

Transitions de phases et
propriétés piézoélectriques de
monocristaux de



Hichem DAMMAK



Laboratoire **S**tructures, **P**ropriétés et **M**odélisation des **S**olides

Maître de conférences à l'ECP depuis Septembre 1994

1994

1999

2003

Ions poly-atomiques C_{60}

Phases ferroélectriques et
piézoélectricité dans PZN-PT



Effets d'irradiation

Simulations numériques



2001

Transitions de phases
Oxydes ferroélectriques



Thèse 91-94

Transitions de phases
dans les métaux purs
induites par irradiations
aux ions **monoatomiques**



94 -

Service de mesures
diélectriques

THALES 99 -

Piézoélectricité géante



Plan

Transitions de **phases** dans les métaux
&
forte excitation électronique

Phases ferroélectriques
&
piézoélectricité de monocristaux de
 $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})_{(1-x)}\text{Ti}_x\text{O}_3$

Transitions de phases dans les métaux & forte excitation électronique

Collaboration

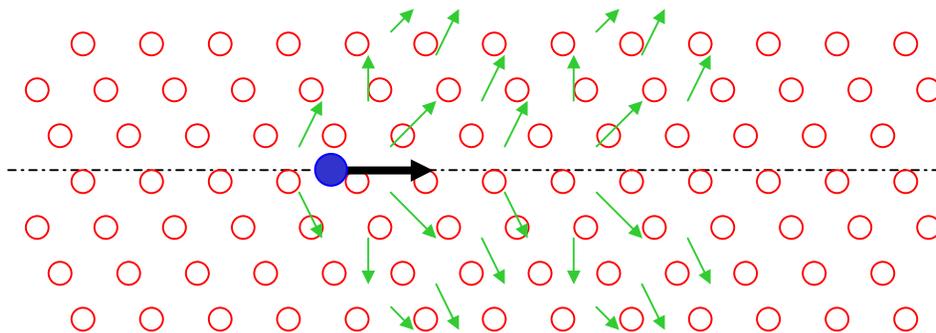
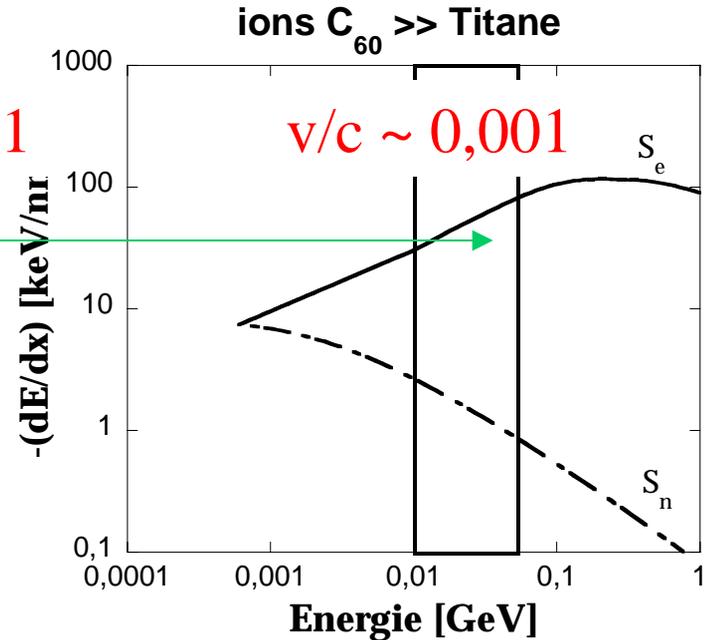
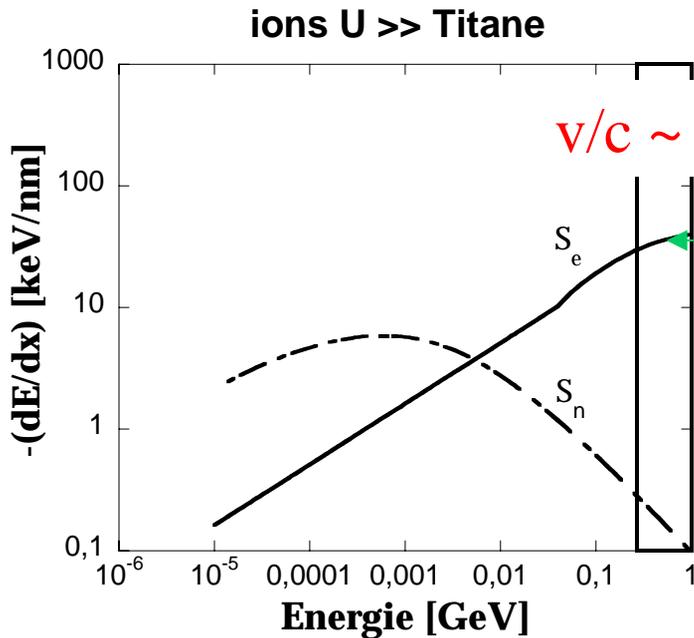
A. Dunlop, M. Angiolini (Post doc.)

