

# ***ETUDES EXPÉRIMENTALES DE L'EFFET D'UNE POLARISATION ÉLECTRIQUE À L'ÉCHELLE ATOMIQUE***

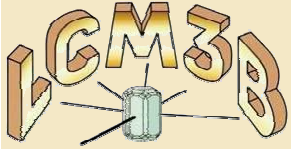
***N.K. Hansen***

*Main collaborators:*

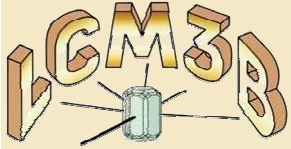
*Régis Guillot, Pierre Fertey & Paul Allé*

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et Modélisation des Matériaux Minéraux et Biologiques*

**Université Henri Poincaré - Nancy I**



1. Champs électriques et Cristaux
2. Techniques Experimentales
3. Effet Piézoélectrique Inverse
4. Effets Structuraux Induits :  $\alpha$ -Quartz et isotypes



## Effects of an electric field on crystals

### ■ *Microscopic Level*

- *Migration*
- *Domain Structure*
- *Dynamics of Domain Walls*

**Microstructure**

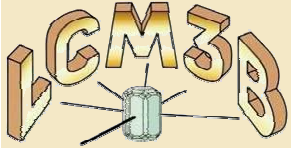
« *Imaging* »  
(topography)

### ■ *Atomic Level*

- *Atomic Displacements*
- *Charge Transfer*
- *Bond Polarisation*

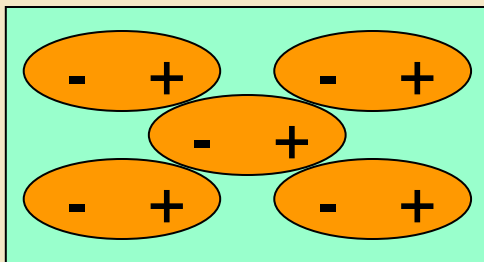
**Polarisation**

*Diffraction*



# Polarisation and Polarisation dependent properties

Linear Properties:



1.) Pyro-electric constants  $\frac{d\bar{P}}{dT}$

2.) Dielectric constants  $\frac{d\bar{P}}{d\bar{E}}$

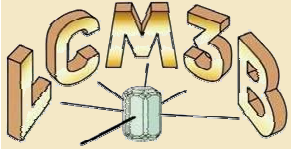
3.) Piezo-electric constants  $\frac{d\bar{P}}{d\underline{\tau}}$

( $\tau$  = stress)

3a.) Converse Piezo-electric effect

$$\frac{d\underline{\underline{\varepsilon}}}{d\bar{E}} = \frac{d\bar{P}}{d\underline{\underline{\tau}}} \quad (\underline{\underline{\varepsilon}} = \text{strain})$$

NB: 3a) Under an electric field as 2.)  
but only Bragg angles must be measured



## *Relation avec les grandeurs mesurables par diffraction*

*Changements des angles de Bragg  $\Delta\theta_B$*

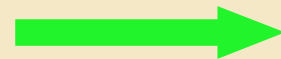


*Coefficients du tenseur piézoélectrique*

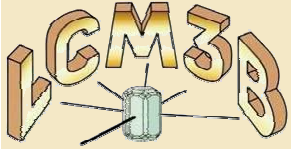
*Changements des intensités de Bragg  $\Delta I_B / I_B$*



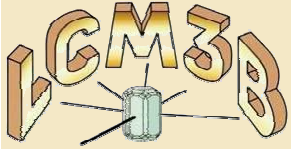
*Modification de la structure atomique*



*Polarisation induite*

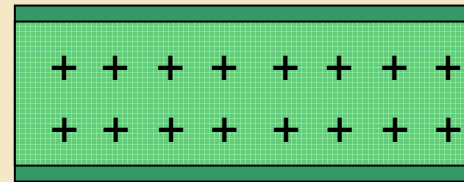


# *Des problèmes fondamentaux*

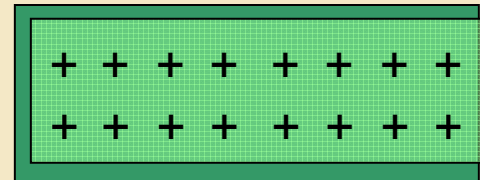


# Effect of an Electric Polarisation of a Crystal

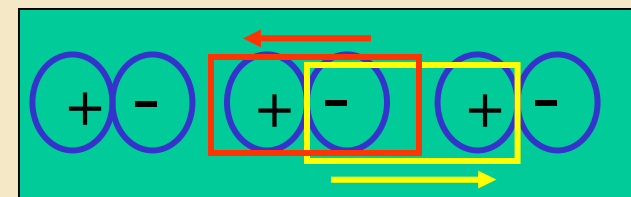
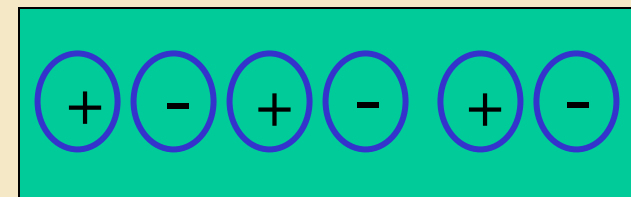
Pb 1: displacement of a diffuse density

