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PARIS 7 - DENIS DIDEROT



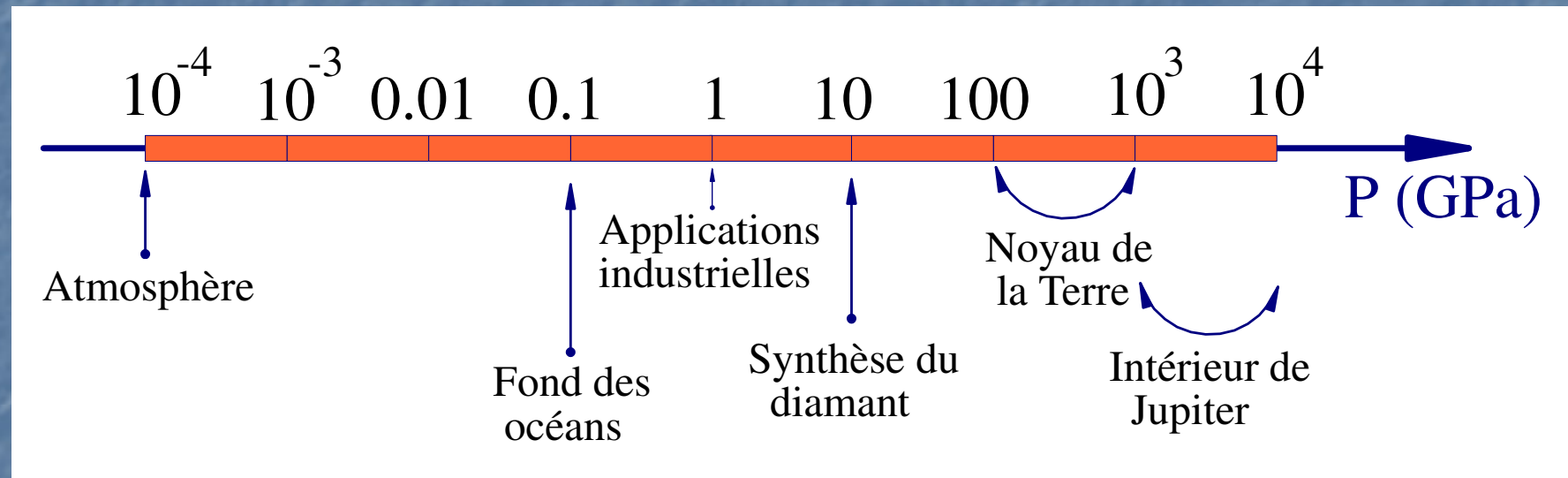
Diffraction sur monocristal en conditions extrêmes

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Institut de Minéralogie et de Physique des Milieux Condensés

Paris

Pourquoi les hautes Pressions ?



Pourquoi les hautes Pressions ?

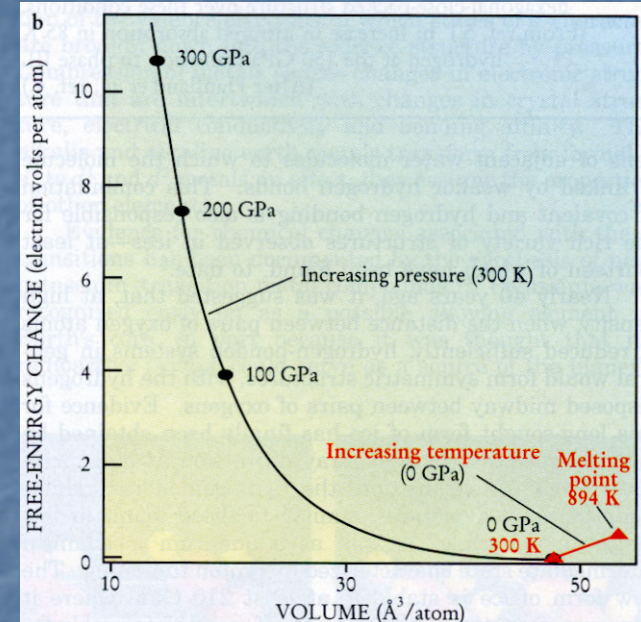
Grandes variations facilement contrôlées

- ✓ des distances interatomiques
- ✓ de l'énergie libre du système

Modifications importantes

- ✓ corrélations électroniques
- ✓ couplages entre modes de vibrations
- ✓ changement de nature des liaisons
- ✓ Nouvelles phases
- ✓ Nouveaux matériaux

- ✓ Test des potentiels
- ✓ ...



Quelle physique ?

La Liaison Interatomique sous conditions extrêmes

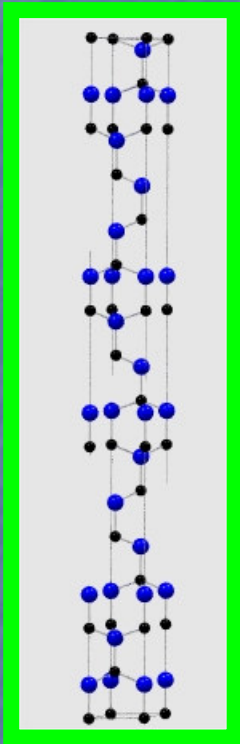
Aspects structuraux et dynamiques

Transfert de Charge			Approche et Mécanismes des transitions de phase			Physique aux Interfaces		
Hydrogène	Liaisons Covalente	Van Der Waals	Compétition ordre désordre	hybridation orbitales Changement coordinance	Nouvelles Phases	Nouveaux Matériaux	Biologie	Chimie
	Stabilité de la liaison intramoléculaire					Ultra durs	Proteines	Synthèse
Glaces H ₂ O CH ₄ , NH ₃ , HF	Halogènes Br ₂ , BrI, Hydrogène	Gaz Rares	Glace Pérovskites	Semiconducteurs		Nanocristaux Piézo		
	Polymérisation Réactivité Nitrométhane							

