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Simulation des propriétés mécaniques, piezoélectriques, électroniques ou optiques de nanostructures à semiconducteurs

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FOTON UMR6082

(26/11/2008)

INSA RENNES

Semiconducteurs III-V :
des nanostructures aux composants

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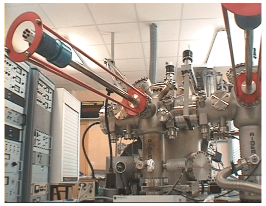
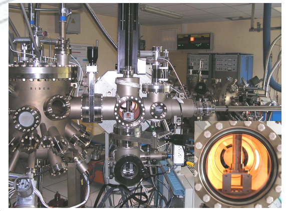


Croissance de nanostructures (EJM)



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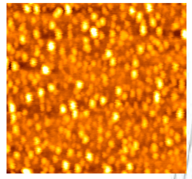
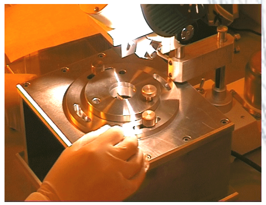
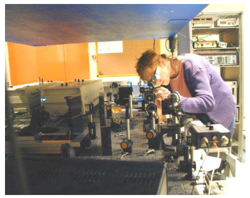


Composants optoélectroniques

Caractérisations optiques et structurales des matériaux

Salle blanche,
Caractérisations
des composants





AFM, RX,
PL, Pompe-sonde…

Géométrie des composants

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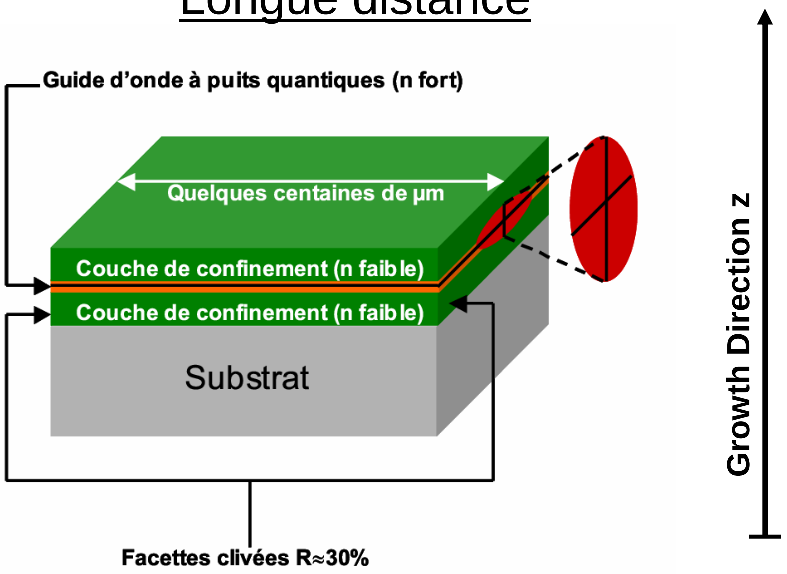
Exemple : laser pour telecoms optiques

Laser à cavité horizontale

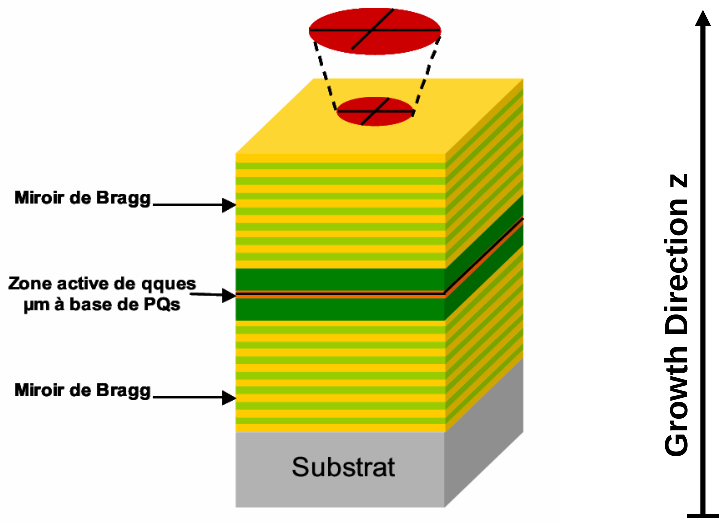
Longue distance



- **λ = 1,55 µm**
- Débit (2.5, 10 et 40 Gbits/sec avec modulation externe)
- Besoin limité en composants
  Composant complexe et cher

Laser à cavité verticale (VCSEL)

Courte distance



- (MAN / LAN) (DATAcom)
  λ = 1,3 et 1,55 µm - λ = 0,85 µm
- Débit (jusqu'à 10 Gbits/sec en modulation directe)
- Besoin important en composants
  Fabrication à grande échelle et cout faible

Plusieurs échelles

- **échelle nano : effets quantiques et anisotropie des nanostructures à semiconducteurs**

- **échelle micro : effets de confinement optique, d'anisotropie, de cross-talk électronique des zones actives et cavités**

- **échelle méso (cm) : effets électrique (contacts) et thermique (évacuation de la chaleur, cross-talk) pour les composants**

- **échelle macro : insertion du composant dans un système (taux d'erreurs, pertes d'insertion …)**

Nanostructures : structures de basse dimensionalité

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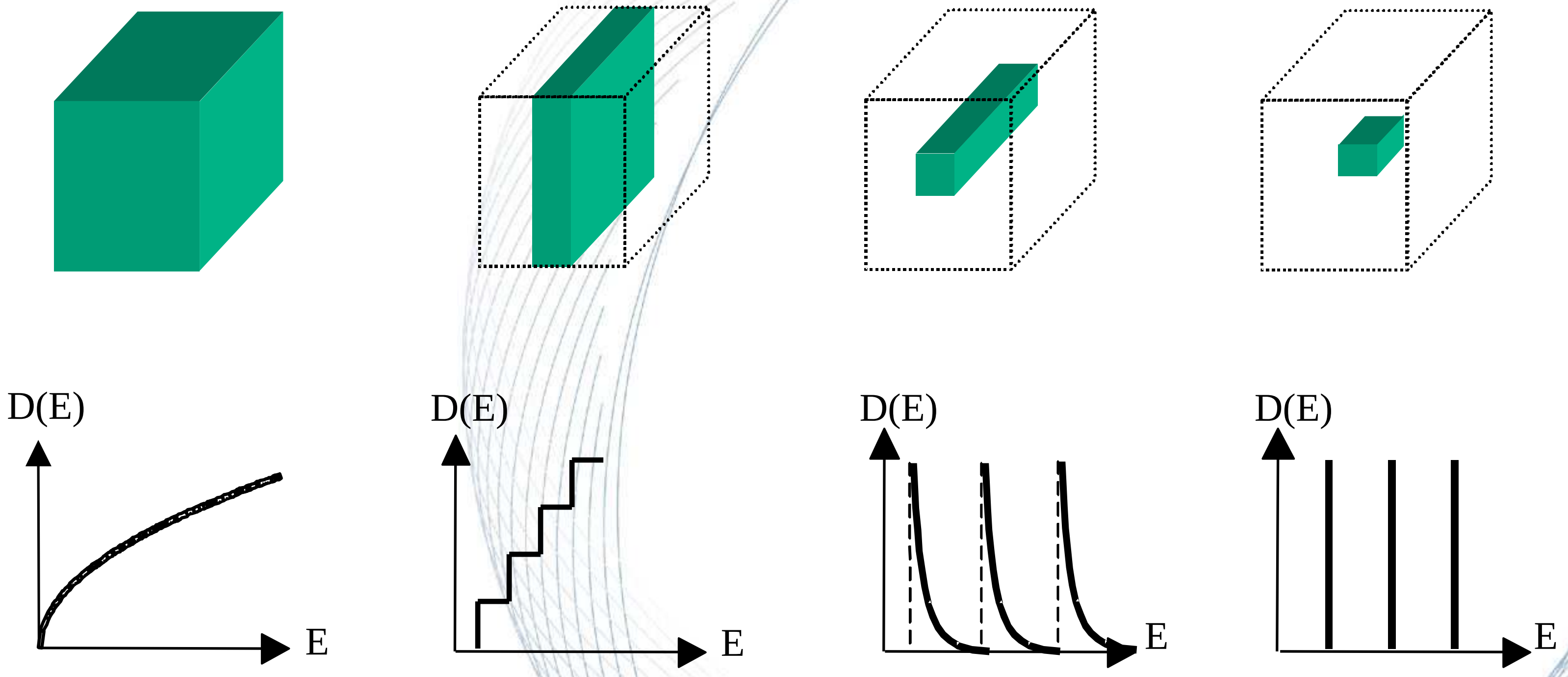
Massif	Puits	Fils	Ilot
3D	2D	1D	0D



Densité d'états électroniques

Coordonnées paraboliques et fonctions hypergéométriques confluentes

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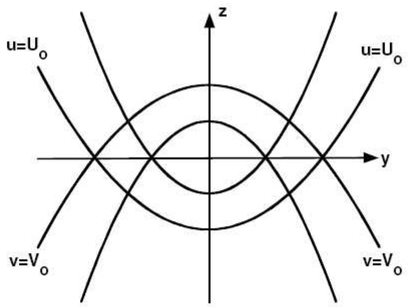
$$x = auv\cos(\theta) \qquad y = auv\sin(\theta) \qquad z = a(u^2 - v^2)/2.$$