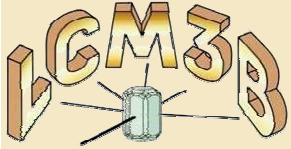


No significant change of the electron density in the bulk



Pb 2: How to choose a unit cell ( yellow or red or ?) such that its dipolemoment is representative of the crystal polarisation





## *Problems with theory*

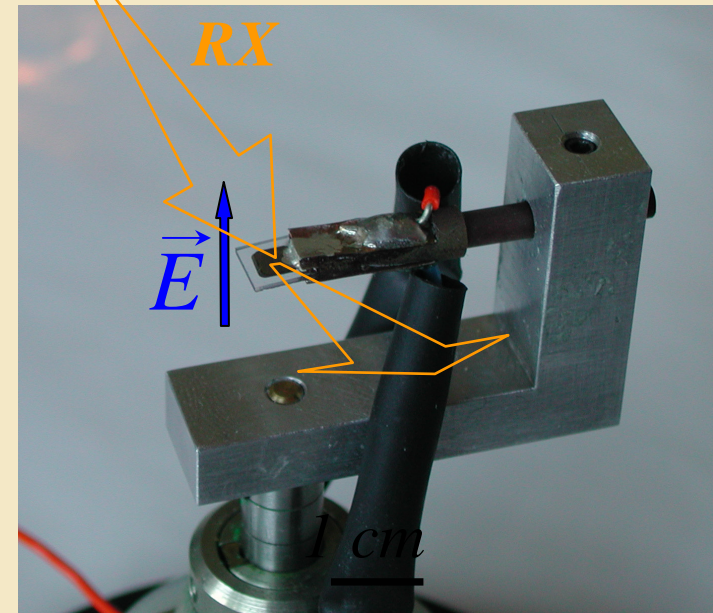
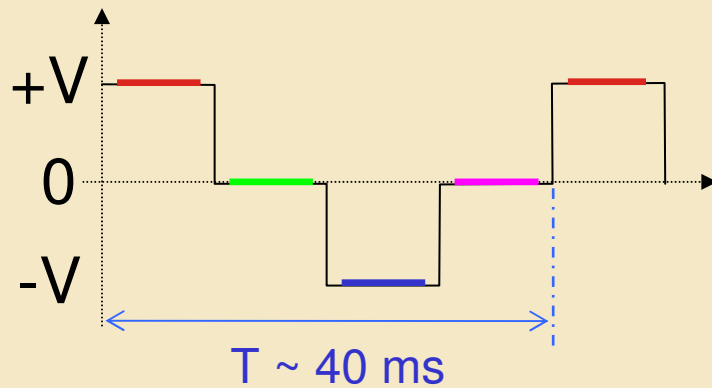
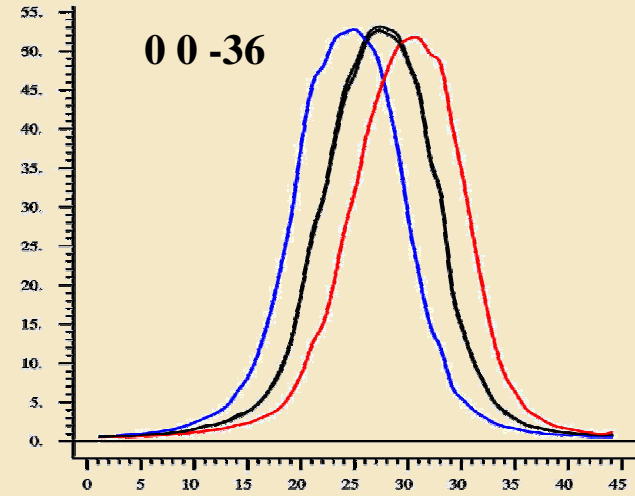
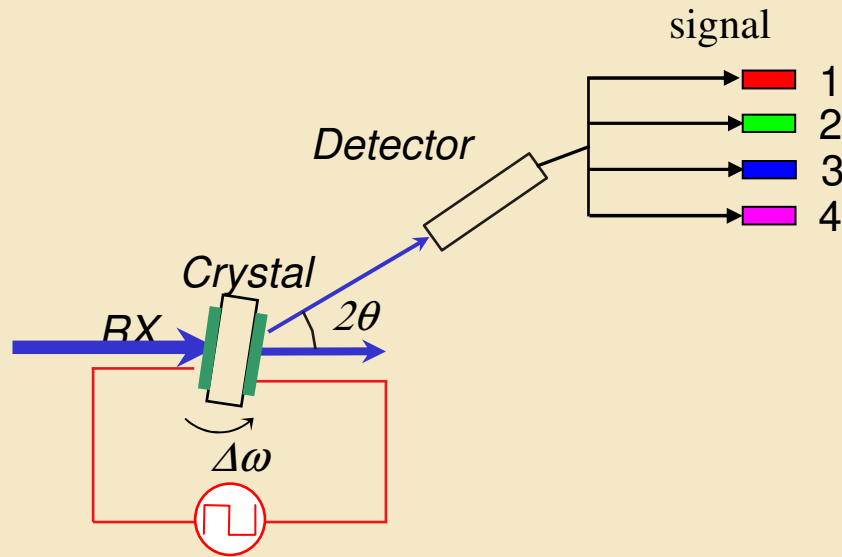
Applying a uniform electric field makes the Hamiltonian in band structure calculations non-periodic