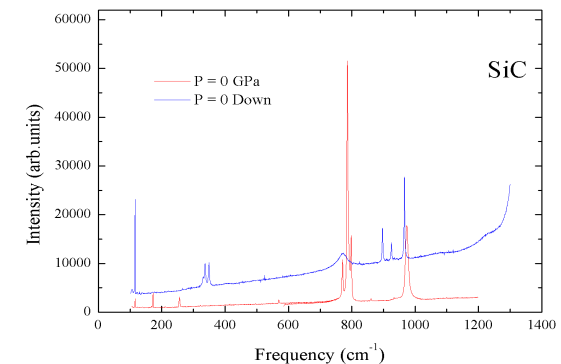
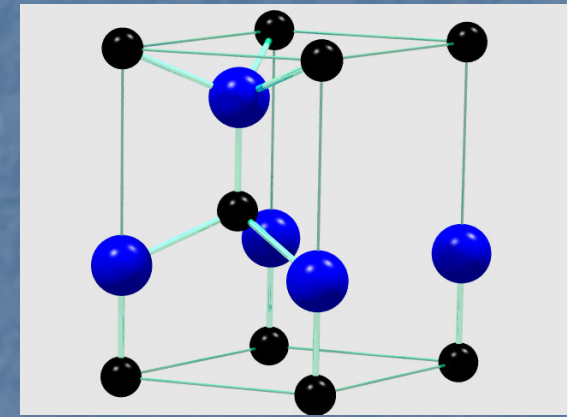
Quelques exemples

- ✓ Matériaux durs (SiC, B_α)
- ✓ Transitions de phase (LGT)
- ✓ Stabilité (Quasicristaux AlPdMn)
- ✓ liaison hydrogène
- ✓ ...

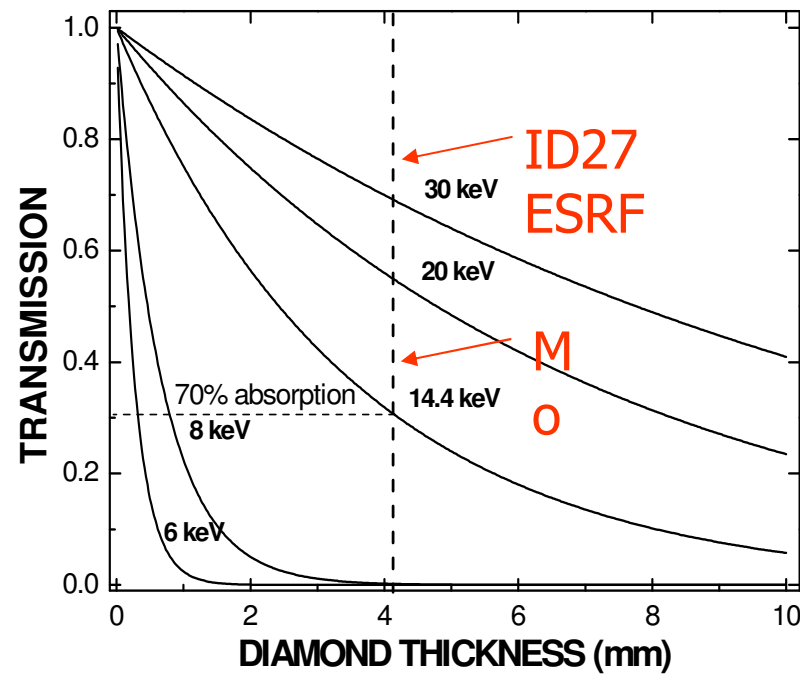
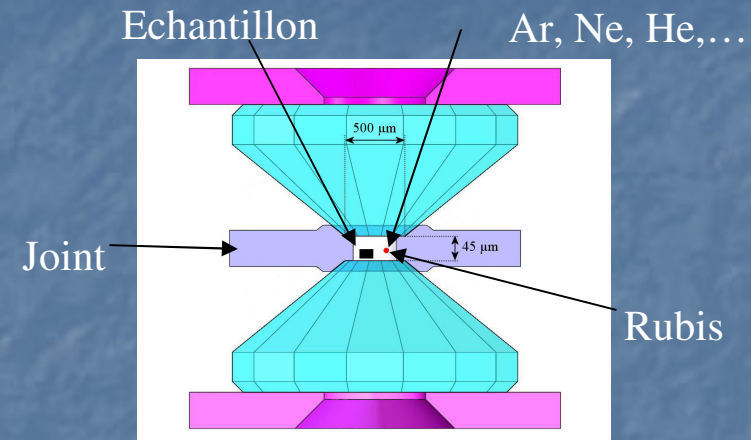
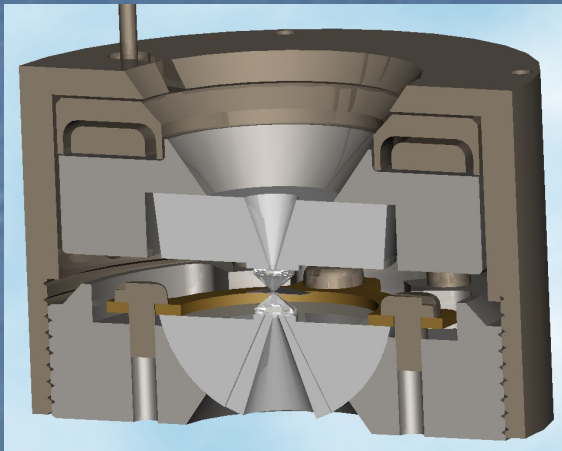
SiC moissanite



- ✓ Matériau dur
- ✓ Riche polytypisme (15R R3m)
- ✓ Transition de phase à P croissante
- ✓ Transition vers une phase ordonnée différente à la descente
- ✓ Equation d'Etat...