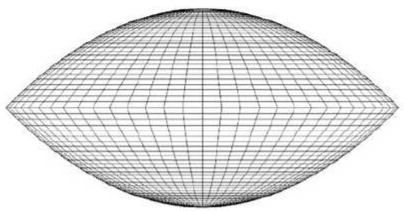
(u, v, θ) $(0 \leqslant u \leqslant \infty, 0 \leqslant v \leqslant \infty$ and $0 \leqslant \theta \leqslant 2\pi)$

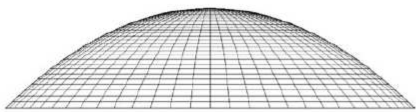
Ilots quantiques lenticulaires en régime de confinement fort



(a)

$$H = \frac{-\hbar^2}{2}\vec{\nabla}\frac{1}{m(\vec{r})}\vec{\nabla} + V(\vec{r}) = -\frac{\hbar^2}{2a^2(u^2+v^2)}\left[\frac{1}{u}\frac{\partial}{\partial u}\frac{u}{m_{(u,v)}}\frac{\partial}{\partial u} + \frac{\partial}{\partial v}\frac{v}{m_{(u,v)}}\frac{\partial}{\partial v}\right] - \frac{\hbar^2}{2a^2u^2v^2m_{(u,v)}}\frac{\partial^2}{\partial\theta^2} + V(u,v).$$

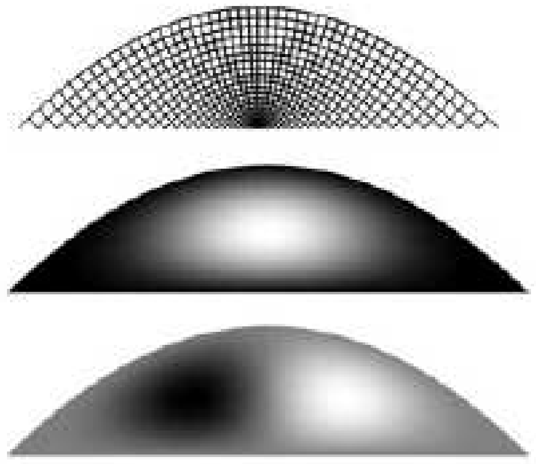

(b)


(c)

$$\Psi(u, v, \theta) = f(u)g(v)\,\mathrm{e}^{in\theta}$$

$$u^2\frac{\mathrm{d}^2 f}{\mathrm{d}u^2} + u\frac{\mathrm{d}f}{\mathrm{d}u} + (Eu^4 - Cu^2 - n^2)f = 0$$

$$v^2\frac{\mathrm{d}^2 g}{\mathrm{d}v^2} + v\frac{\mathrm{d}g}{\mathrm{d}v} + (Ev^4 + Cv^2 - n^2)g = 0$$



$$f(u) = NF(u, C, E, n) = N\,\mathrm{e}^{-\mathrm{i}\sqrt{E}u^2/2}(\mathrm{i}\sqrt{E}u^2)^{n/2}\phi\left(\frac{-\mathrm{i}C}{4\sqrt{E}} + \frac{n+1}{2}, n+1, \mathrm{i}\sqrt{E}u^2\right)$$

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Coordonnées paraboliques et fonctions hypergéométriques confluentes

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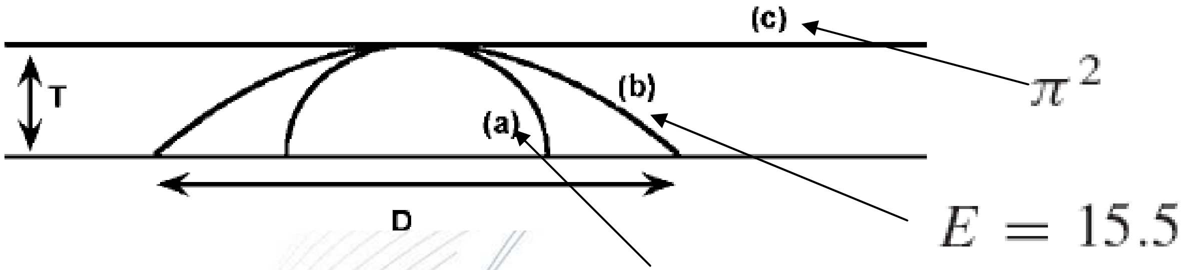
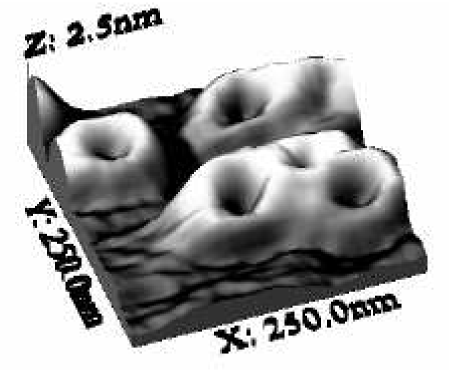
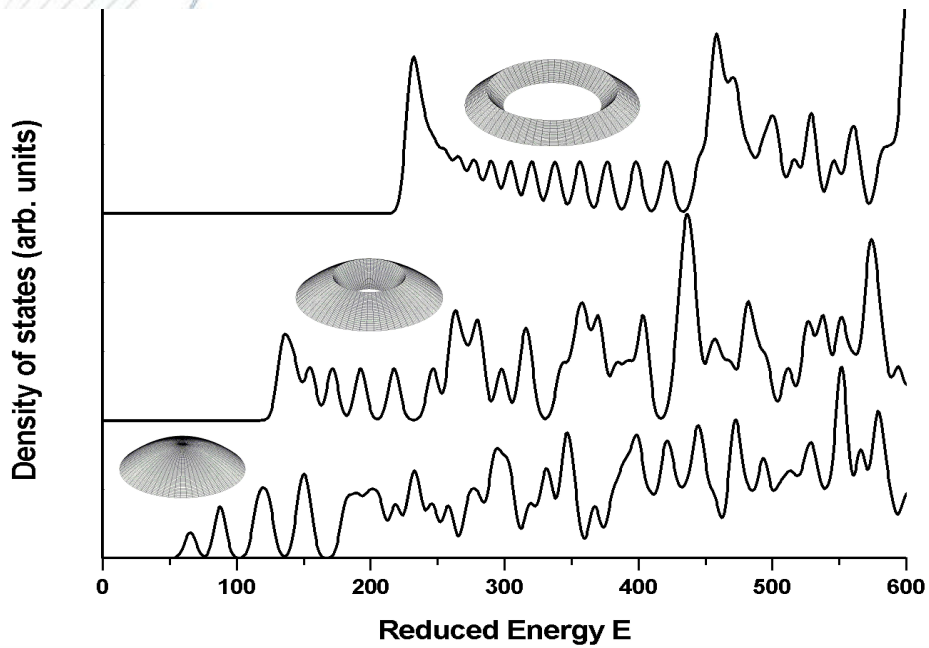


Energie de l'état fondamental (unités réduites)



Anneaux quantiques



$$f(u) = F(u, C, E, m) = \mathrm{e}^{-\mathrm{i}\sqrt{E}u^2/2}(\mathrm{i}\sqrt{E}u^2)^{m/2} \begin{pmatrix} \lambda_f \phi\left(\frac{-\mathrm{i}C}{4\sqrt{E}} + \frac{m+1}{2}, m+1, \mathrm{i}\sqrt{E}u^2\right) \\ +\mu_f \psi\left(\frac{-\mathrm{i}C}{4\sqrt{E}} + \frac{m+1}{2}, m+1, \mathrm{i}\sqrt{E}u^2\right) \end{pmatrix}$$

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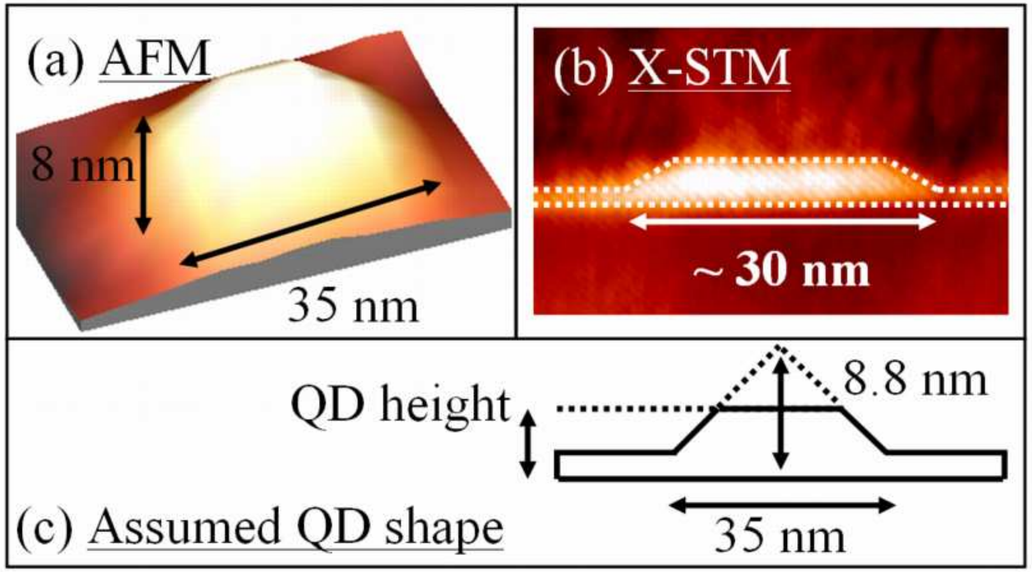
Ilots InAs/InP sur substrat (100) ou (311)