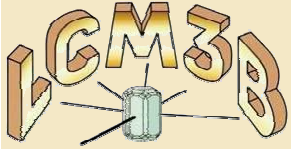
The problem of defining the polarisation of a 'infinite' crystal

Approaches are being developed at present but they use concepts not easily applied to experimental data



# Experimental Technique





# *Experimental Technique*

## Technical Specifications

Strong Fields  $\sim 30$  kV/cm

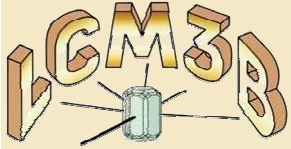
Duration of Steps  $1 \text{ ms} < T_s < 1 \text{ s}$

The parameters for each step can be regulated individually

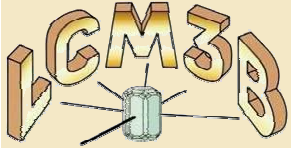
## Speed of Data Collection (Synchrotron, point detector)

1 Set of Profiles ( $10^6 - 10^7$  cts)  $\sim 15$  min.

$\Rightarrow \sim 60$  Reflections per Week of Beamtime  
(each Reflection Remeasured  $\sim 4$  times)

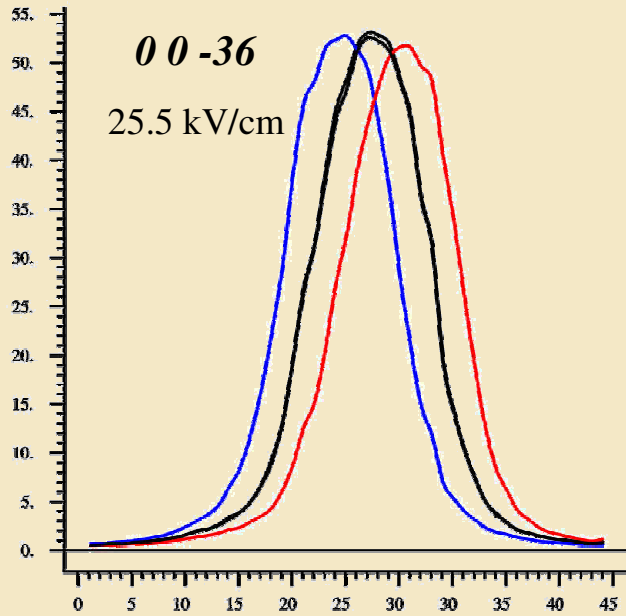


# *Résultats Expérimentaux*

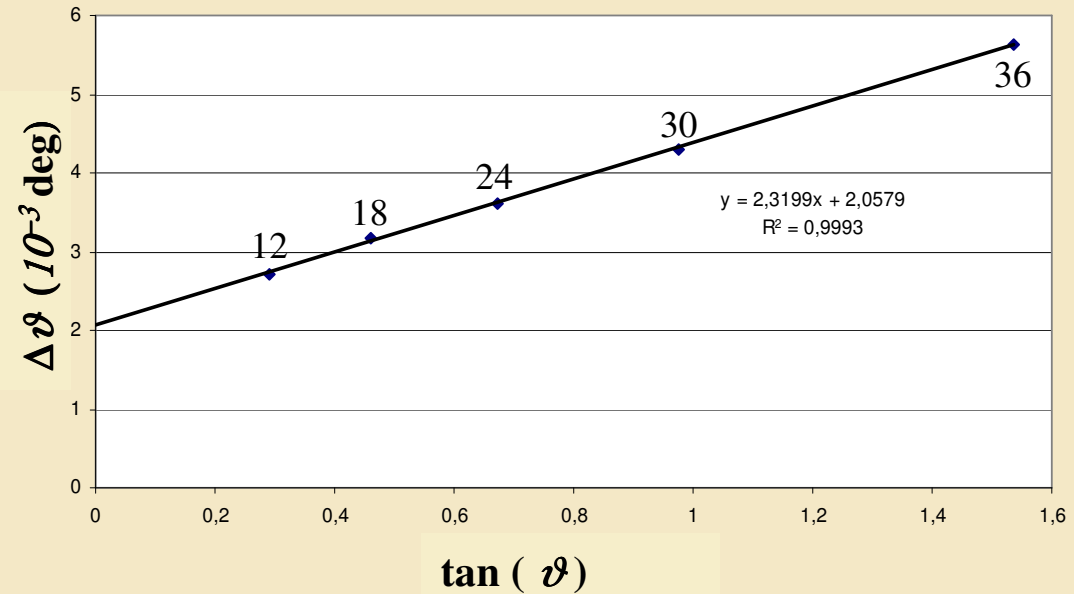


# LiNbO<sub>3</sub> Diffraction Analysis of the Piezo-Electric Effect

00-6l à 19,2 keV a l'ESRF sur LiNbO3



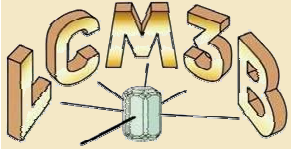
Steps  $\Delta\omega = 0.001$  deg



Piezo-electric constant  $d_{33} = 14$  pC/N

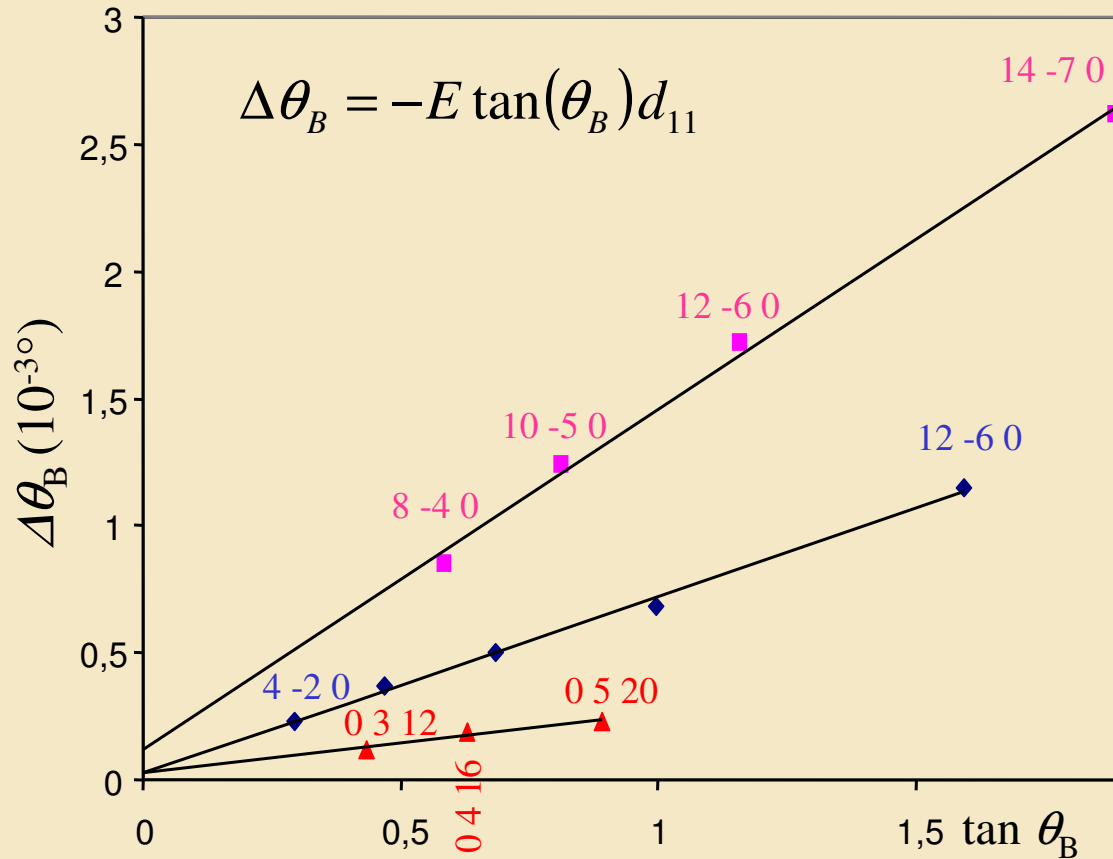
Landolt & Börnstein 8 - 18 pC/N

(Measurements at D2AM of the French CRG at ESRF)