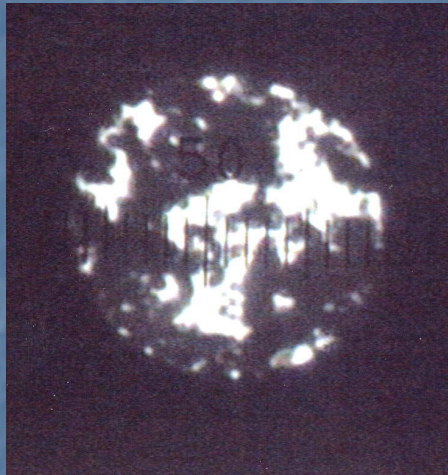


Technique HP

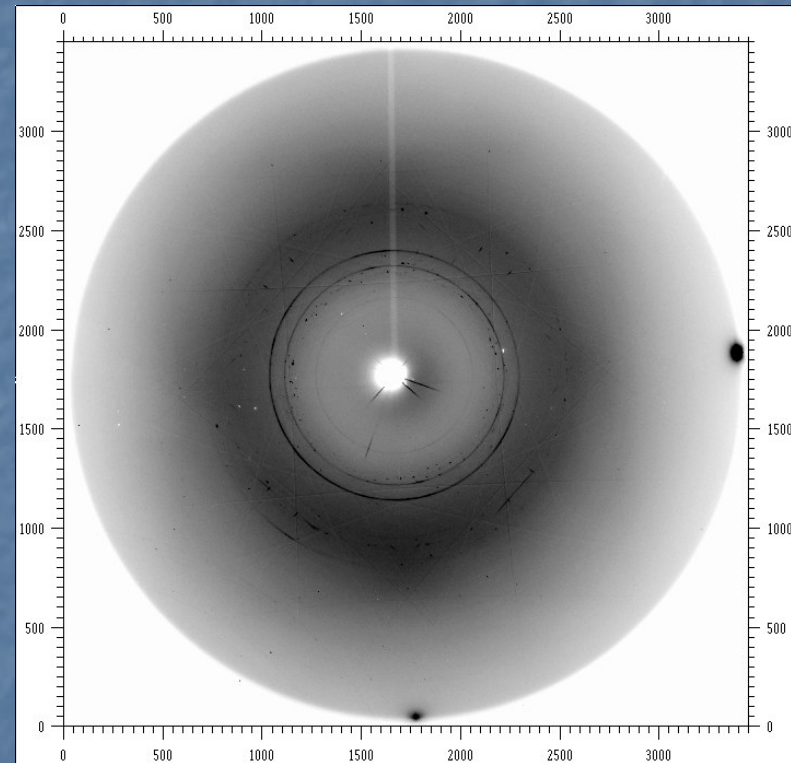


SiC moissanite

Manip Poudre



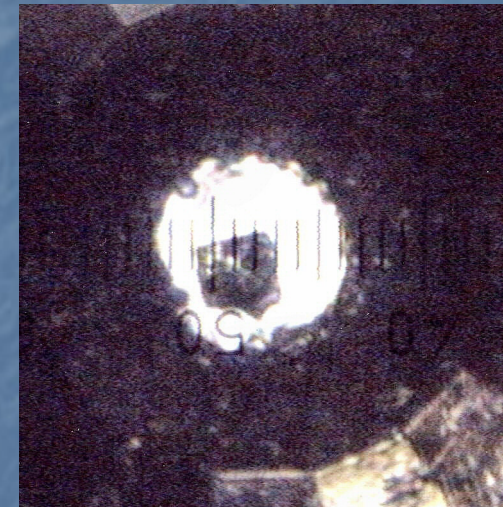
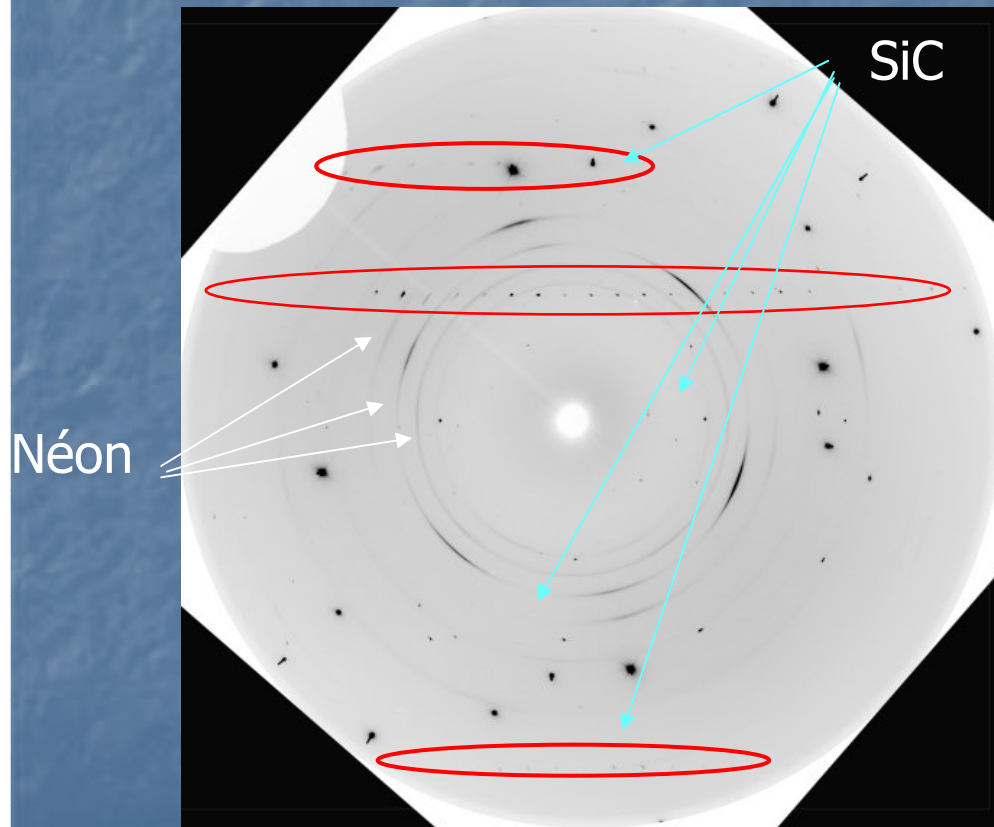
Problèmes variés :
contraintes, bridging,
statistique, intensité,
rubis



ESRF ID30, $\lambda = 0.3738 \text{ \AA}$ (33.166 keV), MAR3450, Fentes 200x200 μm
Multiscan de toute la cellule, temps = 120s