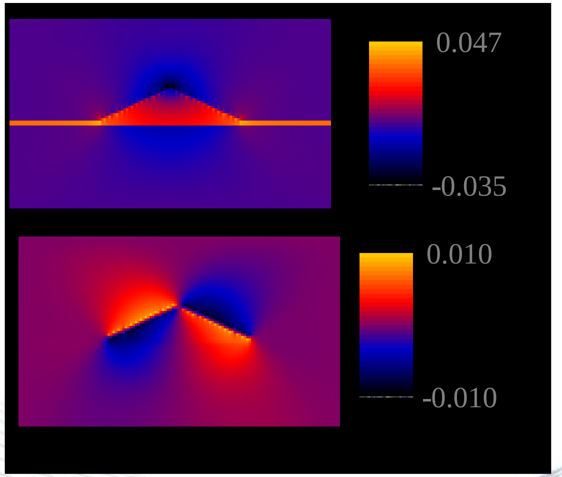
Cornet (Phys. Rev. B 2006) : simulation 3D pour InP(311) ou InP(100) (supercomputer Berlin TUB)

- ***Symétrie Axiale $C_{\infty v}$*** **pour la géométrie sur substrat *(100)***

➢ ***Les contraintes internes aux îlots sont associées au désaccord de maille entre InAs (îlot) et InP (substrat et barrière)***

ε_{zz}

ε_{yz}



- "hydrostatic" component
- "shear" component

Calculs en éléments finis
2D axial (r,z) : comsol/femlab

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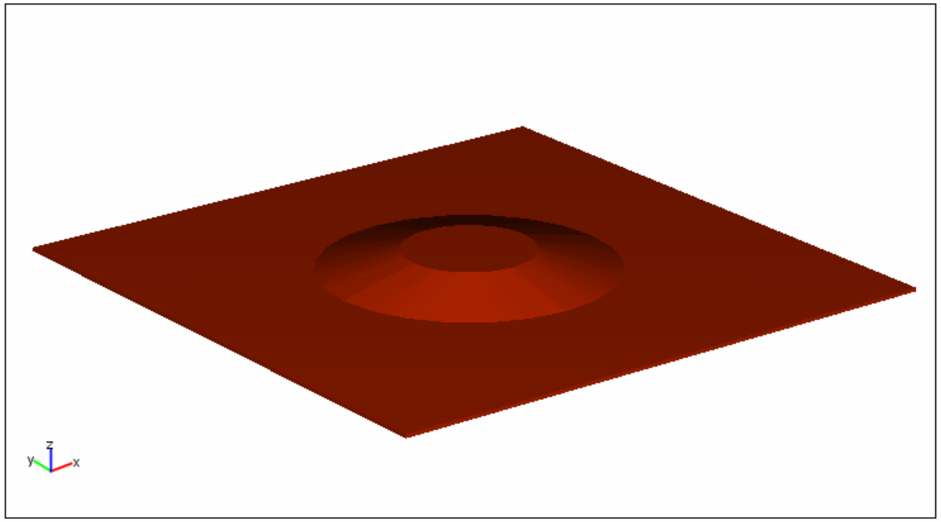
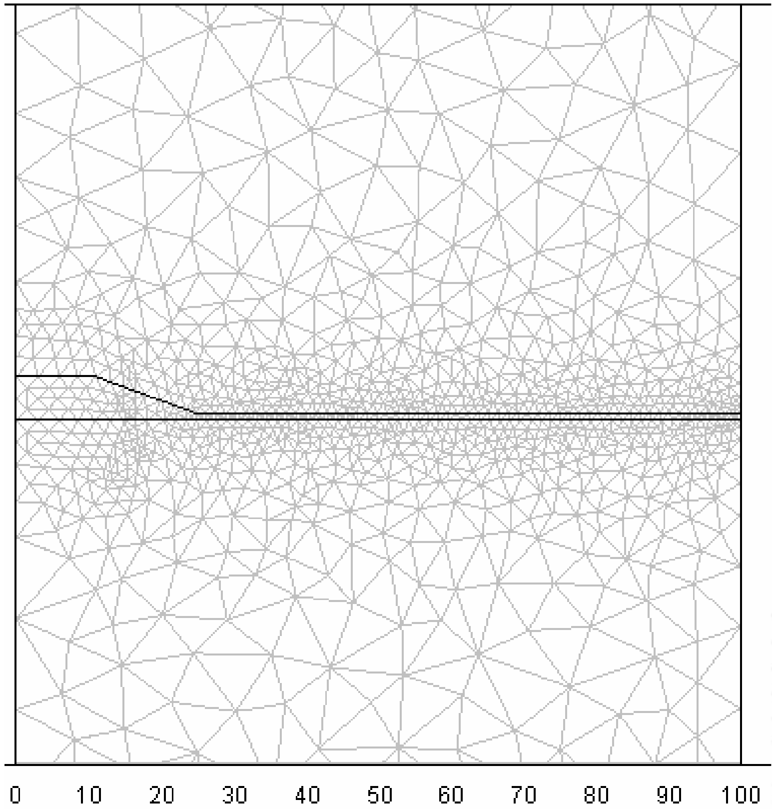




Approximation axiale en élasticité

Description en coordonnées cylindriques : r, ϕ, z $\longrightarrow \varepsilon_{rr}, \varepsilon_{\varphi\varphi}, \varepsilon_{zz}, \varepsilon_{rz}$

approximation "transverse isotrope" pour les matériaux cubiques en maille zinc-blende

$$\begin{pmatrix} C'_{11} & C'_{12} & C_{12} & 0 & 0 & 0 \\ C'_{12} & C'_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \overline{C} \end{pmatrix}$$

$$C'_{11} = \frac{C_{11}+C_{12}}{2} + \overline{C}$$

$$C'_{12} = \frac{C_{11}+C_{12}}{2} - \overline{C}$$

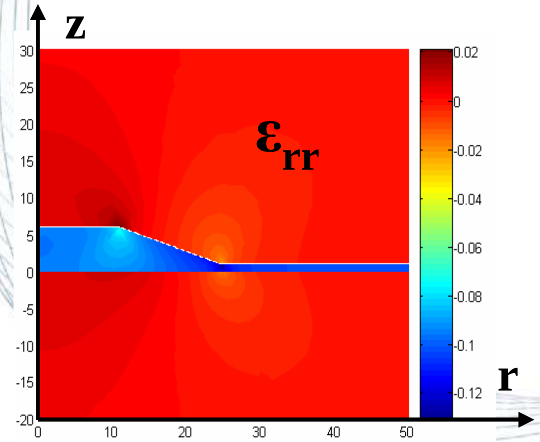
4 paramètres

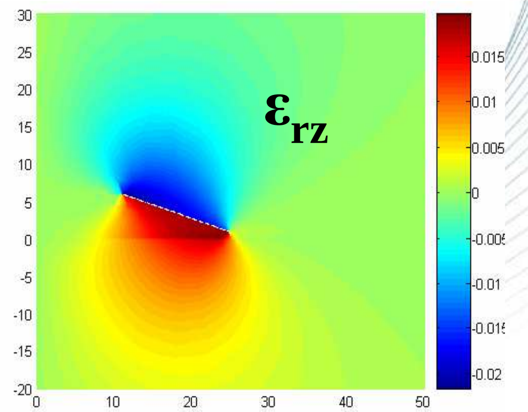
retour en coordonnées cartésiennes $\longrightarrow$

$$\varepsilon_{xx} = \cos^2(\varphi)\varepsilon_{rr} + \sin^2(\varphi)\varepsilon_{\varphi\varphi} \qquad \varepsilon_{xz} = \cos(\varphi)\varepsilon_{rz} \qquad \varepsilon_{xy} = \frac{\sin(2\varphi)}{2}\left(\varepsilon_{rr} - \varepsilon_{\varphi\varphi}\right)$$

$$\varepsilon_{yy} = \sin^2(\varphi)\varepsilon_{rr} + \cos^2(\varphi)\varepsilon_{\varphi\varphi} \qquad \varepsilon_{yz} = \sin(\varphi)\varepsilon_{rz}$$