# Bragg angle variations

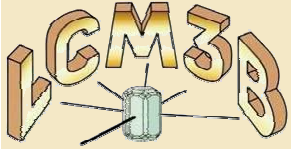
- Linear with E
- Linear with  $\tan(\theta_B)$  for harmonics of a given reflection



$d_{11}(\text{GaPO}_4) = 4,1(2) \text{ pC.N}^{-1}$   
*(literature : 4,5 pC.N<sup>-1</sup>)*

$d_{11}(\text{SiO}_2) = 2,1(1) \text{ pC.N}^{-1}$   
*(literature : 2,31 pC.N<sup>-1</sup>)*

$d_{14}(\text{GaPO}_4) = 1,4 (2) \text{ pC.N}^{-1}$   
*(literature : 1,9 pC.N<sup>-1</sup>)*



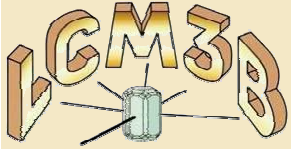
## Reproducibility

### *Comment :*

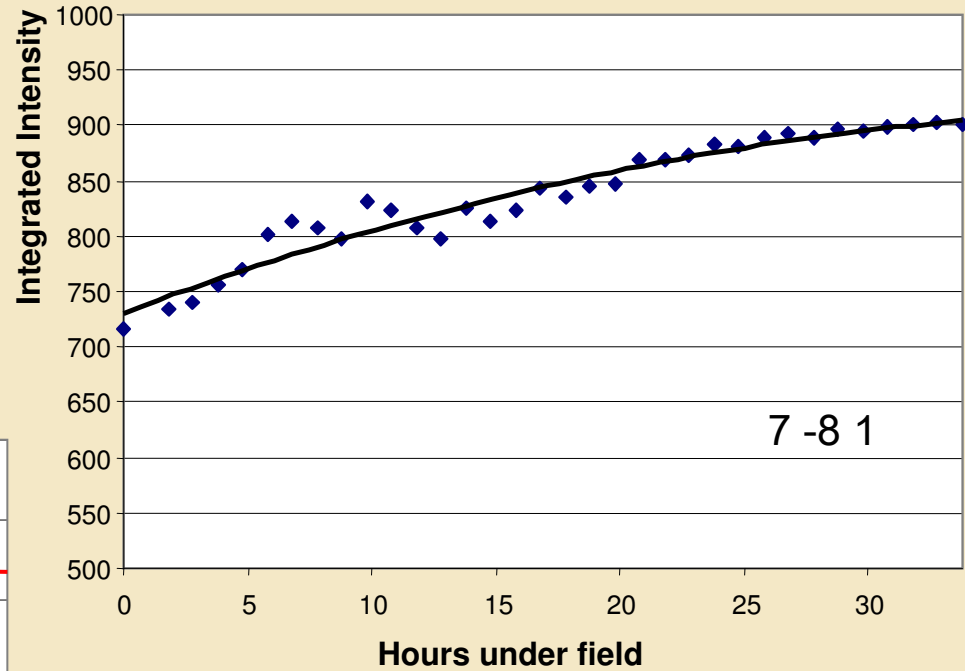
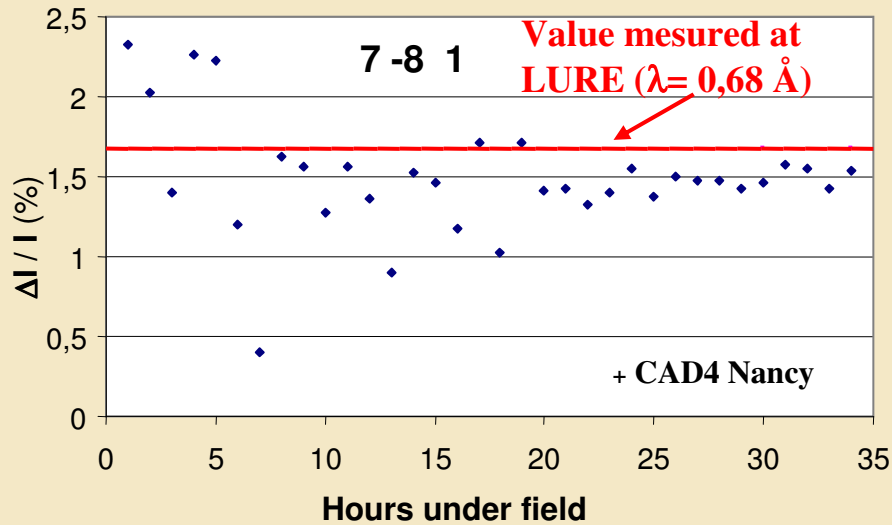
We have always found that the observed shifts in the Bragg angles are very close to what is expected from the known piezo electric constants