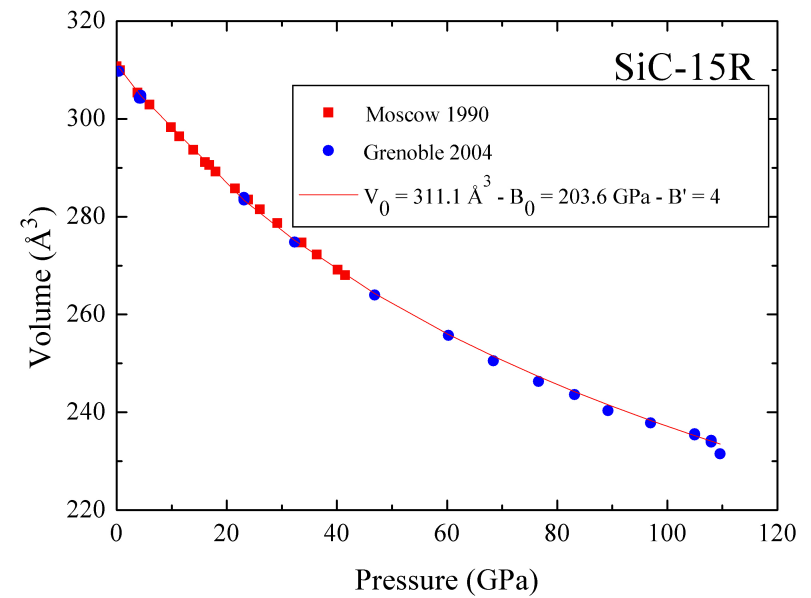
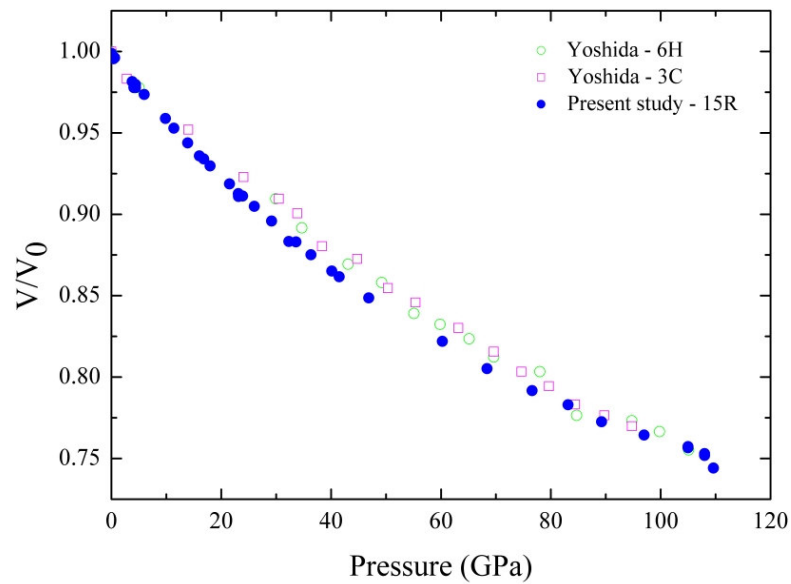
SiC moissanite

Manip Monocristal
P = 54 GPa



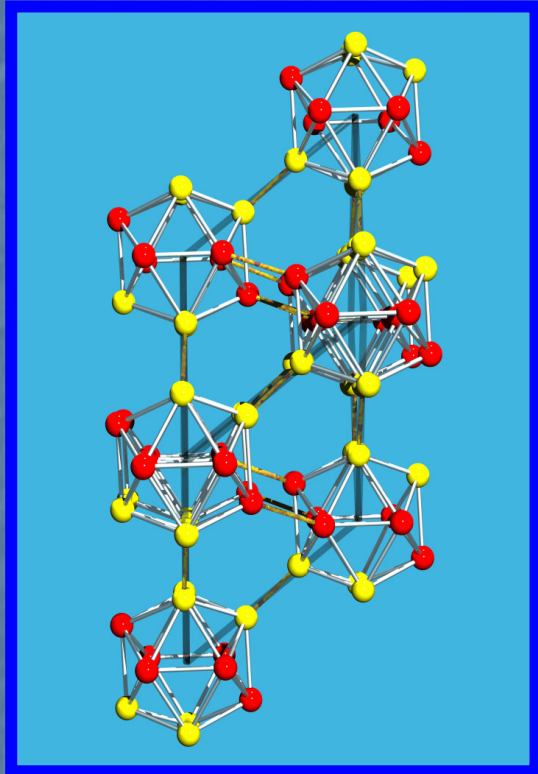
ESRF ID30, $\lambda = .3738 \text{ \AA}$ (33.166 keV)
MAR3450, Fentes /8, temps/3