Exemple : InAs/GaP





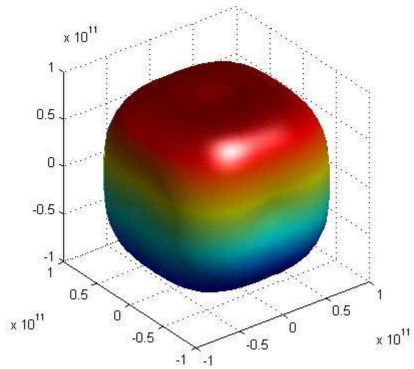
Approximation axiale en élasticité

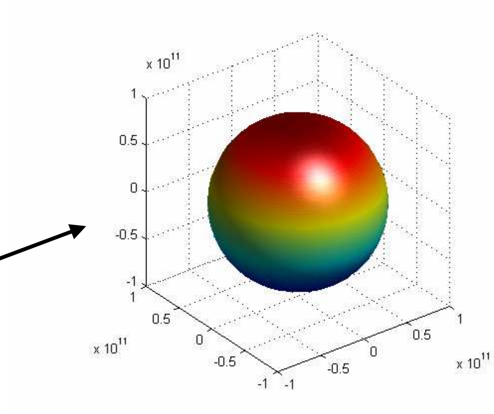
”band warping” des phonons acoustiques

test : → **vitesses du son dans InAs**

Isosurfaces des vitesses longitudinales

Zinc blende



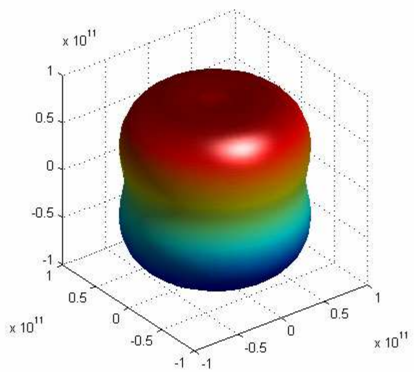


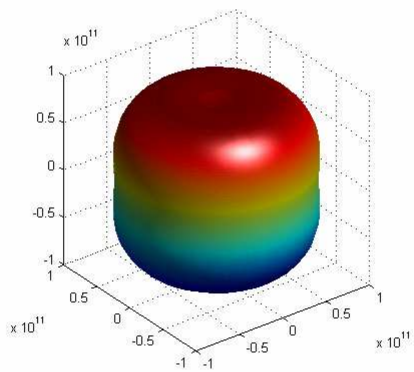
“isotrope 3D“

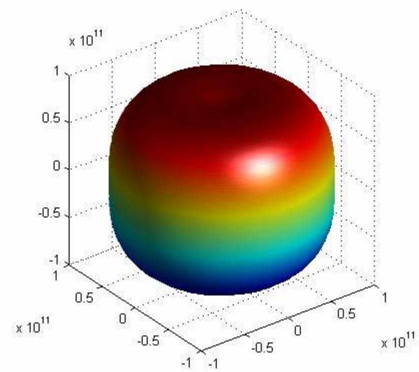
$\boldsymbol{d} = 0$

$\boldsymbol{d} = 0.5$

$\boldsymbol{d} = 1$







Approx. “transverse isotrope“

$$\overline{C} = \frac{C_{11} - C_{12}}{2} + \left(C_{44} - \frac{C_{11} - C_{12}}{2} \right) d$$

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Potentiel piezoélectrique : potentiel électrique associé aux déformations dans l'îlot et dans le substrat

1er ordre : calcul semi-analytique (axial 2D Femlab)

$$\vec{P}_1 = 2e_{14}\left[\sin(2\varphi)\varepsilon_{rz}\vec{u}_r + \cos(2\varphi)\varepsilon_{rz}\vec{u}_\varphi + \frac{\sin(2\varphi)}{2}\left(\varepsilon_{rr} - \varepsilon_{\varphi\varphi}\right)\vec{u}_z\right] \Longrightarrow V_1(r,\varphi,z) = \sin(2\varphi)\, f_1(r,z)$$

J. Even, Appl. Phys. Lett. (2007)

2ème ordre calcul semi-analytique (axial 2D Femlab)

G. Bester, Phys. Rev. Lett. (2006)

Calcul Ab initio **(abinit) des constantes piezoélectriques quadratiques :**

$$\text{InAs} \qquad B_{114} = -0.531\,\mathrm{Cm}^{-2} \quad B_{124} = -4.076\,\mathrm{Cm}^{-2} \quad B_{156} = -0.120\,\mathrm{Cm}^{-2}$$

$$\vec{\mathbf{P}}_2 = \left|\begin{array}{l} \frac{\sin(2\varphi)}{2}\left[2B_{114}\left(\varepsilon_{rr}+\varepsilon_{\varphi\varphi}\right)\varepsilon_{rz} + 2B_{124}\left(\varepsilon_{rr}+\varepsilon_{\varphi\varphi}+2\varepsilon_{zz}\right)\varepsilon_{rz} + 4B_{156}\left(\varepsilon_{rr}-\varepsilon_{\varphi\varphi}\right)\varepsilon_{rz}\right]\vec{u}_r \\ \qquad + \cos(2\varphi)\left[2B_{114}\varepsilon_{\varphi\varphi}\varepsilon_{rz} + 2B_{124}\left(\varepsilon_{rr}+\varepsilon_{zz}\right)\varepsilon_{rz}\right]\vec{u}_\varphi \\ \qquad + \sin(2\varphi)\left[B_{114}\left(\varepsilon_{rr}-\varepsilon_{\varphi\varphi}\right)\varepsilon_{zz} + B_{124}\left(\varepsilon_{rr}^2-\varepsilon_{\varphi\varphi}^2\right) + 2B_{156}\varepsilon_{rz}^2\right]\vec{u}_z \end{array}\right. \Longrightarrow V_2(r,\varphi,z) = \sin(2\varphi)\, f_2(r,z)$$

Potentiel piezoélectrique (femlab)

2 variables

<u>Strains :</u>

Solver Manager - Solve For *Axial Symmetry*

Solver Parameters : *Stationary Linear*

1 variable

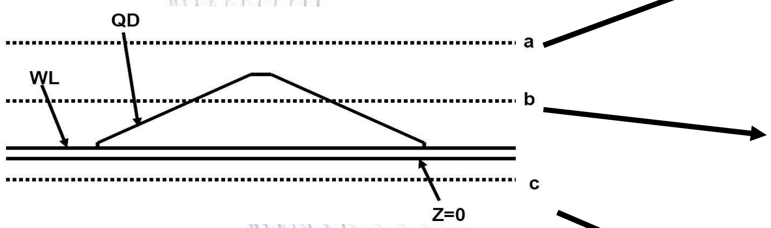
<u>Poisson equation : piezoelectric potential</u>

Solver Manager - Solve For *Coefficient form (c)*

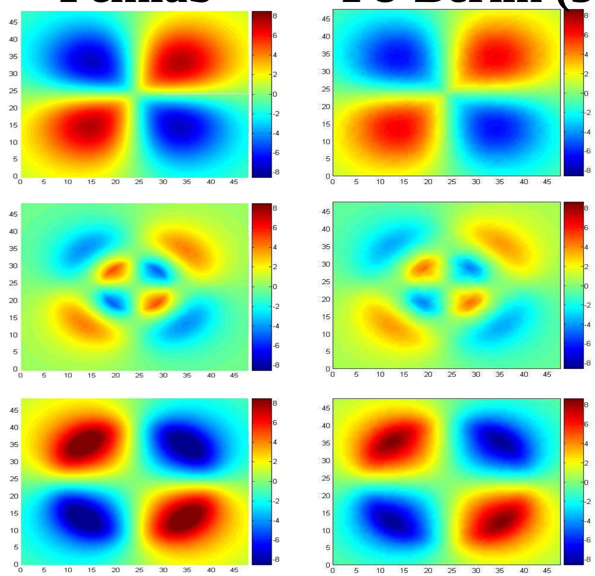
Solver Manager : Initial Value *Stored solution*

Solver Parameters : *Stationary Linear*

Example : Cone InAs/InP



Femlab **TU Berlin (3D)**



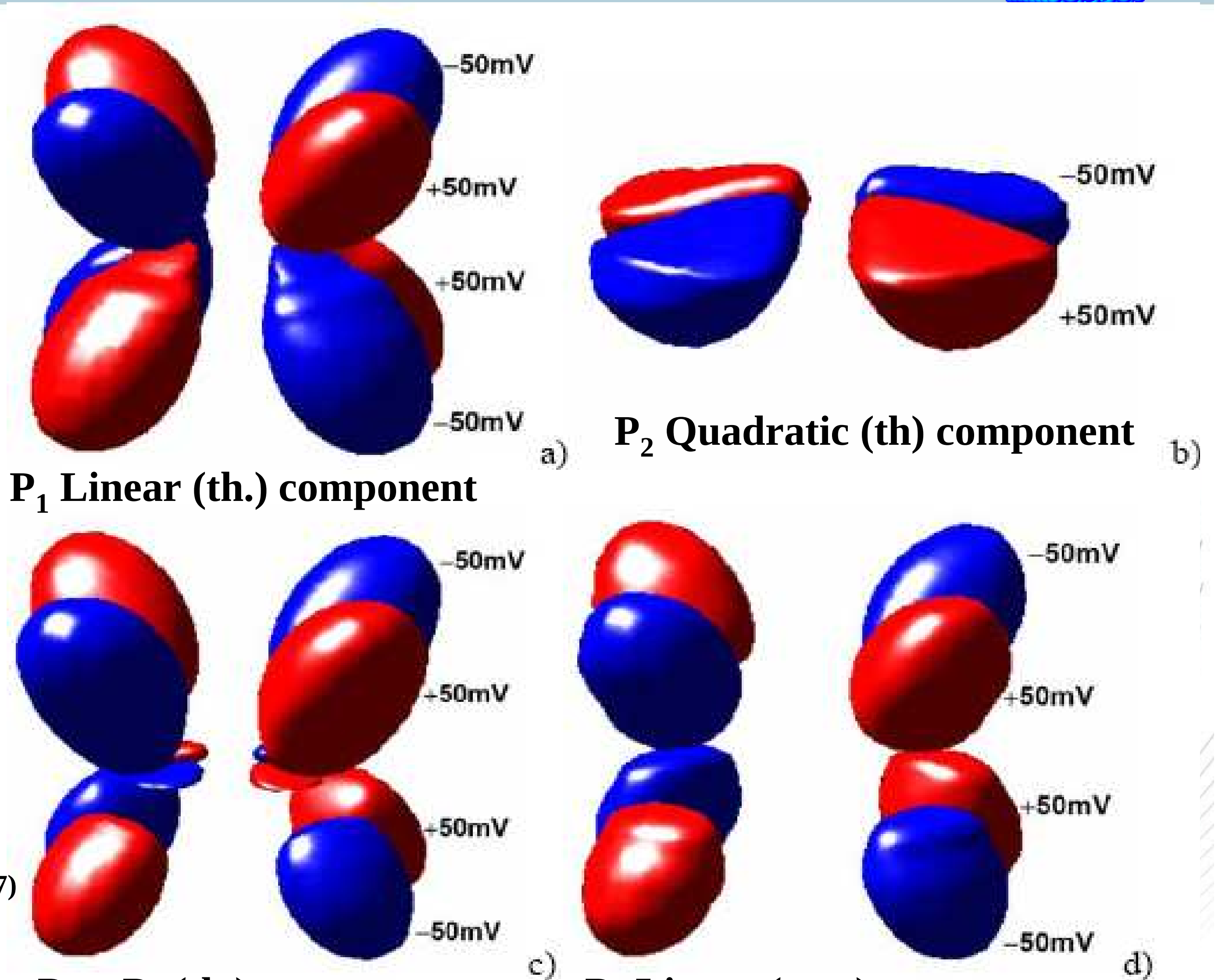
J. Even, Appl. Phys. Lett. (2007)