LSI, Polytechnique

*Irradiations aux ions Fullerènes :
Tandem, Orsay*

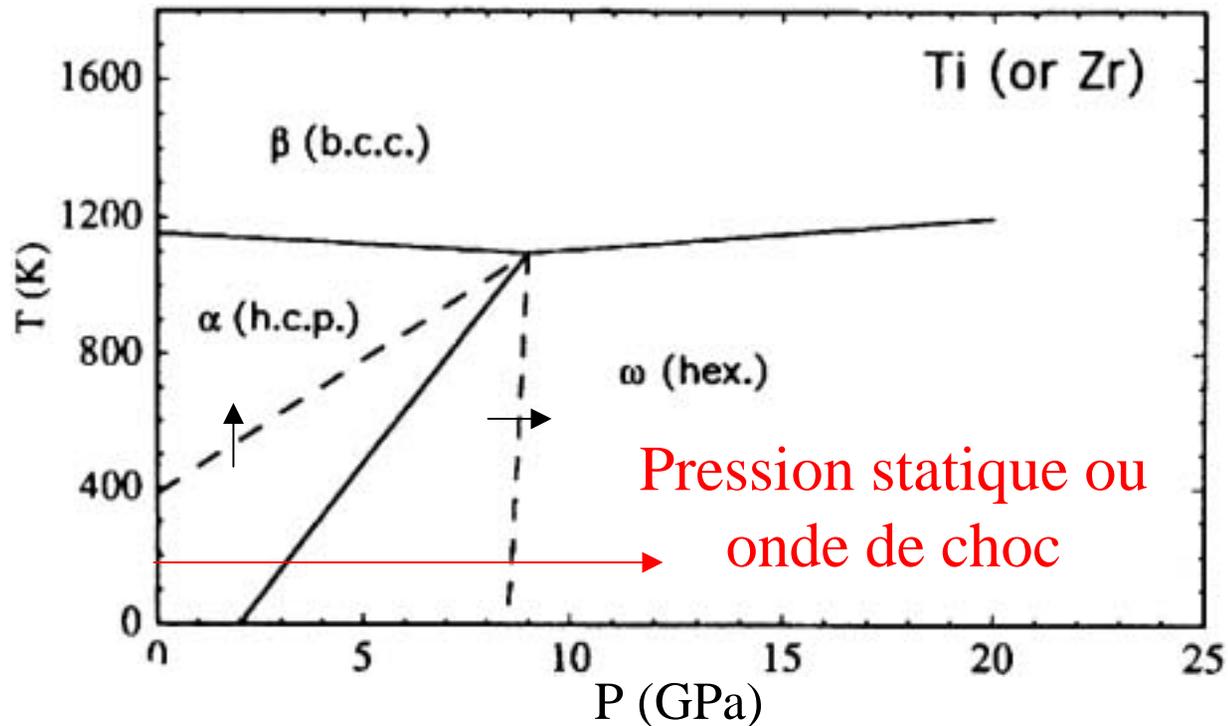


Forte excitation électronique



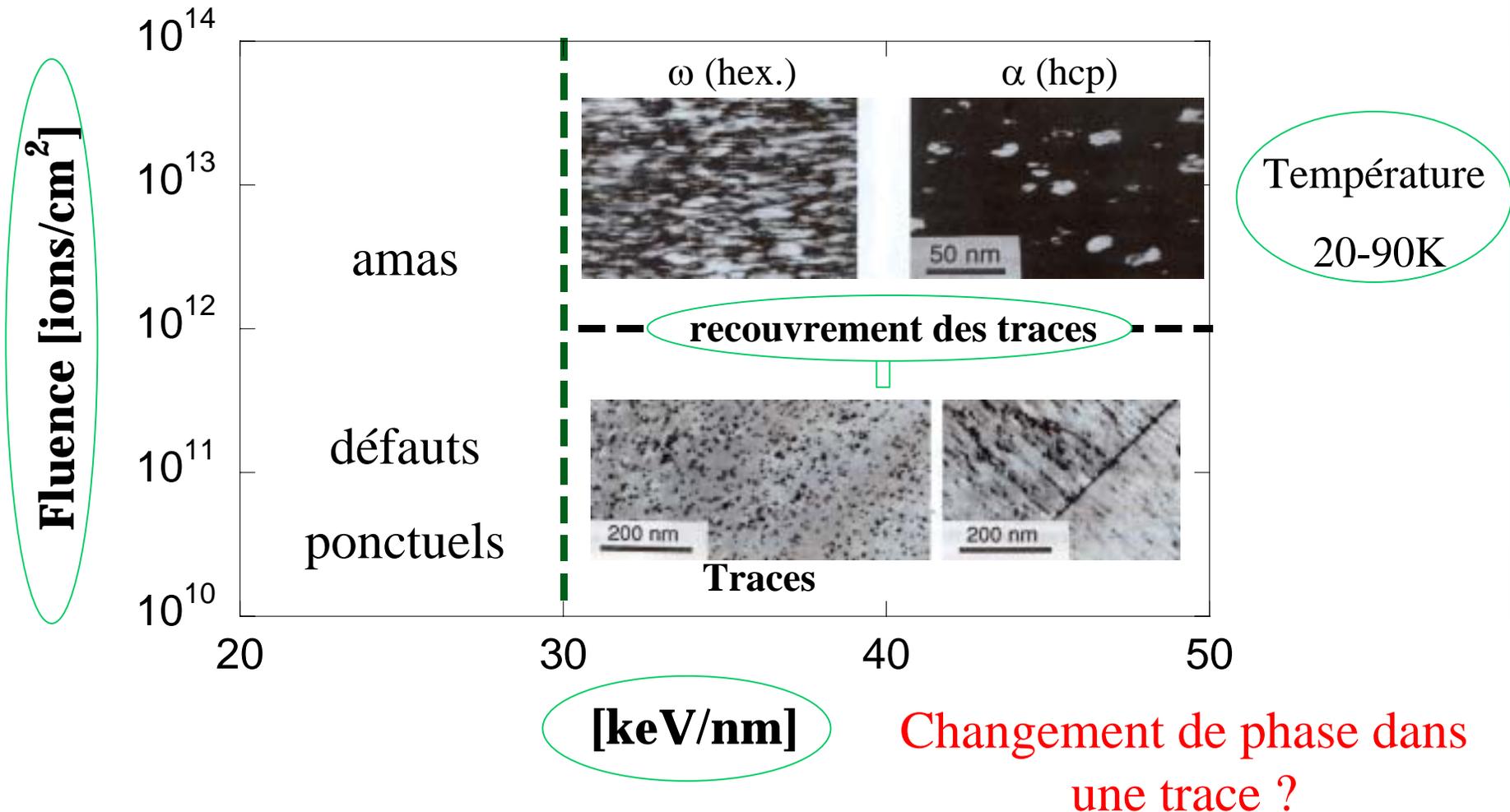
Mécanisme
d'endommagement des
métaux ?

Propriétés du Titane

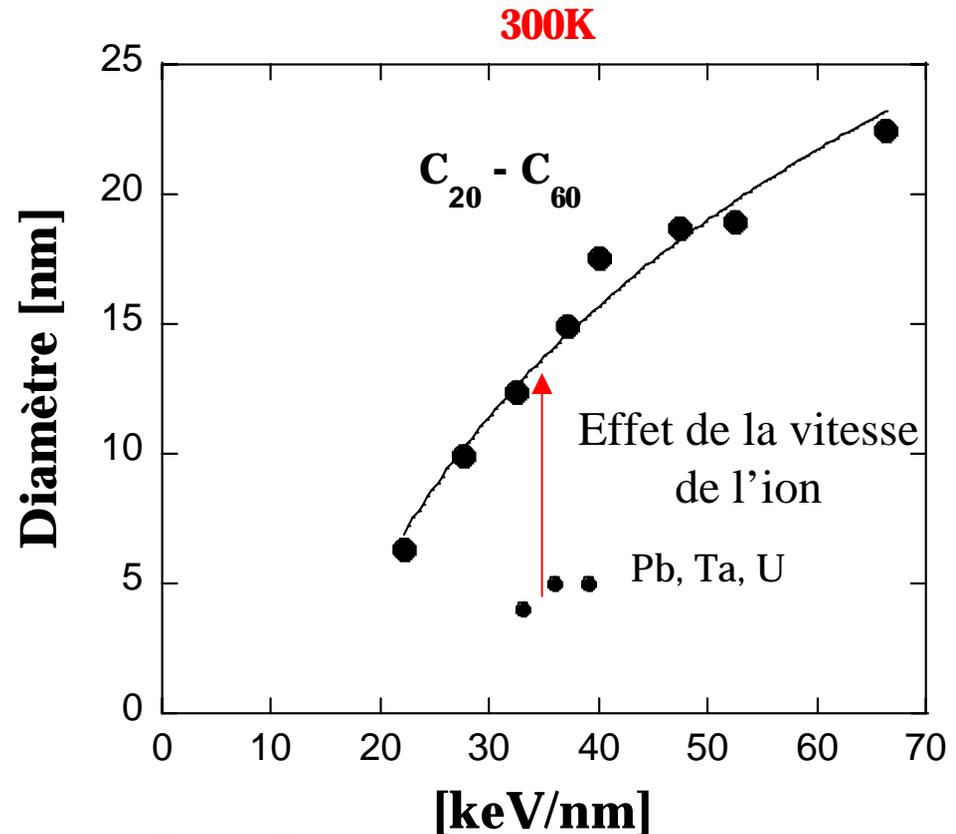
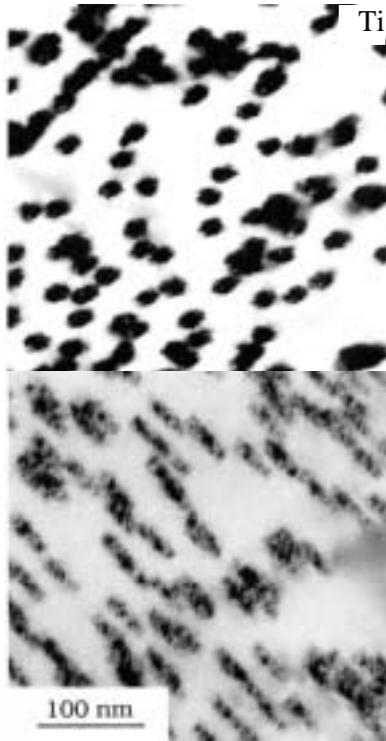
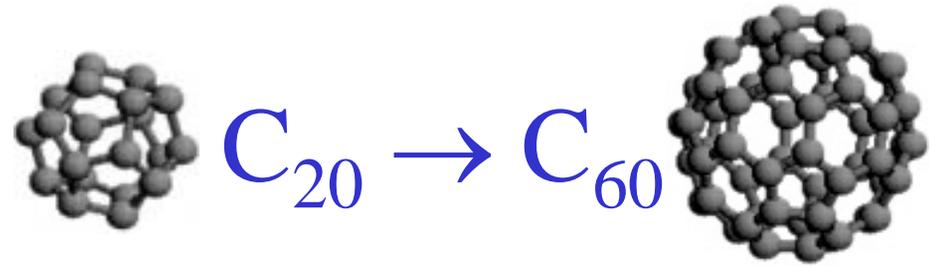


Changement de phase dans une trace ?