SiC moissanite



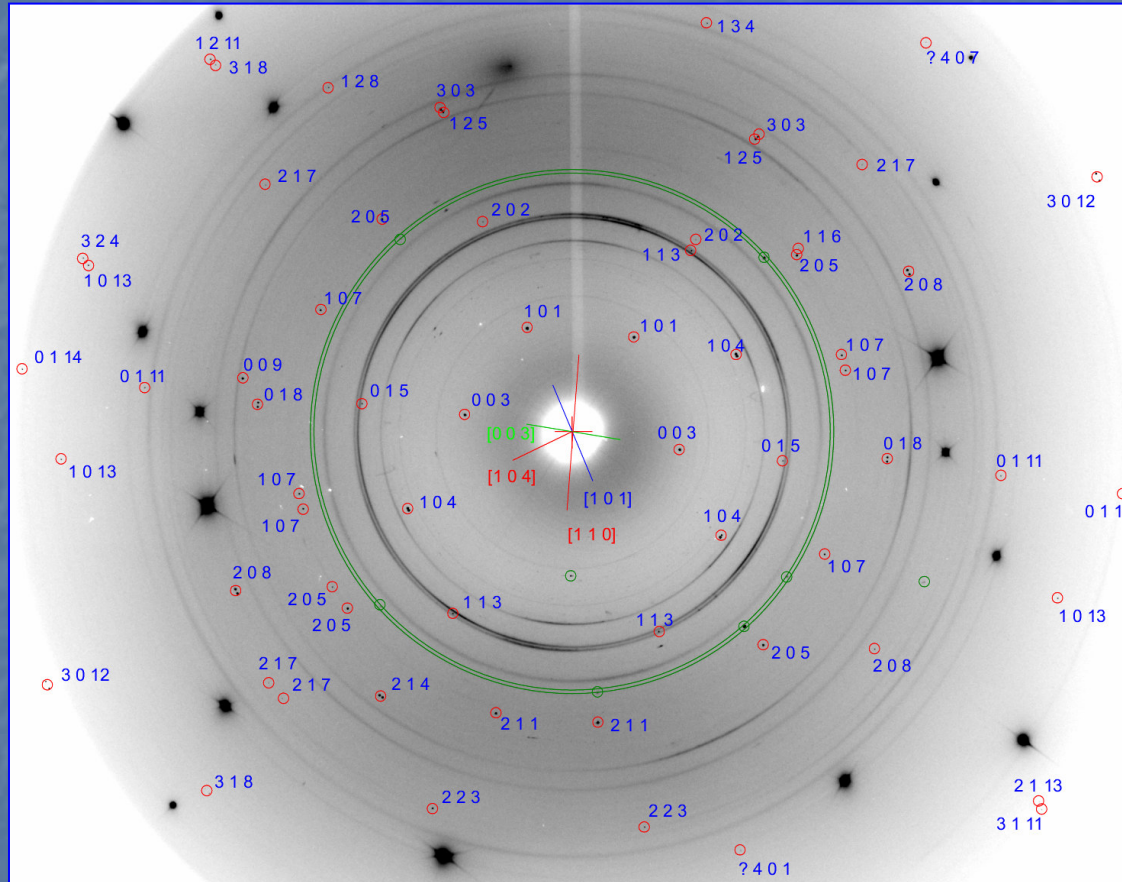
Transition phase HP
EOS

Bore - α

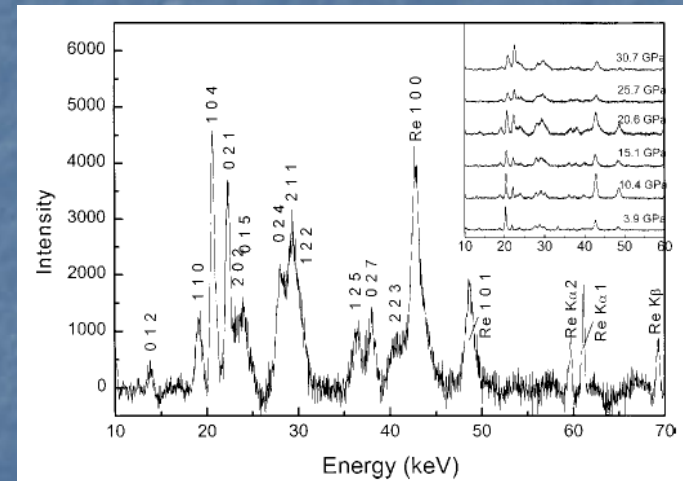


- ✓ liaisons à 3 centres
- ✓ maille contient 1 icosaèdre
- ✓ liaisons inter et intra-icosaèdres...
- ✓ comparaison avec le bore β
- ✓ EOS, stabilité...,

Bore - α



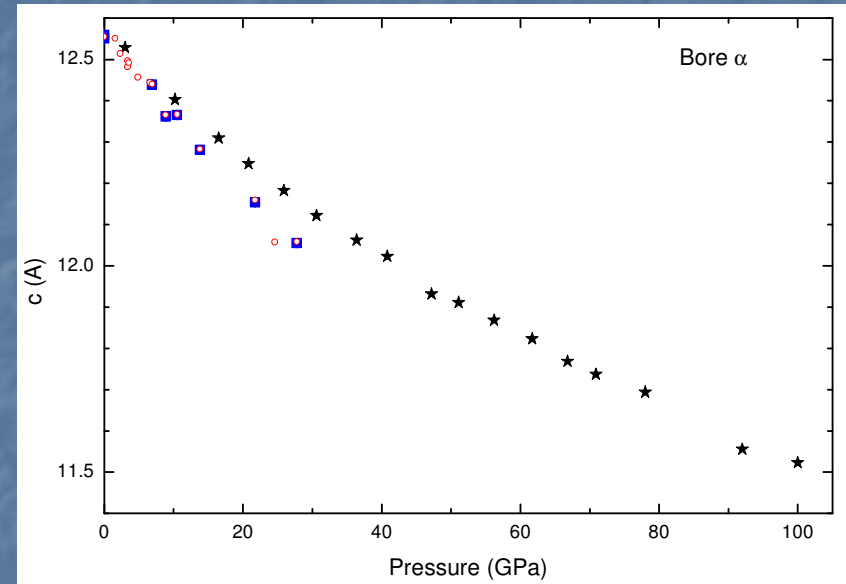
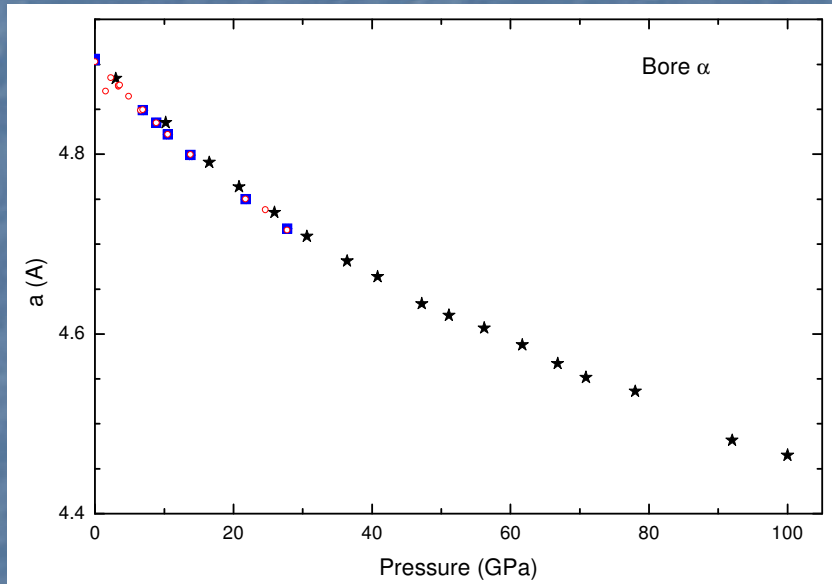
ESRF
ID30 mar3450
ID27 ccd