Potentiel piezoélectrique

potentiel piezo
Isosurfaces
(± 50 mV)
(Export de Femlab)

InAs/GaP cone

J. Even, Appl. Phys. Lett. (2007)



P_1 Linear (th.) component

P_2 Quadratic (th) component

$P_1 + P_2$ (th.) component

P_1 Linear (exp.) component

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Modèle k.p à 8 bandes

Approximation k.p 8x8 :

- **Pour un matériau massif : 8 fonctions de Bloch**
- **Pour un îlot : 8 fonctions enveloppes associées**

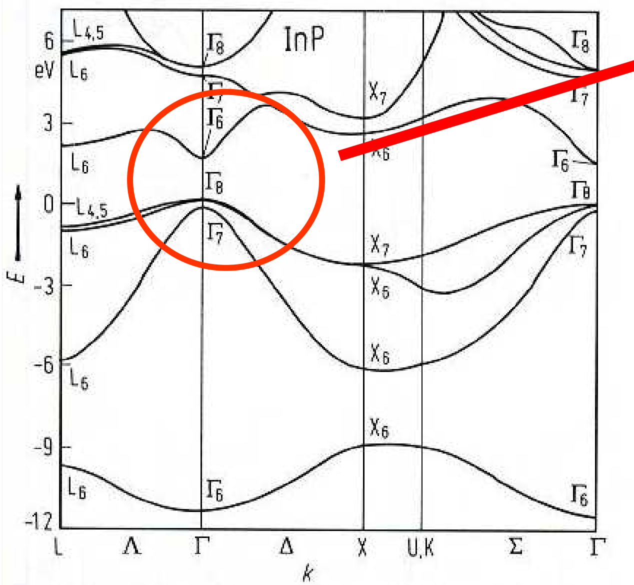

Fig. 1. InP. Band structure obtained with a non-local pseudopotential method [76C].

$$
\begin{pmatrix}
A & 0 & V^* & 0 & \sqrt{3}V & -\sqrt{2}U & -U & \sqrt{2}V^* \\
0 & A & -\sqrt{2}U & -\sqrt{3}V^* & 0 & -V & \sqrt{2}V & U \\
V & -\sqrt{2}U & -P+Q & -S^* & R & 0 & \sqrt{\frac{3}{2}}S & -\sqrt{2}Q \\
0 & -\sqrt{3}V & -S & -P-Q & 0 & R & -\sqrt{2}R & \frac{1}{\sqrt{2}}S \\
\sqrt{3}V^* & 0 & R^* & 0 & -P-Q & S^* & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R^* \\
-\sqrt{2}U & -V^* & 0 & R^* & S & -P+Q & \sqrt{2}Q & \sqrt{\frac{3}{2}}S^* \\
-U & \sqrt{2}V^* & \sqrt{\frac{3}{2}}S^* & -\sqrt{2}R^* & \frac{1}{\sqrt{2}}S & \sqrt{2}Q & -P-\Delta & 0 \\
\sqrt{2}V & U & -\sqrt{2}Q & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R & \sqrt{\frac{3}{2}}S & 0 & -P-\Delta
\end{pmatrix}
$$

Stier Phys. Rev. B 1999

Modèle k.p axial à 8 bandes

Hamiltonien sans déformations :

$$R = -\sqrt{3}\,\frac{\hbar^2}{2m_0}\left[\gamma_2\left(k_x^2 - k_y^2\right) - 2i\gamma_3 k_x k_y\right] \approx -\sqrt{3}\,\frac{\hbar^2}{2m_0}\,\bar{\gamma}\,k_-^2$$

$$k_\pm = -ie^{\pm i\varphi}\left(\frac{\partial}{\partial r} \pm \frac{i}{r}\frac{\partial}{\partial\varphi}\right)$$

Hamiltonien avec déformations :

$$\boldsymbol{R}_\varepsilon = \frac{\boldsymbol{b}\sqrt{3}}{2}\left(\boldsymbol{\varepsilon}_{rr} - \boldsymbol{\varepsilon}_{\varphi\varphi}\right)\cos(2\boldsymbol{\varphi}) - \boldsymbol{i}\frac{\boldsymbol{d}}{2}\left(\boldsymbol{\varepsilon}_{rr} - \boldsymbol{\varepsilon}_{\varphi\varphi}\right)\sin(2\boldsymbol{\varphi}) \approx \frac{\bar{\boldsymbol{b}}\sqrt{3}}{2}\left(\boldsymbol{\varepsilon}_{rr} - \boldsymbol{\varepsilon}_{\varphi\varphi}\right)\boldsymbol{e}^{-i2\boldsymbol{\varphi}}$$

Even Phys. Rev. B 2008

Diagonalisation par blocs Fz de l'Hamiltonien :

"Bon" nombre quantique : le moment angulaire total $F_z = J_z + L_z$

Developpement de la fonction d'onde : $\left|\boldsymbol{J},\boldsymbol{J}_z\right\rangle\left|\boldsymbol{L}_z = \boldsymbol{F}_z - \boldsymbol{J}_z\right\rangle$

Base des 8 fonctions de Bloch
du massif u_i (i=1…8)

8 fonctions enveloppes de (r,z)
correspondant aux RI de $C_{\infty v}$

Modèle k.p axial à 8 bandes

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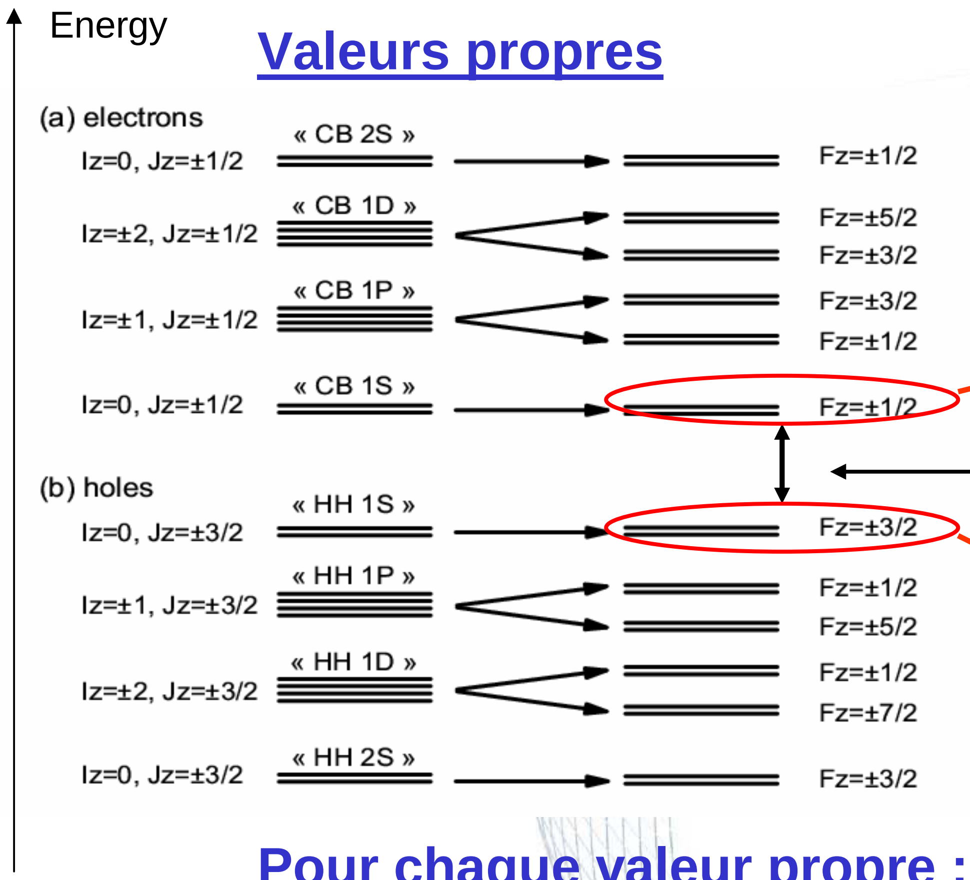
Valeurs propres



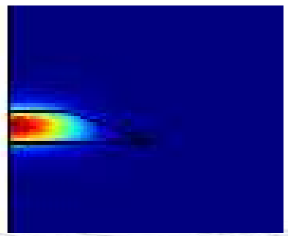
Bande de Conduction : état fondamental

Gap en énergie de l'îlot

Bande de Valence : état fondamental

Pour chaque valeur propre : 8 fonctions enveloppes

Exemple : BC état fondamental Fz= +1/2



Type S
BC (electron)
u_2 fonction enveloppe

Condition : Neumann

Modèle k.p axial à 8 bandes (femlab)

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2 variables

Strains :