Endommagement du Ti Ar, ... U (~1GeV)

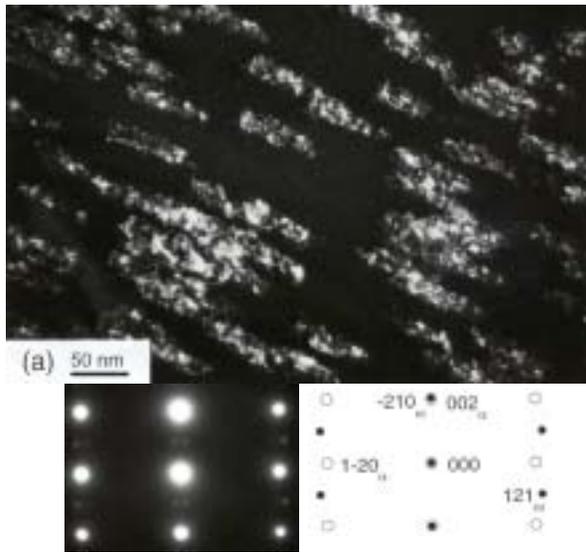


Traces géantes

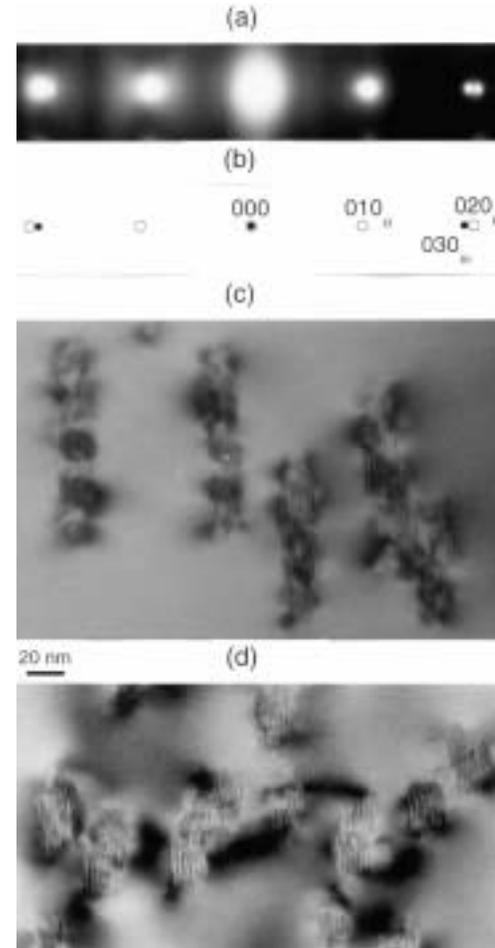


**Densité d'énergie
déposée keV/nm³**

Changement de phase dans une trace C_{60} , 30 MeV



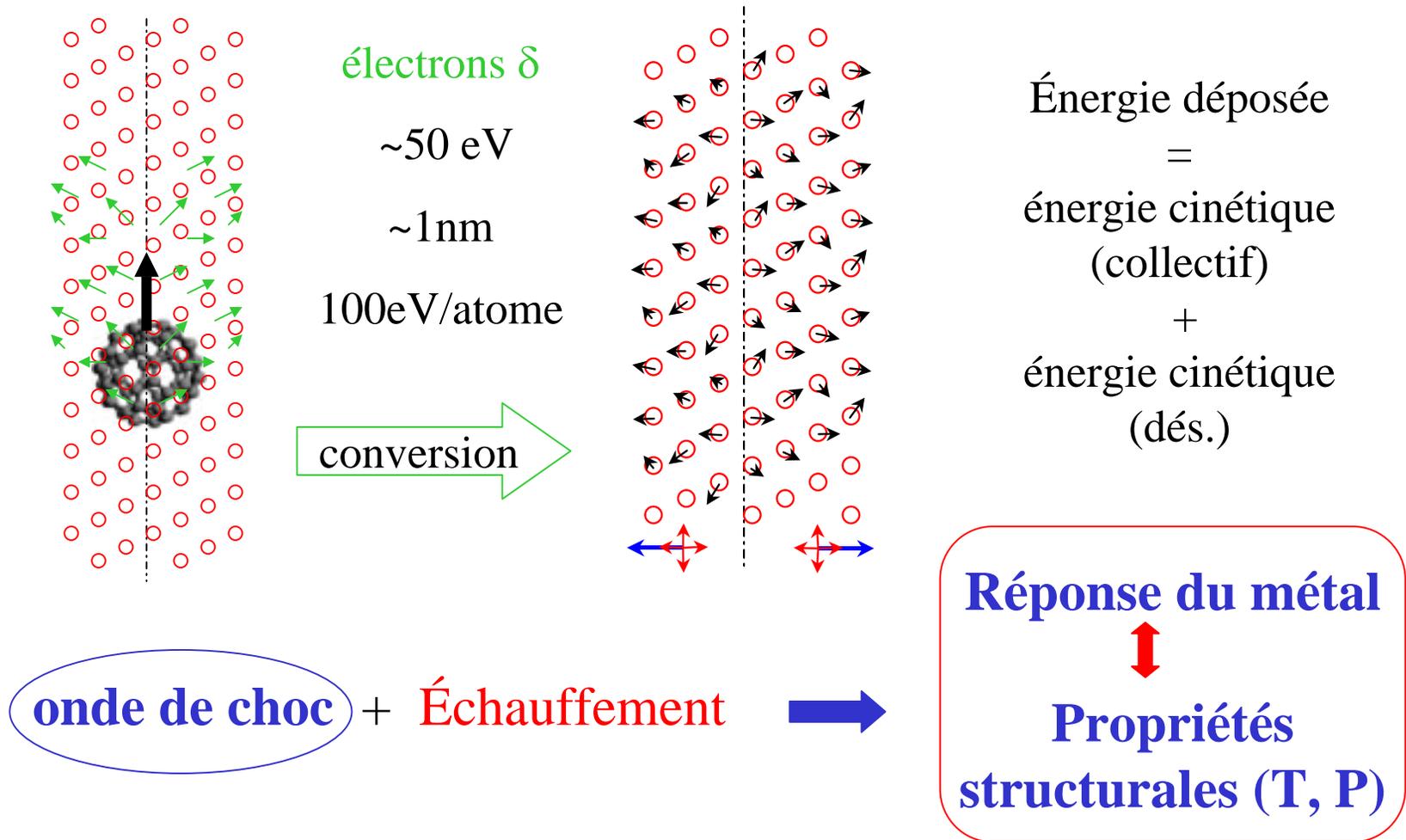
90 K



300 K

90 K

Résultat de la conversion d'énergie



Phases ferroélectriques
&
piézoélectricité de monocristaux de
 $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})_{(1-x)}\text{Ti}_x\text{O}_3$

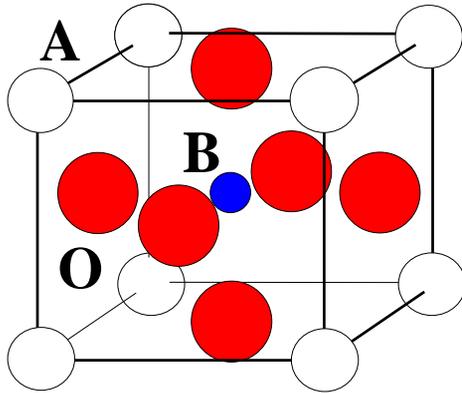


THALES

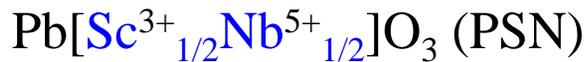
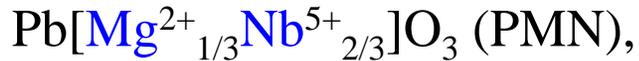
Contexte & Moyens