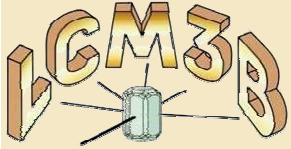
From this we conclude that the electric field inside the sample

- has the strength we expect
- is homogeneous inside the diffracting volume



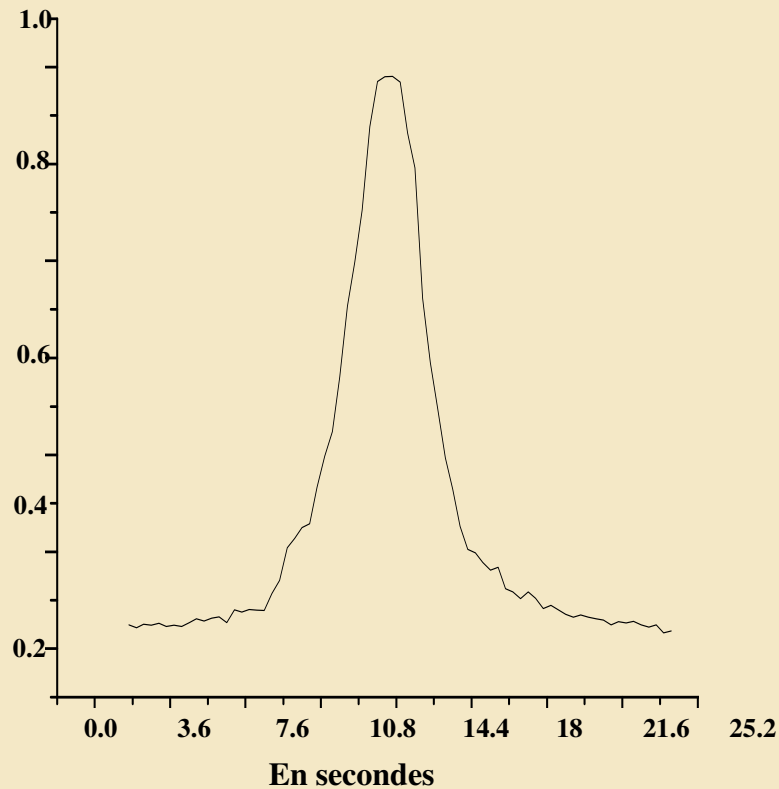
# Transient behaviour of $\alpha$ -quartz (?)



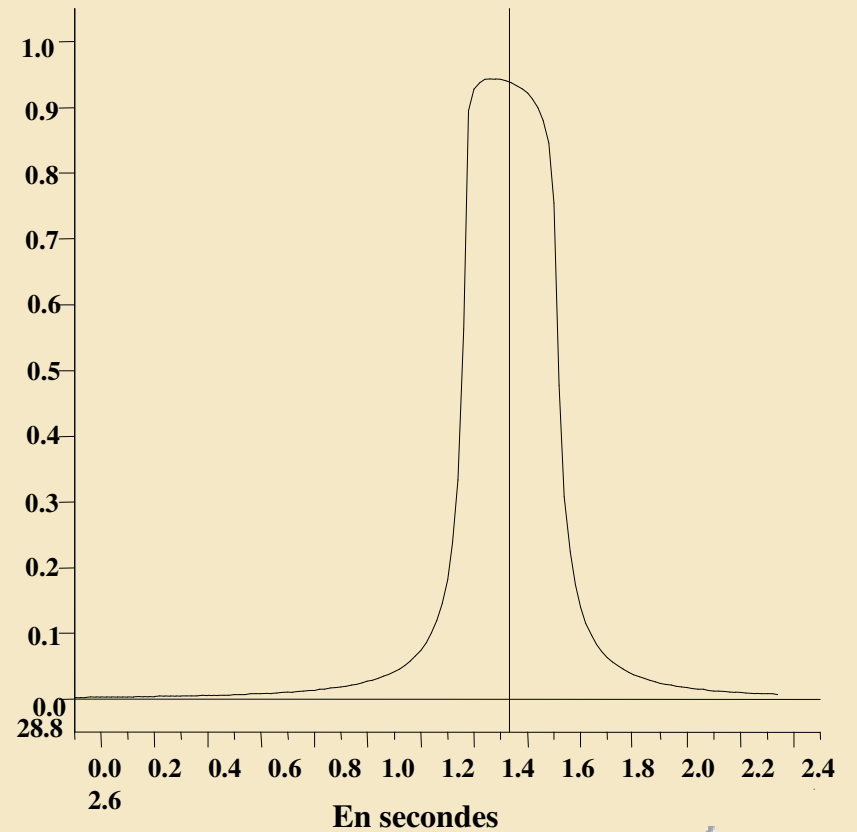


## Pour la raie (4 -2 0) du quartz

Profil mesuré à haute résolution angulaire  
(diffractomètre de B. Capelle à LURE).  
La largeur à mi-hauteur = 3.99 sec.