Solver Manager - Solve For ***Axial Symmetry***

Solver Parameters : ***Stationary Linear***

8 variables

Hamiltonian : Ground state CB

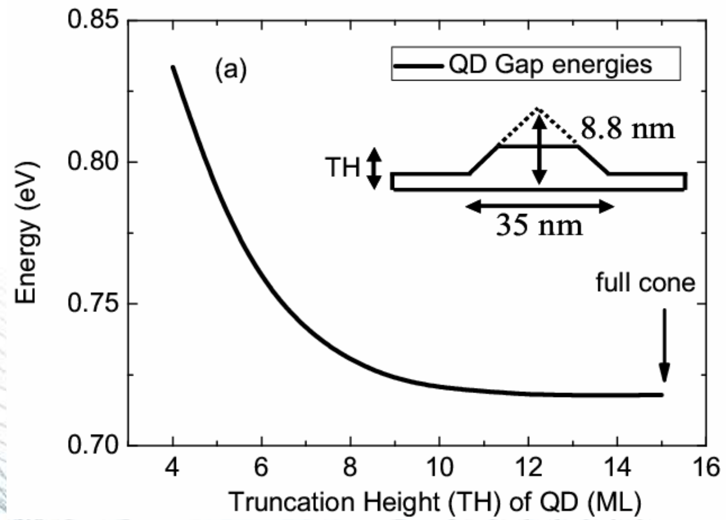
Options - Constants ***Fz = 1/2***

Solver Manager - Solve For ***Coefficient form (c)***

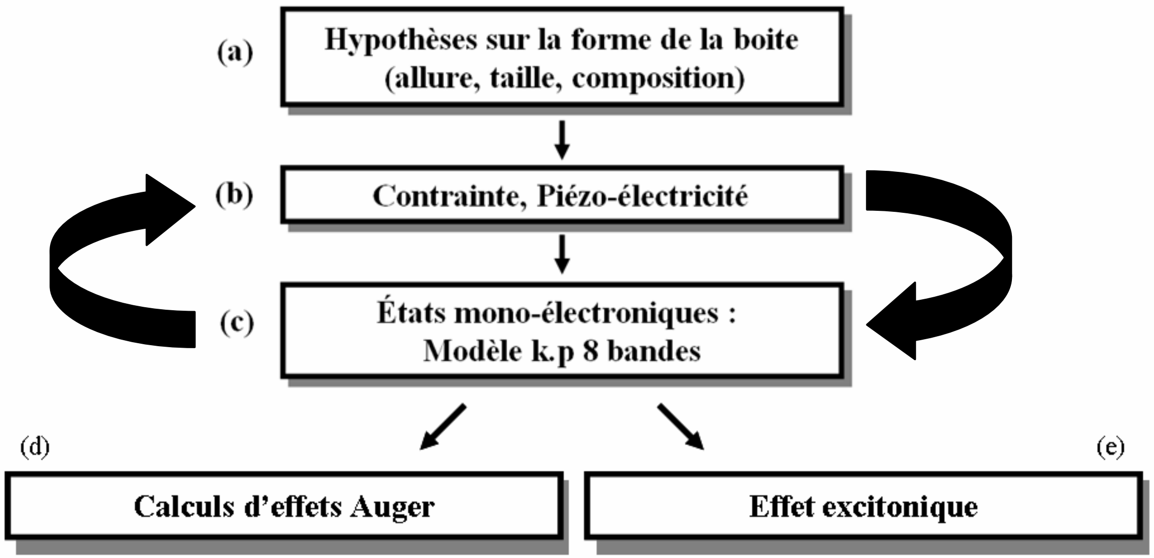
Solver Manager : Initial Value ***Stored solution***

Solver Parameters : ***Eigenvalue 0.27***

Exemple : variation du gap (InAs/InP)



Applications : un “toolbox” extensible



Application no1 :
Pertubation piezoélectrique (femlab)

Hamiltonian : Ground state CB

Options - Constants *Fz = 1/2*

Solver Manager - Solve For ***Coefficient form (c)***

Solver Manager : Initial Value ***Stored solution***

Solver Parameters : ***Eigenvalue 0.27***

Strains :

Solver Manager - Solve For ***Axial Symmetry***

Solver Parameters : ***Stationary Linear***

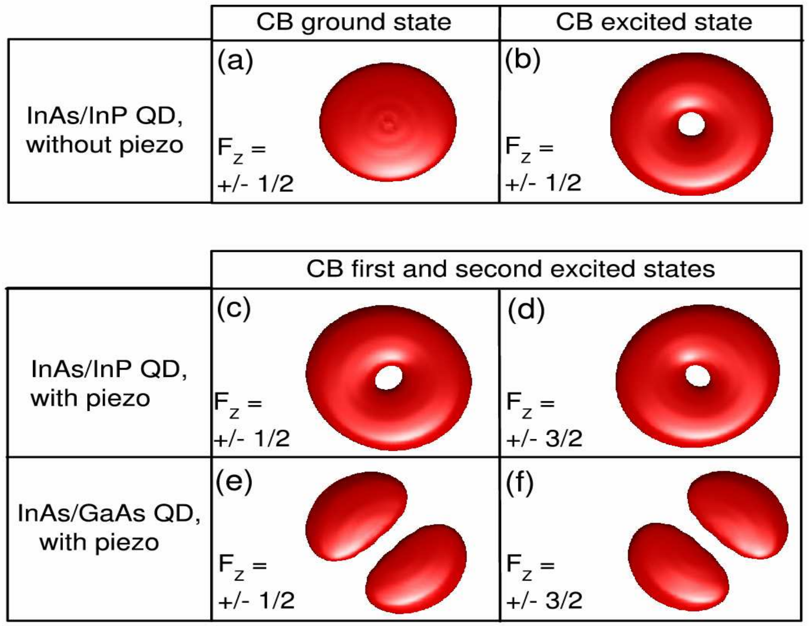
matlab

Poisson equation : piezoelectric potential

Solver Manager - Solve For ***Coefficient form (c)***

Solver Manager : Initial Value ***Stored solution***

Solver Parameters : ***Stationary Linear***



Application no2 : Pertubation excitonique (femlab)

Energie de liaison de l'exciton : interaction electron-trou

Approximation de Hartree et résolution auto-cohérente de l'équation de Poisson *(O. Stier Phys. Rev. B59 (1999))*

$$[H+V_h]\Psi_e=\tilde{E}_e\Psi_e \longleftarrow e|\Psi_h|^2=\epsilon_0\nabla(\epsilon_s\nabla V_h)$$

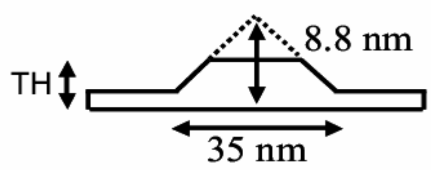
CB Ground state — **VB Hartree potential**

$$-e|\Psi_e|^2=\epsilon_0\nabla(\epsilon_s\nabla V_e) \longrightarrow [H+V_e]\Psi_h=\tilde{E}_h\Psi_h$$

CB Hartree potential — **VB Ground state**

$$\Rightarrow E_X=(E_e-E_h)-(\tilde{E}_e-\tilde{E}_h)-(\langle\Psi_h|V_e|\Psi_h\rangle-\langle\Psi_e|V_h|\Psi_e\rangle)/2$$

Exemple de calcul autocohérent dans Femlab : InAs/InP cone tronqué (TH=9ML)



sans confinement dielectrique ($\varepsilon_{InAs}=\varepsilon_{InP}$) :

E_X= 14 meV

avec confinement dielectrique ($\varepsilon_{InAs}\neq\varepsilon_{InP}$) :

E_X= 17 meV

Application no2 :
Pertubation excitonique (femlab)

FOTON

Strains :

Solver Manager - Solve For *Axial Symmetry*

Solver Parameters : *Stationary Linear*

Hamiltonian : CB Ground state

Options - Constants *Fz = 1/2*

Solver Manager - Solve For *Coefficient form (c)*

Solver Manager : Initial Value *Stored solution*

Solver Parameters : *Eigenvalue 0.27*

Poisson equation : CB Hartree potential Ve

Solver Manager - Solve For *Coefficient form (c3)*

Solver Manager : Initial Value *Stored solution*

Solver Parameters : *Stationary Linear*

Hamiltonian : VB Ground state

Options - Constants *Fz = 3/2*

Solver Manager - Solve For *Coefficient form (c)*

Solver Manager : Initial Value *Stored solution*

Solver Parameters : *Eigenvalue - 0.45*

Poisson equation : VB Hartree potential Vh

Solver Manager - Solve For *Coefficient form (c4)*

Solver Manager : Initial Value *Stored solution*

Solver Parameters : *Stationary Linear*

Matlab (+ Femlab) : 12 variables

Convergence (self-consistency): export

Matlab Integration :

$$\langle \Psi_h | V_e | \Psi_h \rangle$$

Matlab Integration :