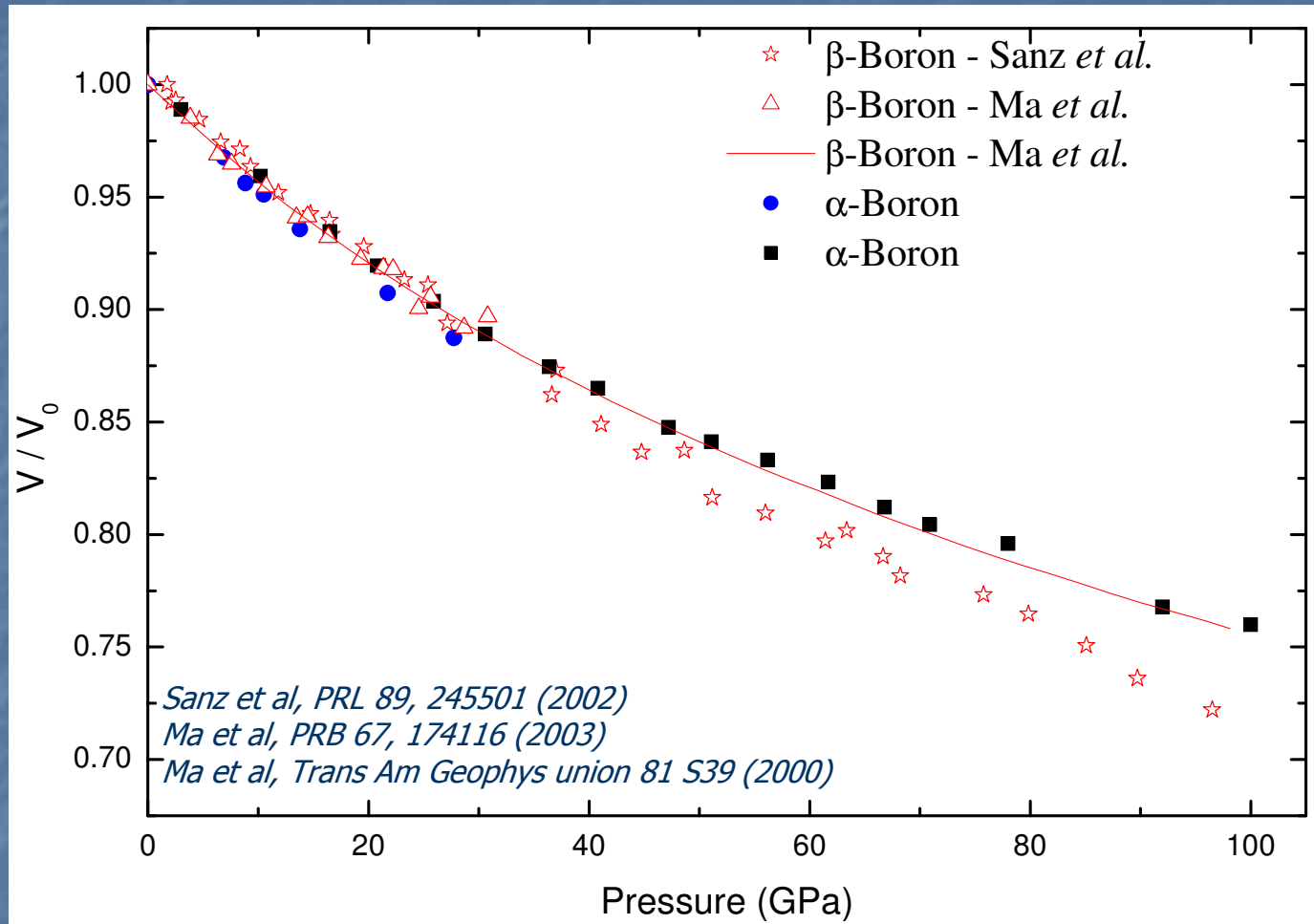
X17C NSLS

Ma et al, PRB 67, 174116 (2003)

Bore - α

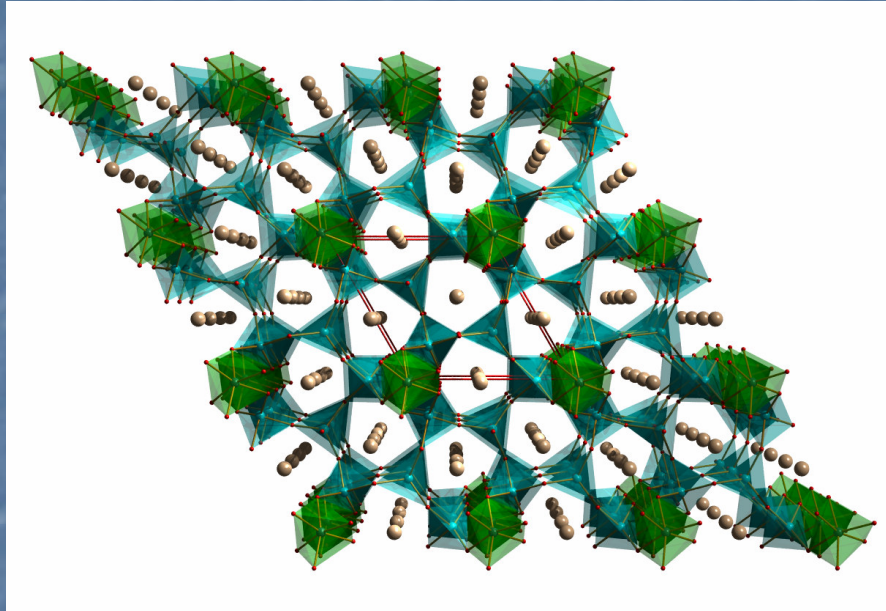


Bore - α

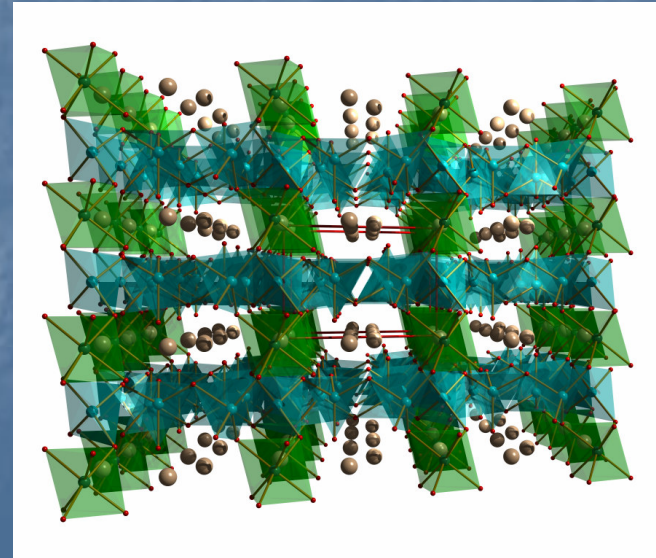


bore- α est-il différent du bore β ?