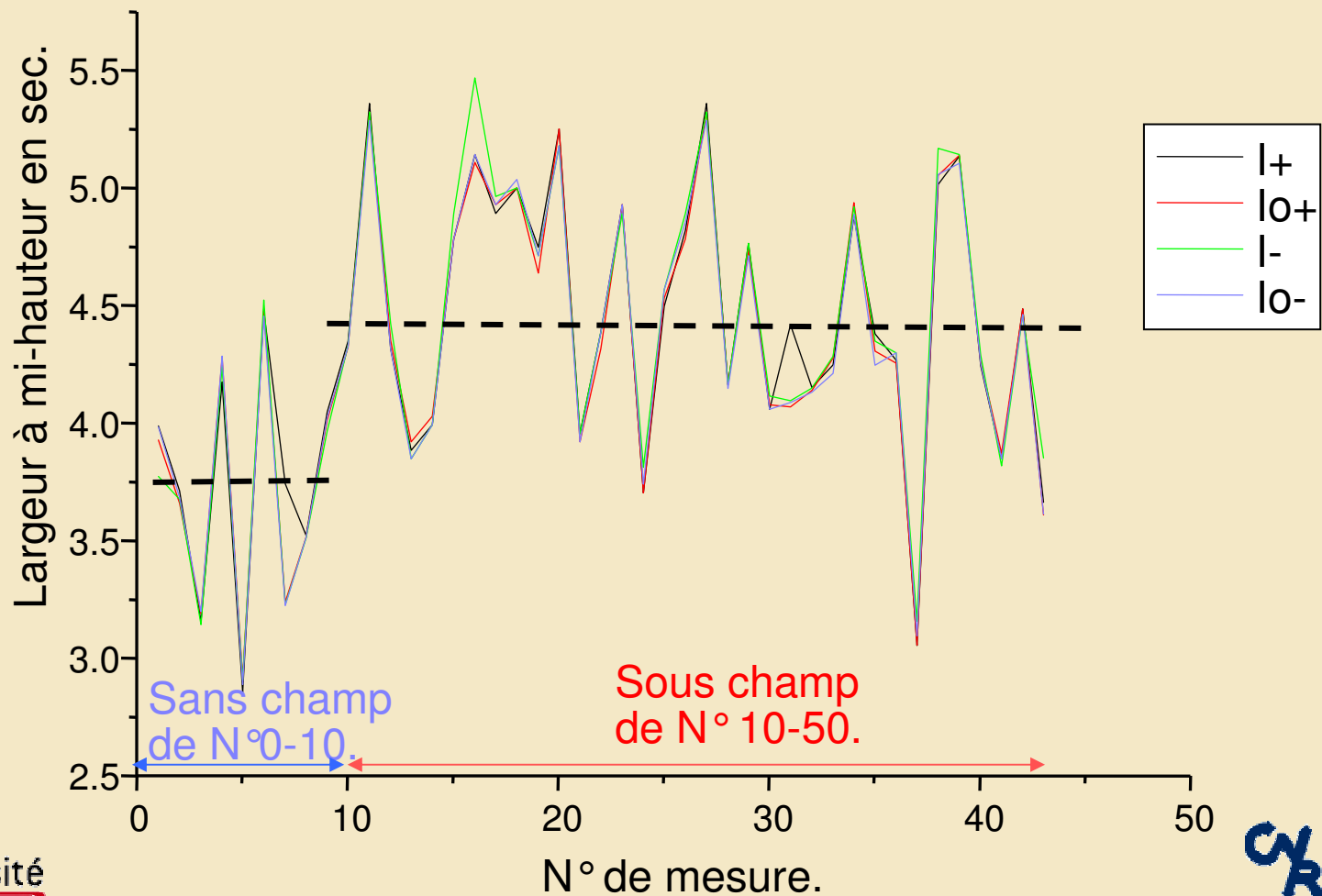
Profil simulé pour un cristal parfait  
La largeur à mi-hauteur = 0.5 sec.