- **Thèses:** A. Idoumou Ould (1997), A. Lebon (2001),
A. Renault (2002)
- **Collaboration:** P. Gaucher, M. Pham Thi
Thales (TRT Orsay, TUS Sofia)
Sonars, Sondes échographiques
- **Synthèse:** ECP (SPMS), Thales (TRT)
- **Structure:** Diffraction RX (SPMS), Raman (Amiens)
- **Diélectrique-Piézoélectrique:** SPMS, TRT

Pérovskites complexes et solutions solides

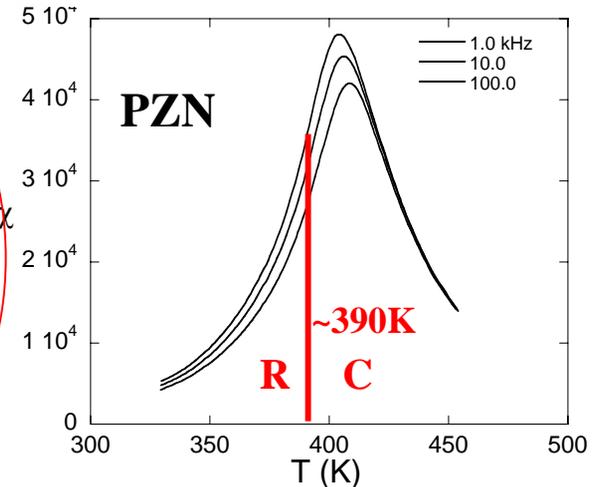
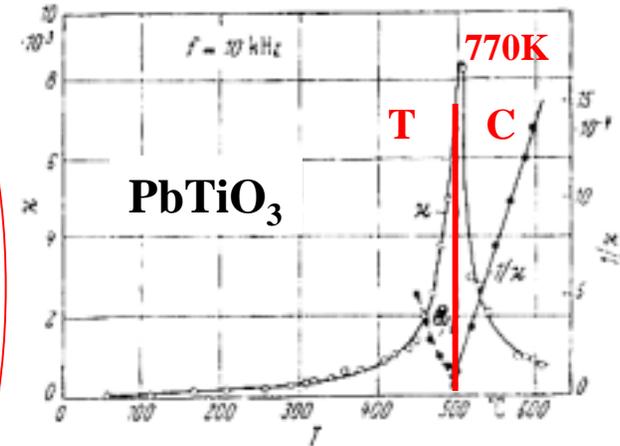


- Simple: $\text{Ba}^{2+}\text{Ti}^{4+}\text{O}_3$, PbTiO_3 (PT),
- Complexe désordonnée:



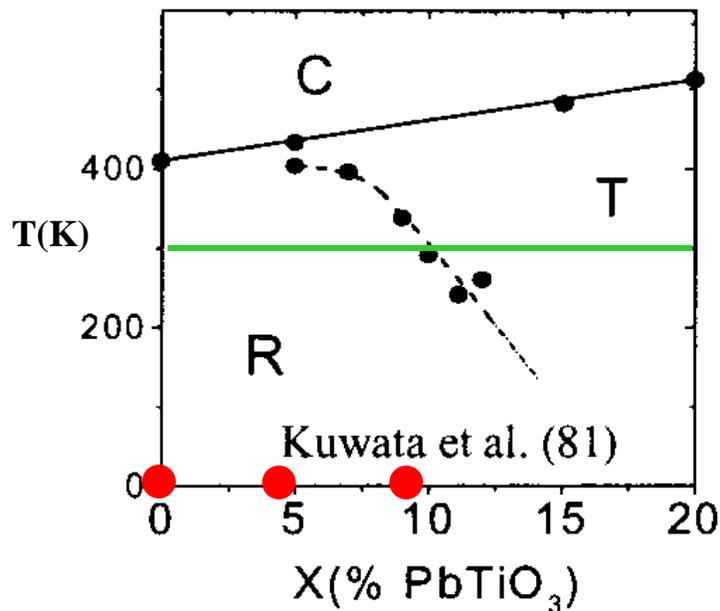
- Solution: PMN-x%PT, **PZN-x%PT**

Relaxeur → Ferroélectrique

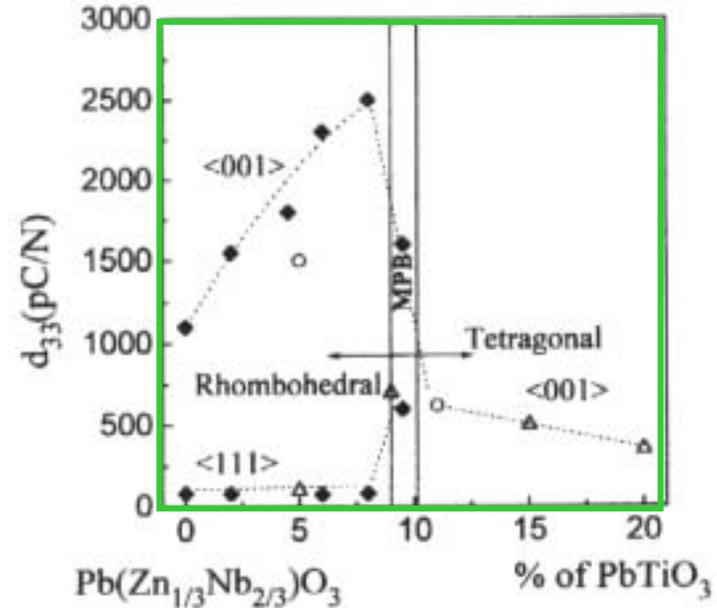


Les composés PZN-x%PT

Structure



Piézoélectricité



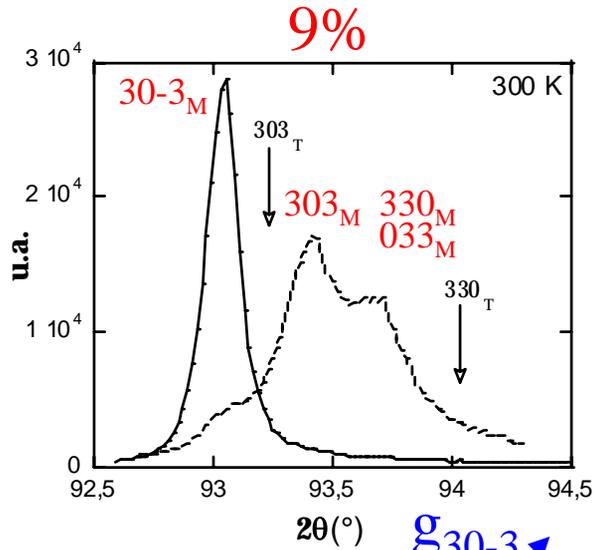
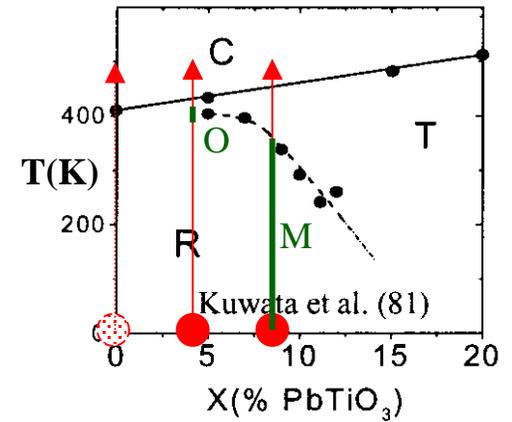
$$S_3 = d_{33} E_3$$