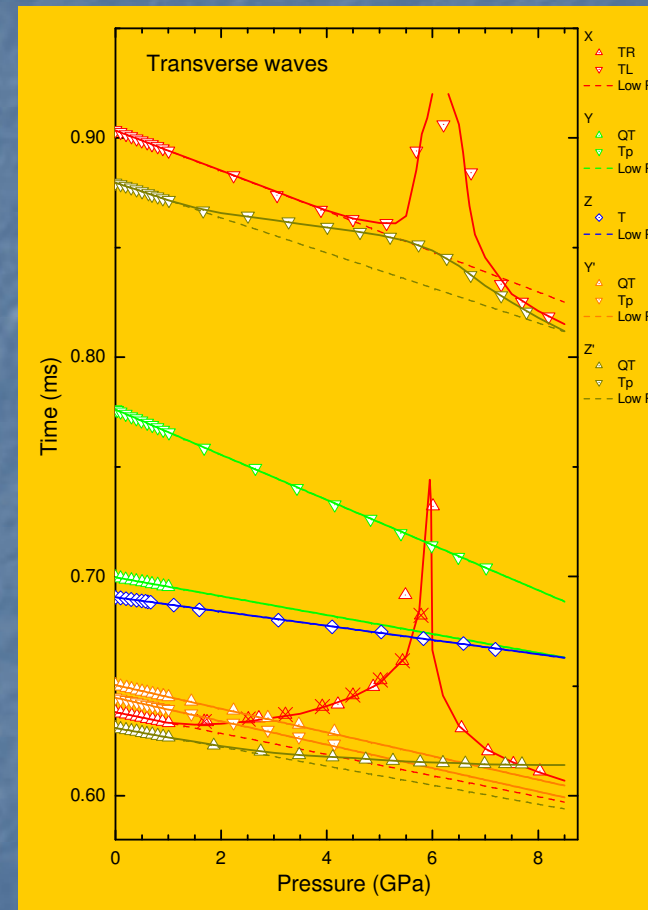
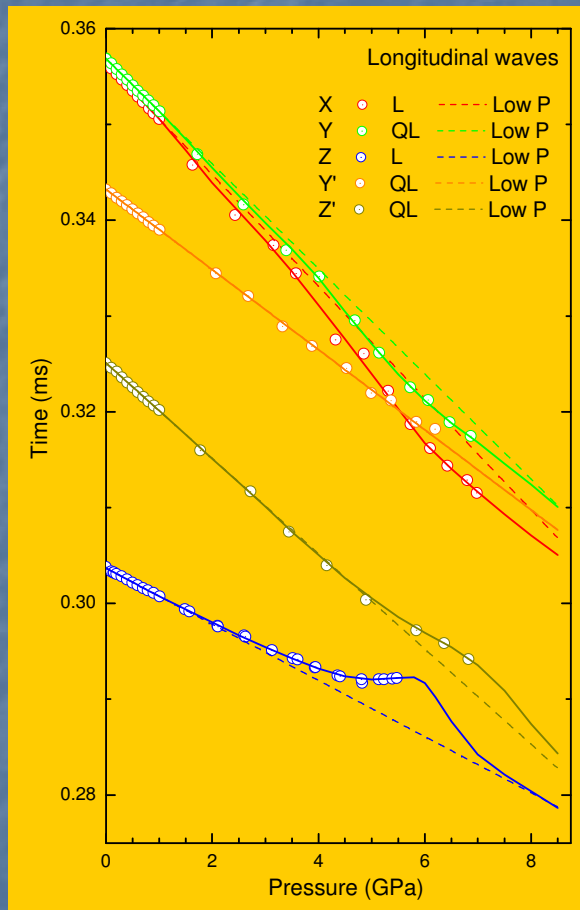
Langatate $\text{La}_3\text{Ga}_5(\text{Ga}_{.5},\text{Ta}_{.5})\text{O}_{14}$



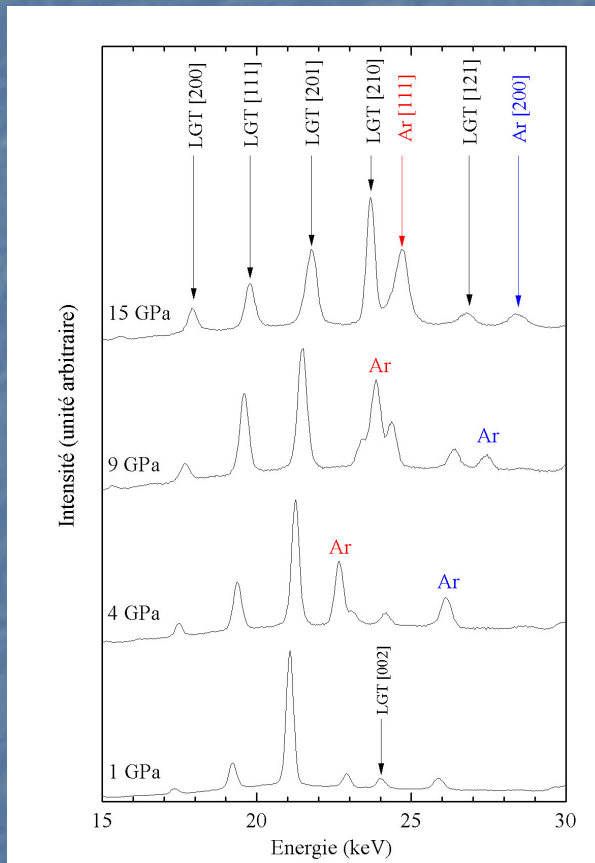
- ✓ Piézoélectrique
- ✓ stable en Température
- ✓ forts coefficients de qualité
- ✓ ...
- ✓ EOS ?
- ✓ Propriétés mécaniques ?