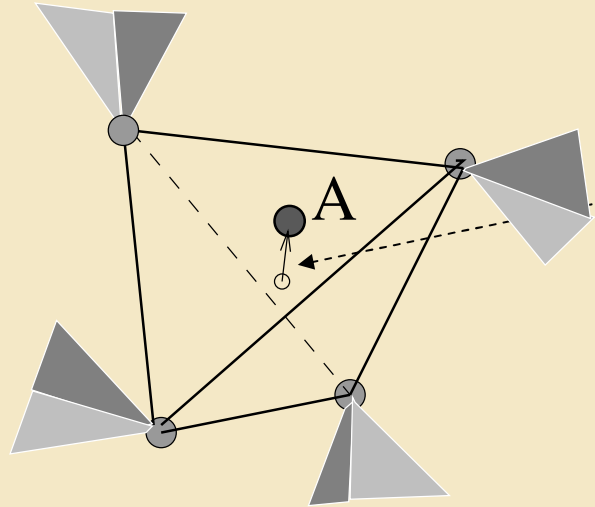


# Modification du profil

Evolution de la largeur à mi-hauteur de la raie (4-20) du quartz

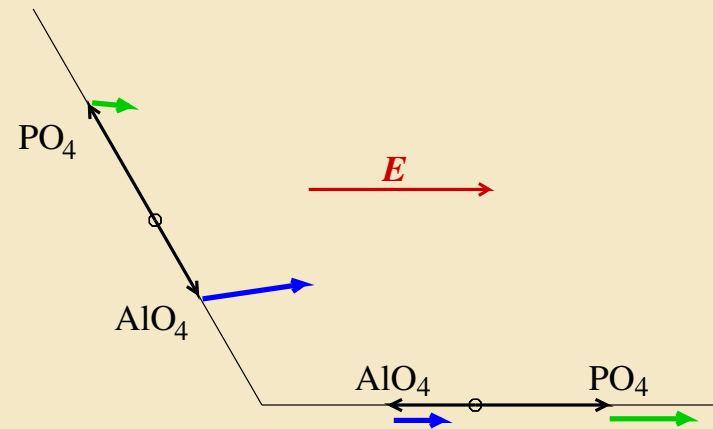


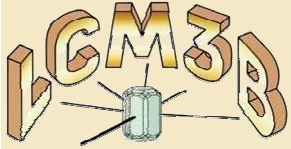
# Effet du champ électrique sur la déformation des tétraèdres $AO_4$



Vecteur de déformation  
 = vecteur du barycentre des O  
 à l'atome A ;  
 peut être assimilé à un moment  
 dipolaire local

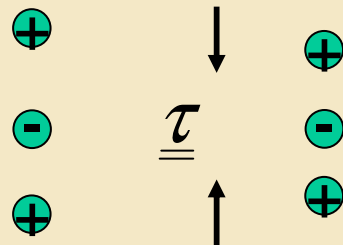
$AlPO_4$  : en noir les vecteurs de déformation hors champ.  
 En couleur les modifications pour un champ de 30 kV/cm (x10)





## *Comparaison des conditions extrêmes contrainte mécanique ~ champ électrique*

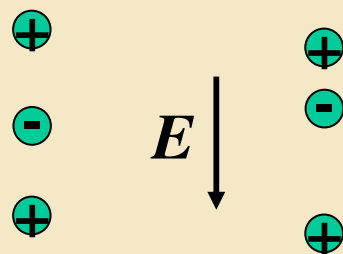
Contraintes mécaniques



~ constantes d'élasticité

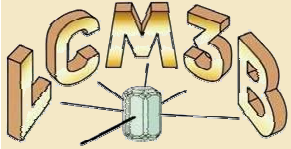
~ dispersion des phonons  
acoustiques  
au point  $\Gamma$

Champ électrique



~ constantes diélectriques

~ dispersion des phonons optiques  
au point  $\Gamma$



## *Aknowledgements*

Instrumentation & GaPO<sub>4</sub>

*U. Pietsch, S. Gorfman*

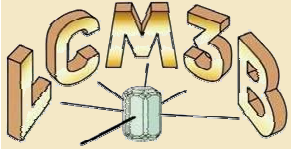
Universität Potsdam / Universität Siegen

Experimental set-up at *HASYLAB*, Hamburg

Instrumentation

*H. Graafsma*

*ESRF*, Grenoble / *HASYLAB*, Hamburg



## ***Aknowledgements***

***P. Fertey, R. Guillot, P. Allé, C. Lecomte***

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***E. Elkaim***

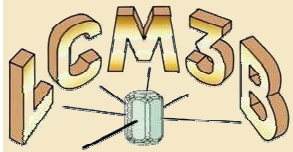
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***J.-F. Bérar, N. Boudet***

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***O. Cambon, J. Haines***

*LPCM, Université Montpellier II, France*



***FIN***