Structure cristallographique

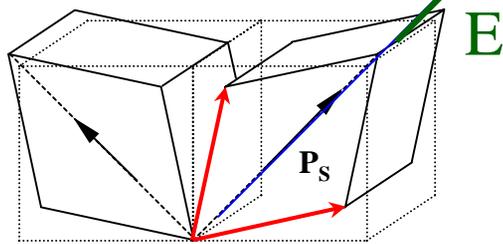
Structure en domaines

Morphotropique

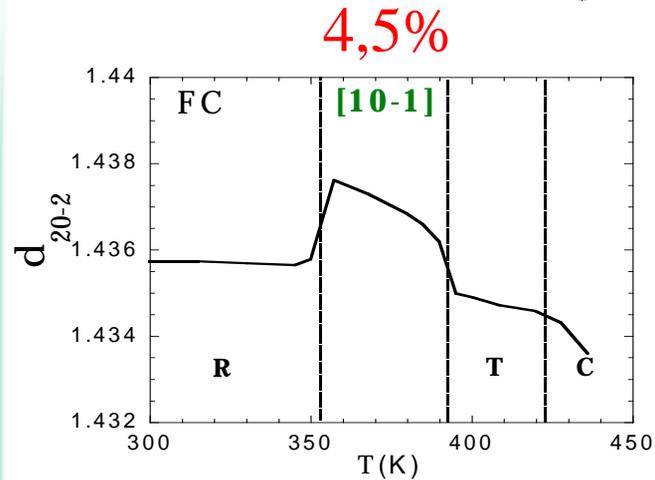
Nouvelles phases



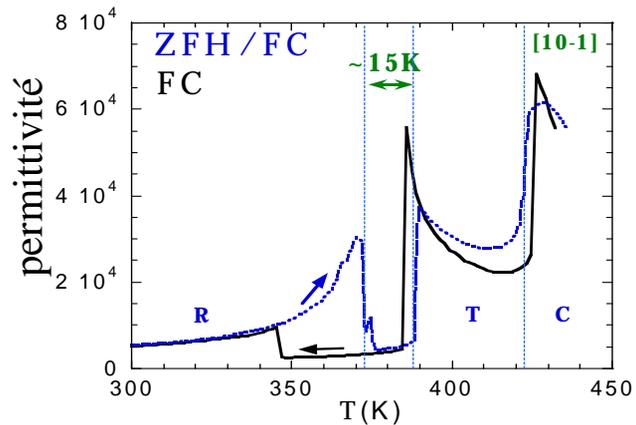
monoclinique



$a = 4,0617$; $c = 4,0628$
 $b = 4,027 \text{ \AA}$; $\beta = 90,19^\circ$

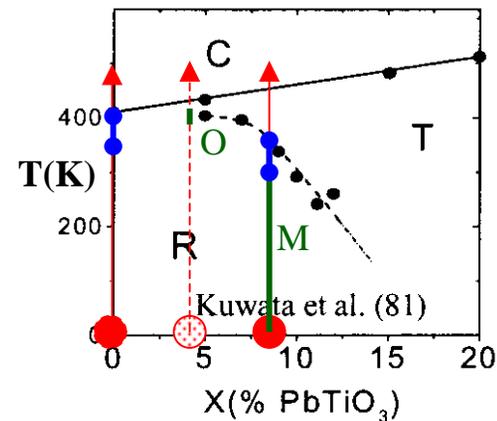


Orthorhombique

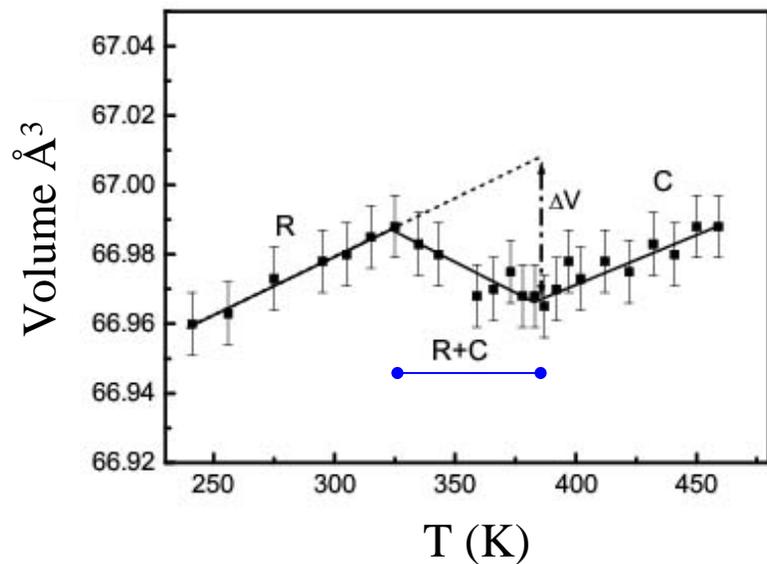


Coexistence de phases

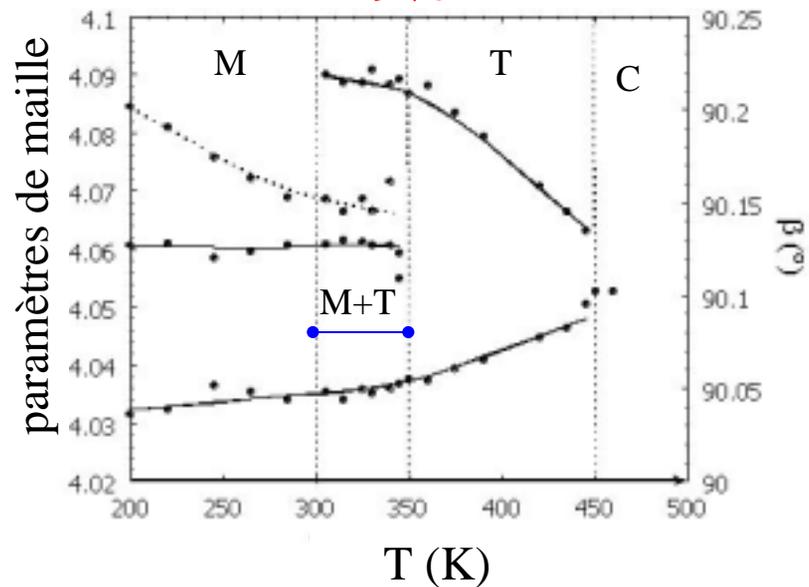
~ 50K



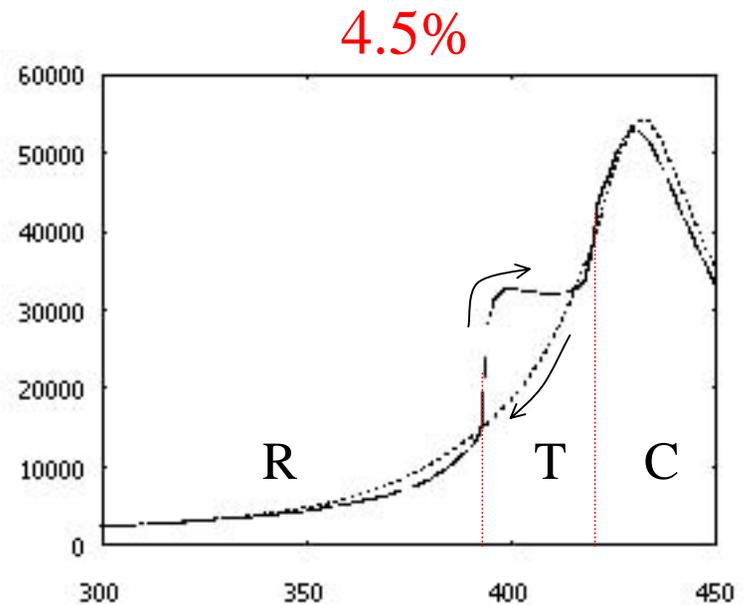
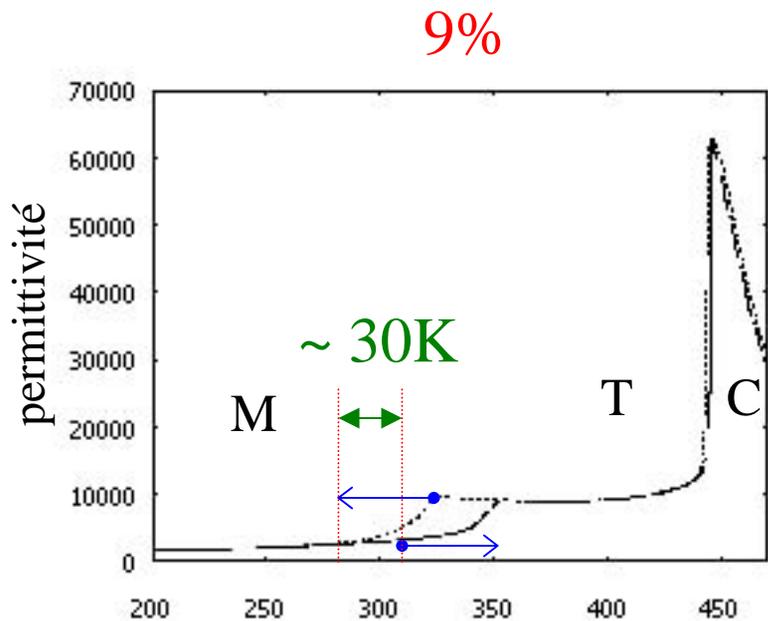
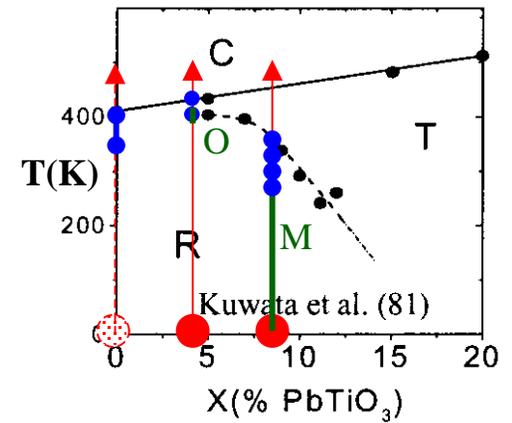
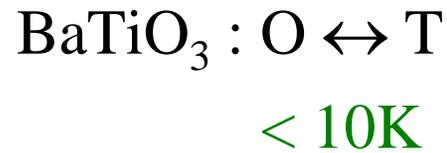
PZN