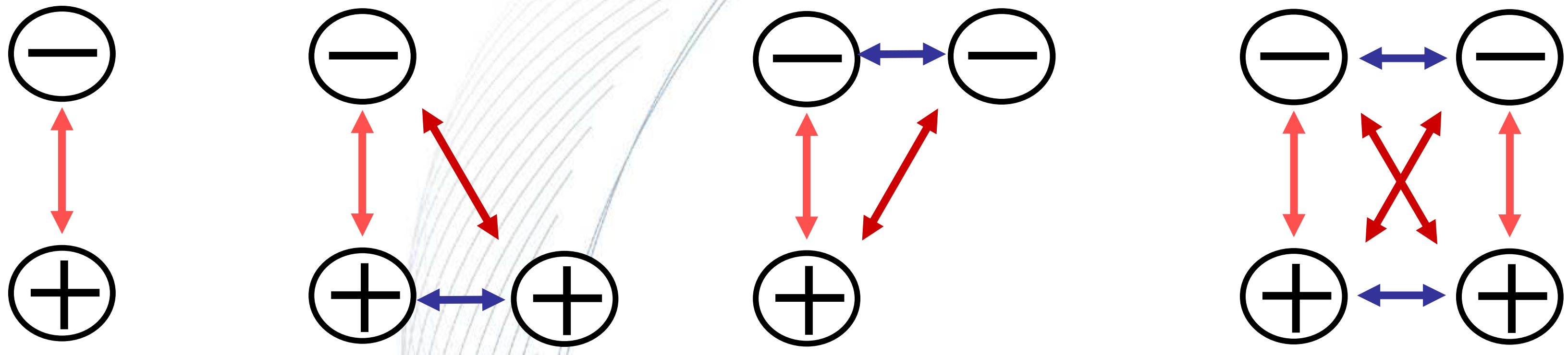
$$\langle \Psi_e | V_h | \Psi_e \rangle$$

Exciton energy :

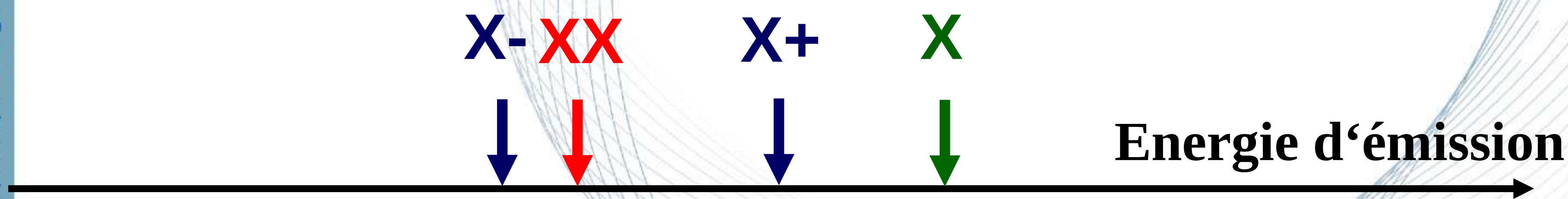
Ex=Ee'-Eh'+<psie|Vh|psie>/2 - <psih|Ve|psih>/2

Application no3 :
Effets à n-corps multiexcitoniques

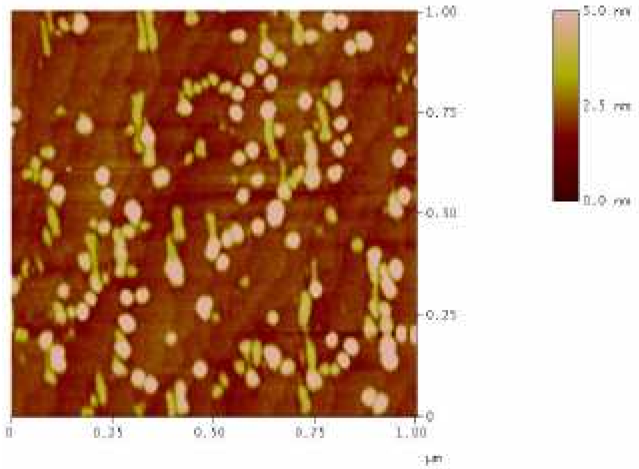
Exciton	Trion Positif	Trion Négatif	Biexciton
X	X+	X-	XX



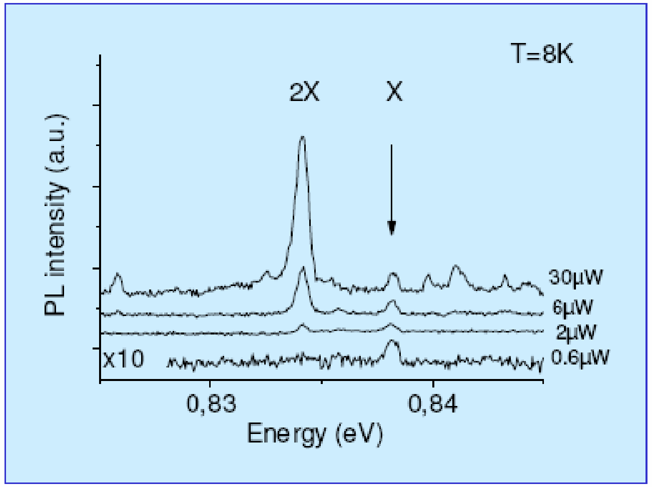
$E_{bx} = 16.0$ meV	$E_{bx+} = 0.5$ meV	$E_{bx-} = 4.0$ meV	$E_{bxx} = 3.6$ meV

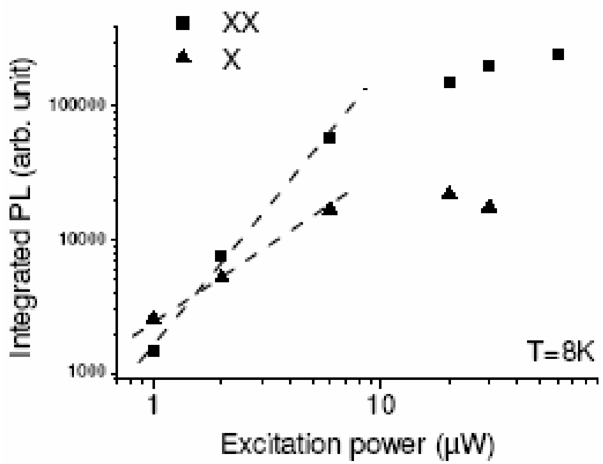


Application no3 :
Effets à n-corps multiexcitoniques



Petits îlots
Densité faible
Emission à 1.55µm
(N. Chauvin 2006)

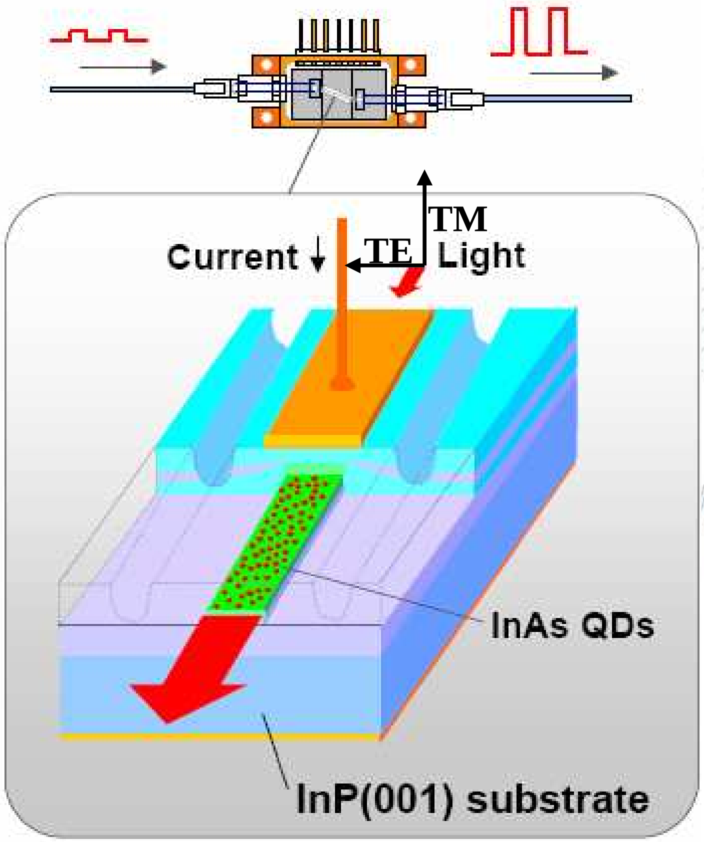




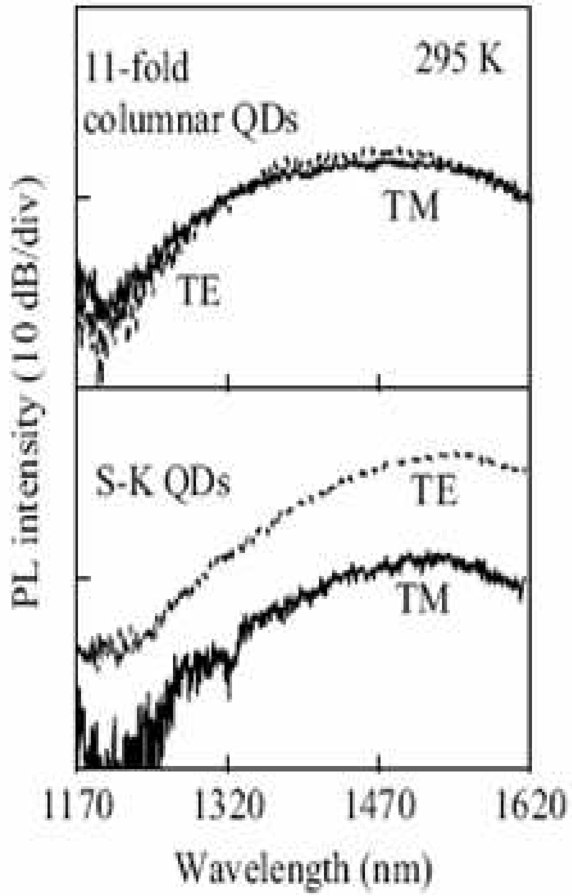
Energie de liaison du biexciton ~5meV !!

