text{N}$   $\leftrightarrow$  0.50 – 0.82 eV

*(these energies correspond to the first hydrogen like energy level of an exciton of the structure)*

# Optical phenomena....(ctn)

## 4. Qualitative reason for both excitons of the structure and tunnel optical absorption in InN and related alloys

It is necessary that a minimum in the conduction band and a maximum in the valence band to be close. It determines:

- significant binding energy forming excitons of the structure if electron is located in the minimum and hole occupies the maximum;
- determines overlapping between the wave functions  $|i\rangle$  and  $|f\rangle$  giving tunnel optical absorption if electron occupies the maximum and there is no electron in the minimum.

**Thank you!**

**Q & A**