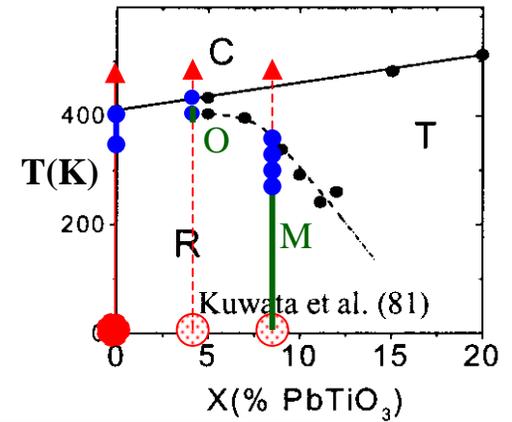
9%



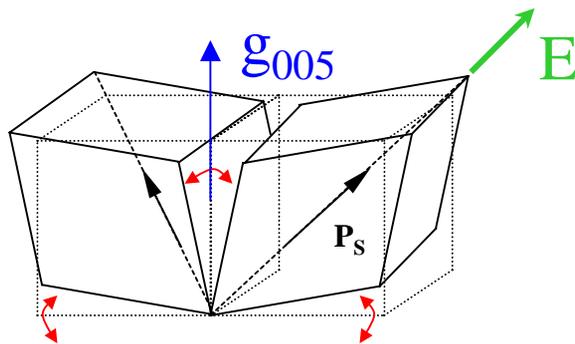
Hystérésis thermique



Contraintes aux interfaces entre domaines

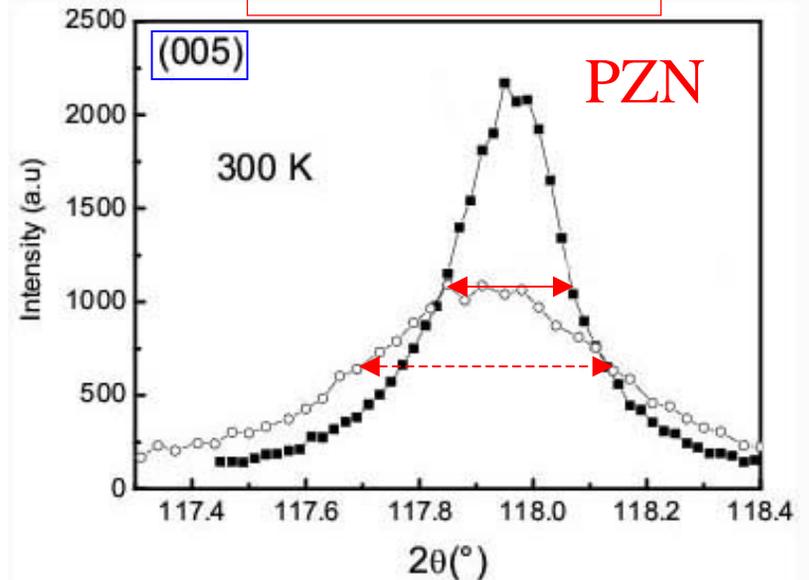


100 nm – 10 μm



- Interprétation des profils des raies de diffraction !

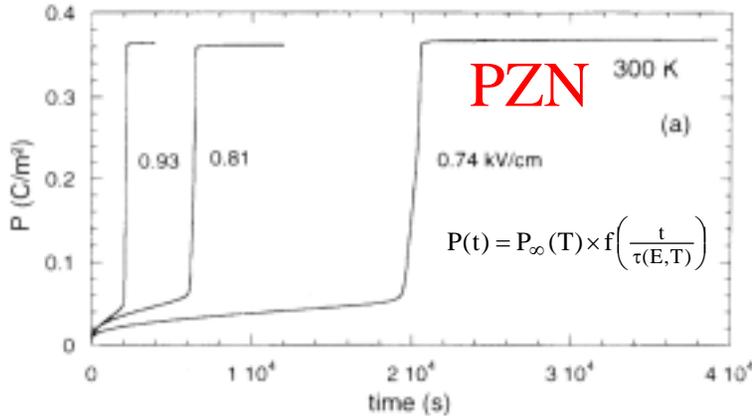
Monodomaine



Polydomaine

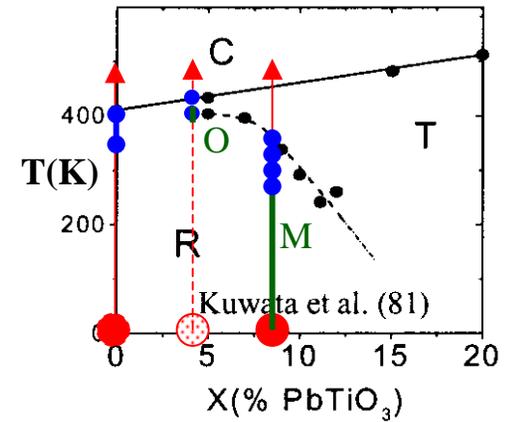
Cinétiques Lentes

Polarisation

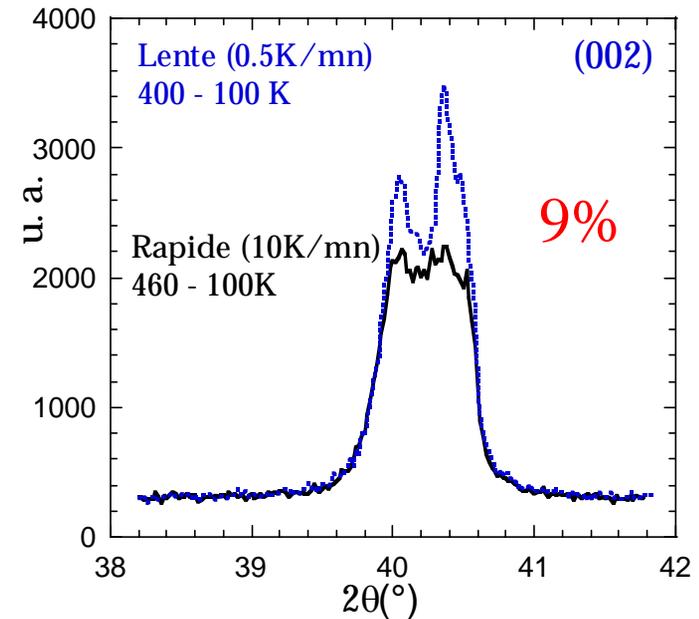


- Paramètres importants !