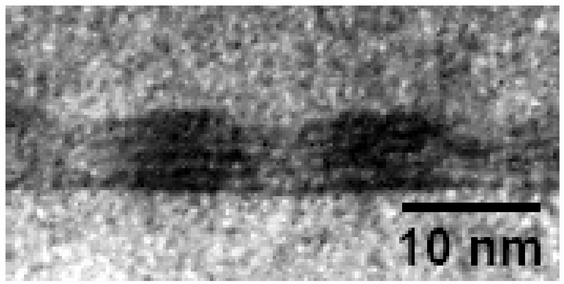
FOTON

Application no4 :
Insensibilité à la polarisation



Kawagushi (Fujitsu, 2006)

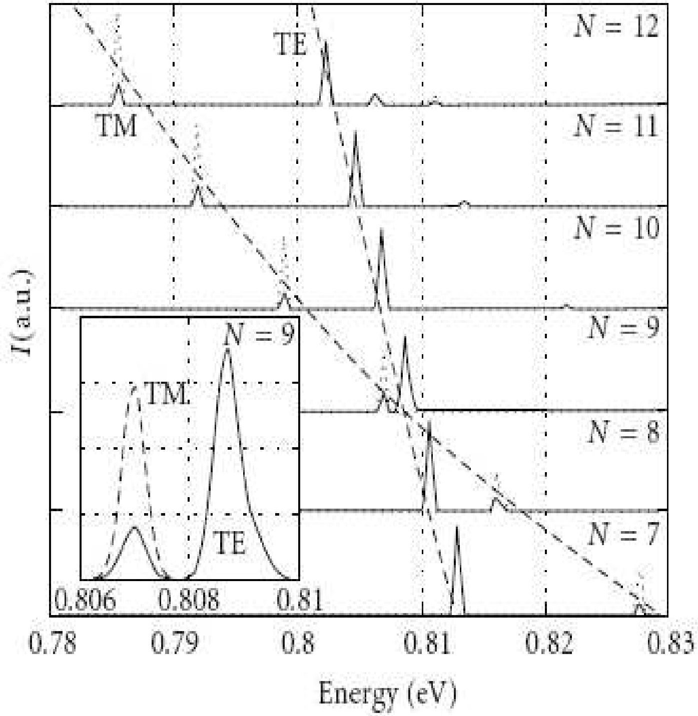


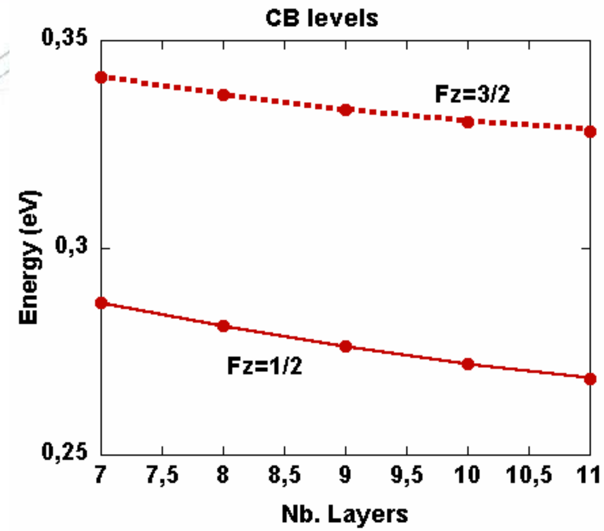


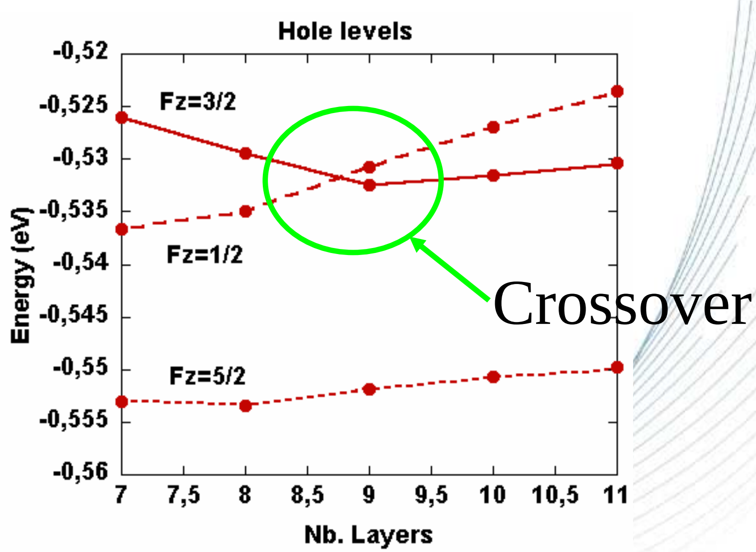
Amplificateurs optiques

Institut National des Sciences Appliquées
Ecole publique d'ingénieurs

Application no4 :
Insensibilité à la polarisation

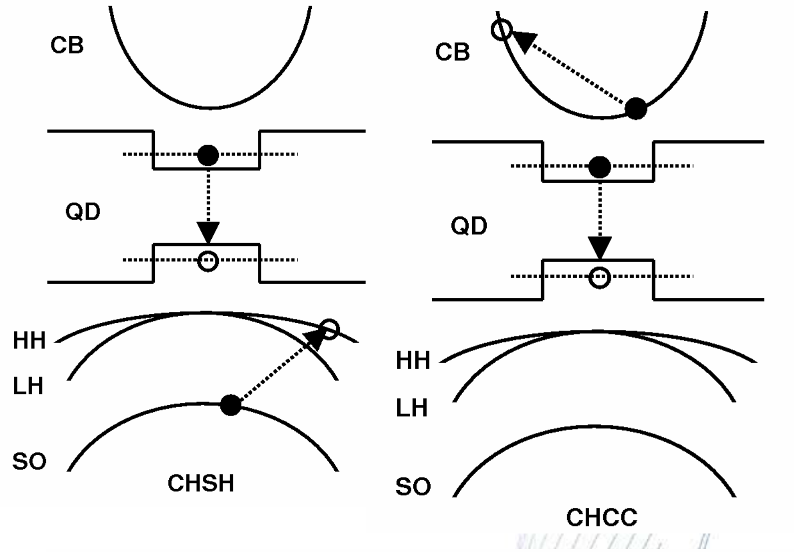


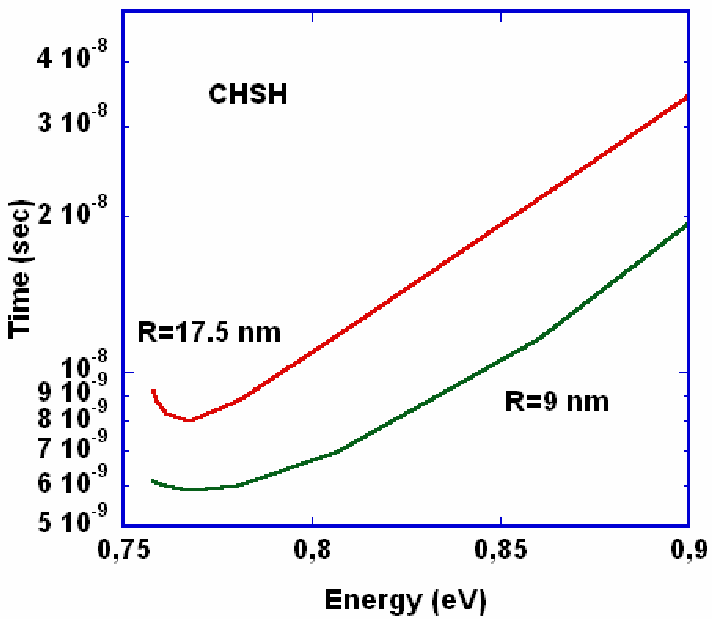


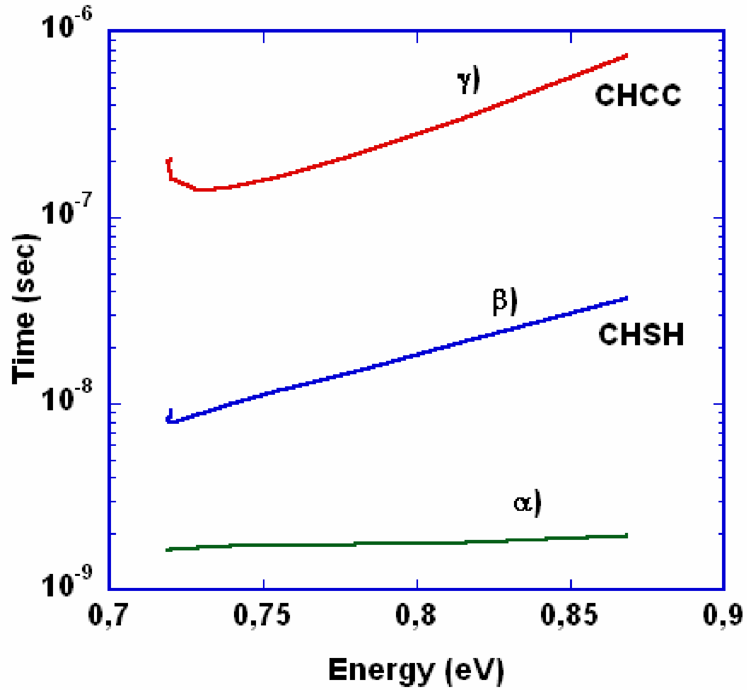


Insensibilité à la polarisation d'ilots columnaires

Application no5 :
Effet Auger dans les lasers à îlots







Conclusion :

-Il existe d’autres applications (en dehors des telecoms)
-Il existe d’autres types de nanostructures
-Il existe d’autres classes de matériaux (wurtzite …)
-Il existe d’autres méthodes de calcul (ab initio, liaisons fortes …)