$dT/dt, E, dE/dt$



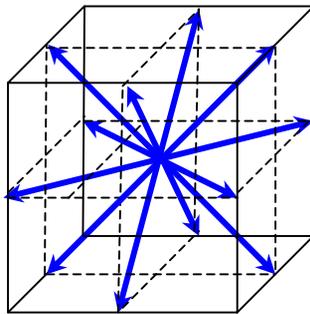
Changement de phases



États polarisés

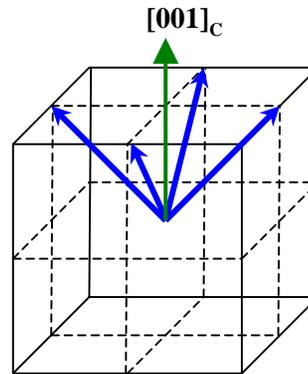
Etat spontané

12M
12O

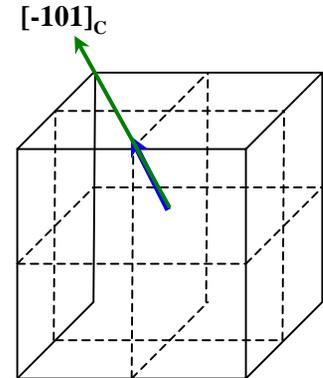


Etats polarisés

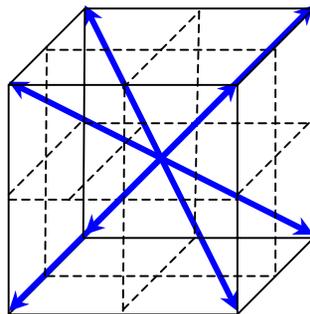
4M
4O



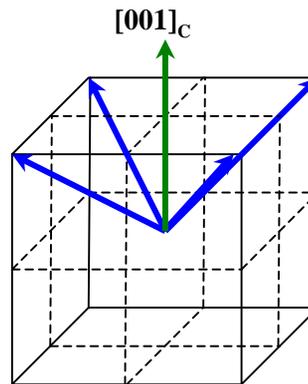
1M
1O



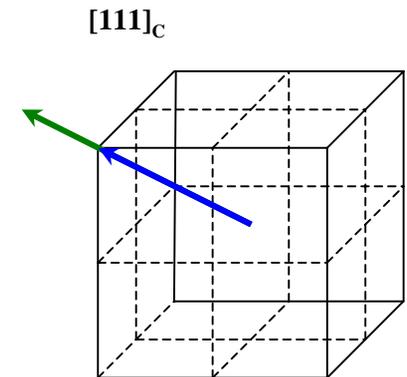
8R



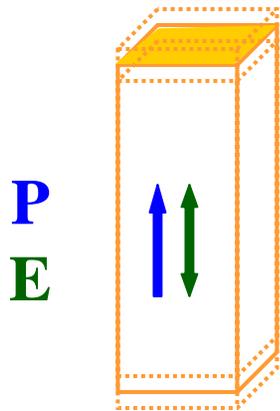
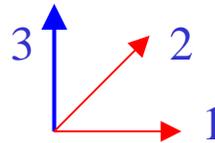
4R



1R

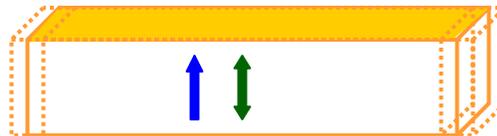


Modes de déformation piézoélectrique



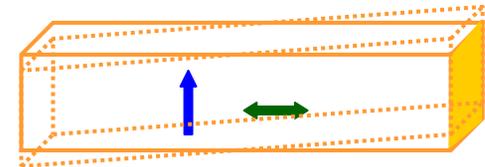
Mode (33)

$$d_{33}, s_{33}$$



Mode (31)

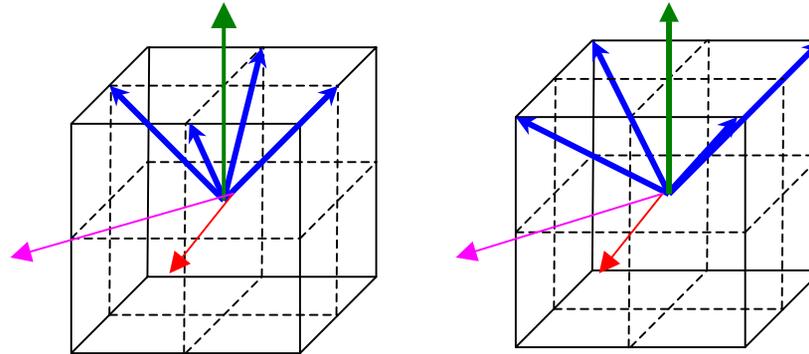
$$d_{31}, s_{11}$$



Mode (15)

$$d_{15}, s_{55}$$

Piézoélectricité du poly-domaine



| État poly-domaines [001] | | PZN9%PT | PZN4.5PT | BaTiO ₃ |
|--------------------------|-------------------------------|---------|----------|--------------------|
| | | 4M | 4R | 4O |
| Longitudinal [001] | s_{33} (pN/m ²) | 184 | 112 | ~ 15 |
| | d_{33} (pm/V) | 2730 | 2048 | ~ 400 |
| | k_{33} | 93% | 89% | ~ 67% |
| Transverse [100] | d_{31} | 1840 | 827 | |
| | k_{31} | 84% | 38% | |
| [110] | d_{31} | 1110 | 1114 | |
| | k_{31} | 85% | 86% | |

Changement de symétrie

Faible champ électrique ~ 1 kV/cm

PZN

$R \rightarrow M_A$

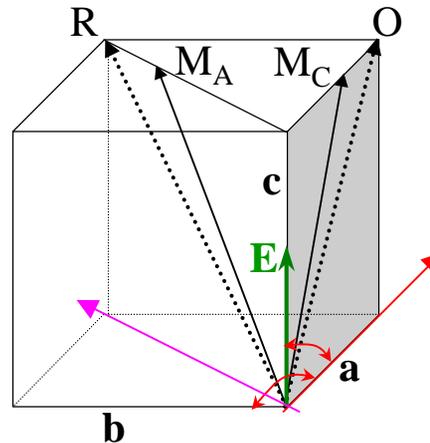
$c-a : 0,000 \rightarrow 0,002 \text{ \AA}$

$\alpha : 89,93 \rightarrow 89,85^\circ$

4,5%

$R \rightarrow M_A$

Ohwada 2001



9%

Distorsion
monoclinique

$c-a : 0,001 \rightarrow 0,004 \text{ \AA}$

$\beta : 90,19 \rightarrow 90,17^\circ$

Fort champ électrique $> \sim 5$ kV/cm

8%

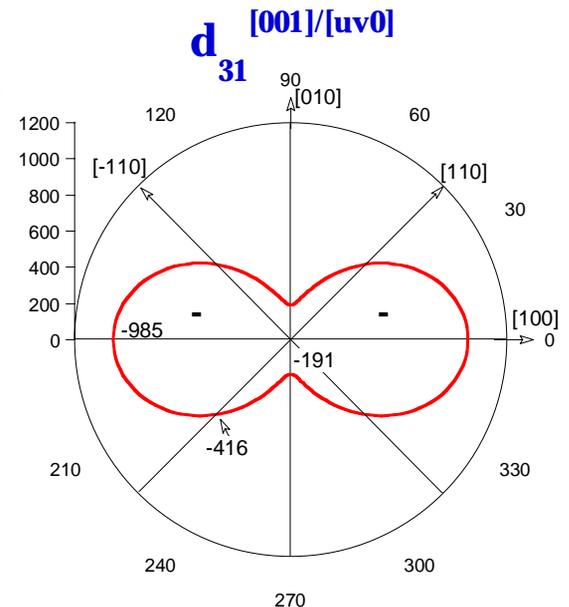
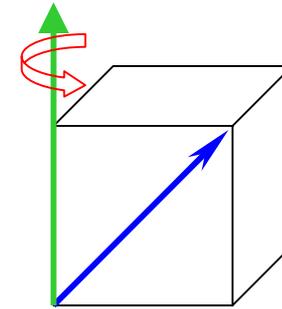
$R \rightarrow M_A \rightarrow M_C \rightarrow T \rightarrow O$

Ohwada 2001

Noheda 2002

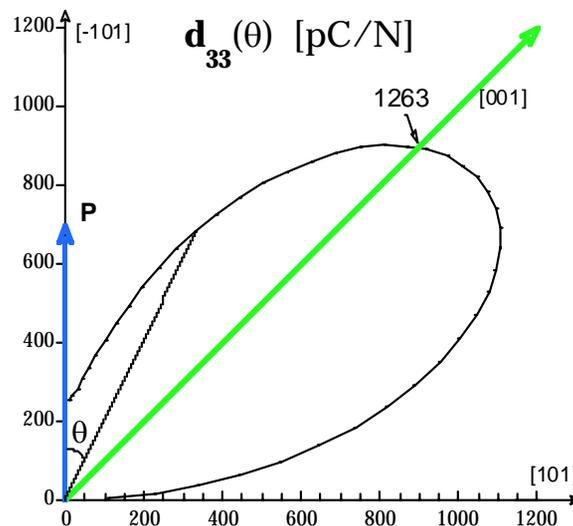
Piézoélectricité du mono-domaine

| État Mono-domaine [10-1] | | PZN9%PT | KNbO ₃ |
|-----------------------------|-------------------------------|---------|-------------------|
| | | 1M | 10 |
| Cisaillement [001],[100] | s_{55} (pN/m ²) | 190 | 40 |
| | d_{15} (pm/V) | 3200 | 214 |
| | d_{15}/d_{33} | 13 | 7 |
| | k_{15} | 80% | 90% |



Forte anisotropie

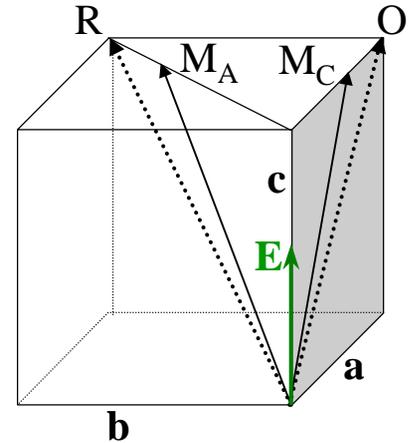
Approximation
Phase O



Origine de la piézoélectricité géante

Microscopique

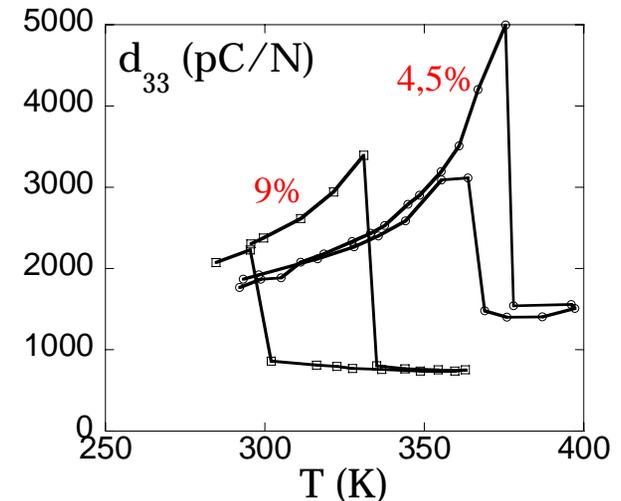
- Aptitude à changer de symétrie
- Énergies des phases très proches
- Phénomènes pré-transitionnels



Morphotropique



Proximité d'une transition de phase



Origine de la piézoélectricité géante

Macroscopique

Forte compliance élastique $s_{\alpha\beta}$

Faible distorsion ferroélectrique



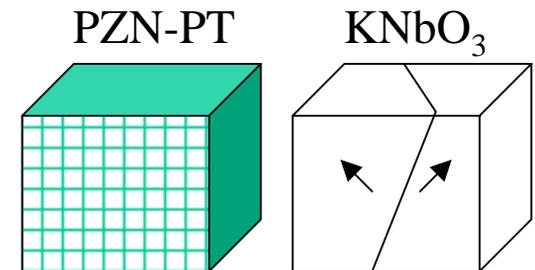
- Forte densité de domaines:

+

- Forte anisotropie



- Contraintes dynamiques induites



$$d_{i\alpha}^{\text{eff}} = f(d_{i\alpha}, s_{\alpha\beta})$$

Perspectives

- **Extension à d'autres composés :**
 - PMN-PT, PSN-PT (R. Haumont, B. Dkhil, J.M. Kiat)
- **Étude de transducteurs large bande utilisant les monocristaux:**
(C. Augier, P. Gaucher, M. Pham Thi)

Perspectives

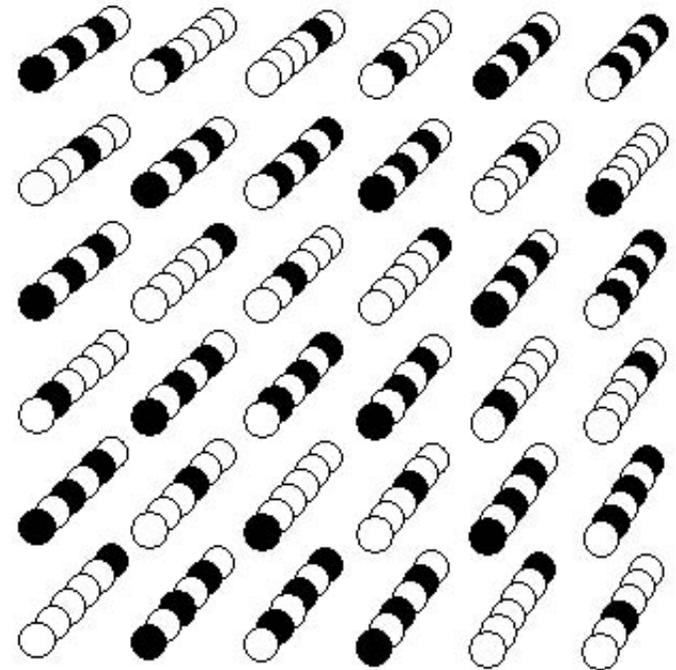
- Rôle du désordre microscopique: (+2; +5)
simulation numérique

Phase cubique en
moyenne

Moment dipolaire
électrique local

Monte Carlo

M. Hayoun, LSI, Polytechnique



Perspectives

- Nanopoudres – Nanomatériaux « Relaxeurs »

Cristal



micro-grain



nano-grain

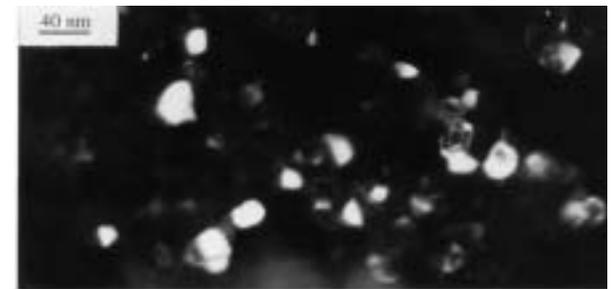
microstructure
des domaines

Nanodomaines
polaires ~50 nm

Lyophilisation

(J. Carreaud, C. Bogicevic, B. Dkhil, J.M. Kiat)

nanopoudre → Céramique
Homogénéité



Grains de BaTiO₃

THALES



Laboratoire **S**tructures, **P**ropriétés et **M**odélisation des **S**olides