Langatate $\text{La}_3\text{Ga}_5(\text{Ga}_{.5},\text{Ta}_{.5})\text{O}_{14}$



Langatate $\text{La}_3\text{Ga}_5(\text{Ga}_{.5},\text{Ta}_{.5})\text{O}_{14}$



Dispersion d'énergie
LURE DW11

LGT
P= 0 - 18 GPa

ESRF - ID27
16 / 7 / 2006

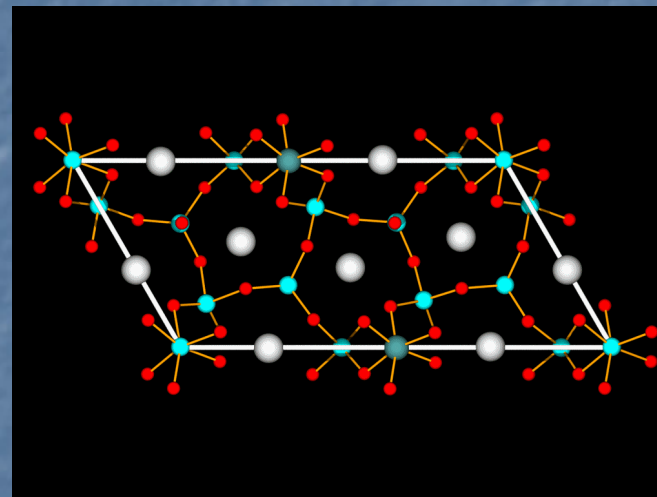
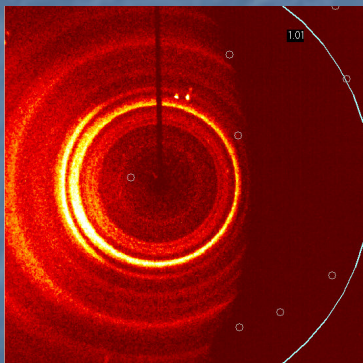
M Gauthier, A Polian, P Munsch
W Crichton

LGT-esrf

ESRF (ID27) CCD
XDS

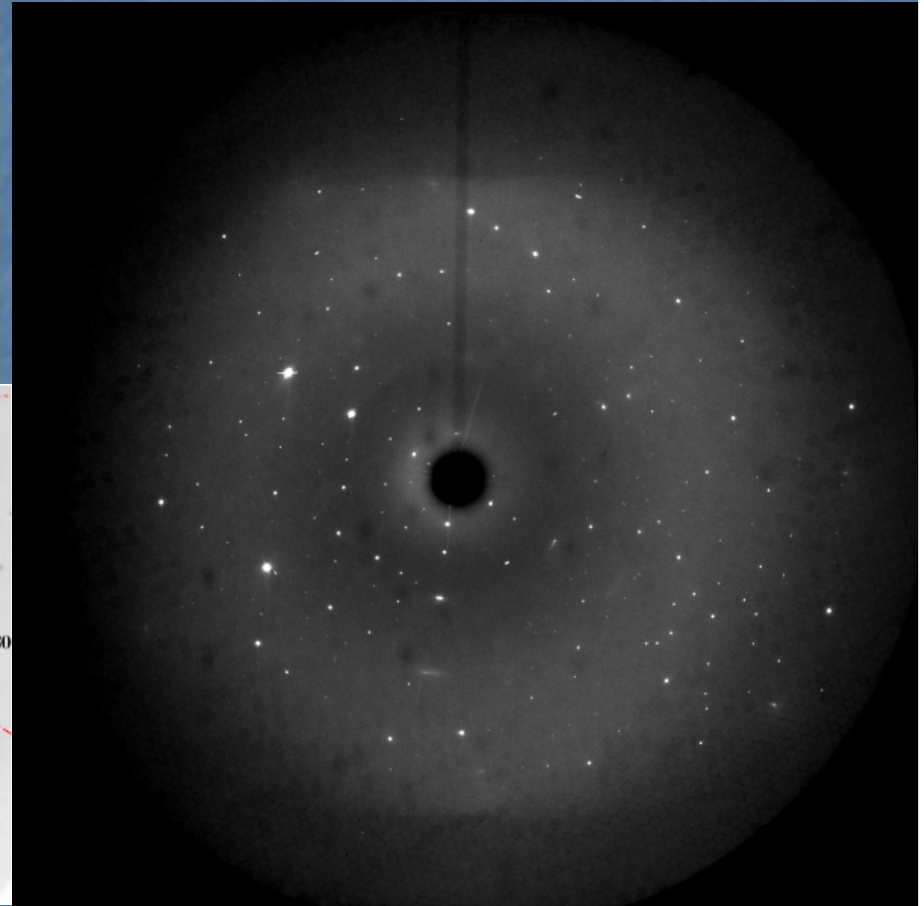
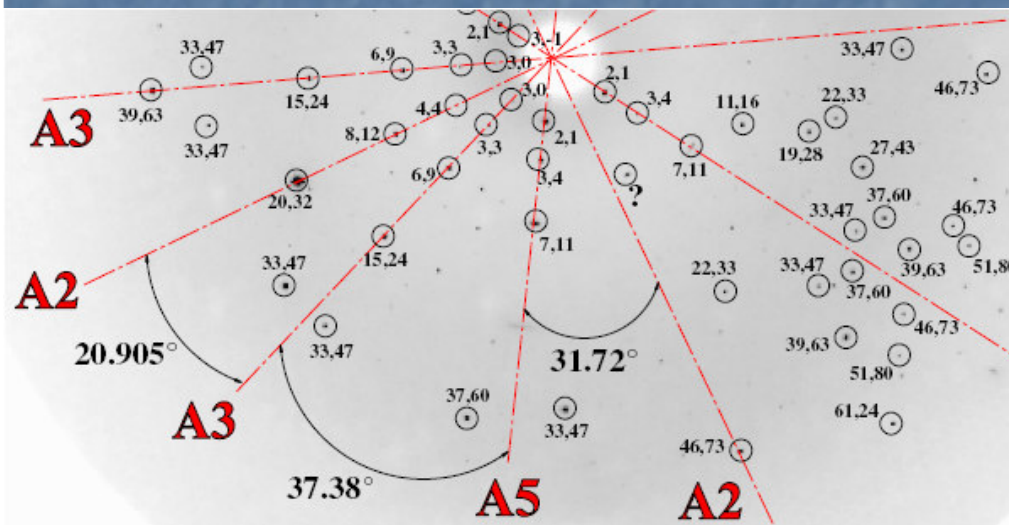
Langatate $\text{La}_3\text{Ga}_5(\text{Ga}_{.5},\text{Ta}_{.5})\text{O}_{14}$

- ✓ Paramètres insuffisants
- ✓ correction d'intensité
- ✓ correction d'ombrage
- ✓ ...

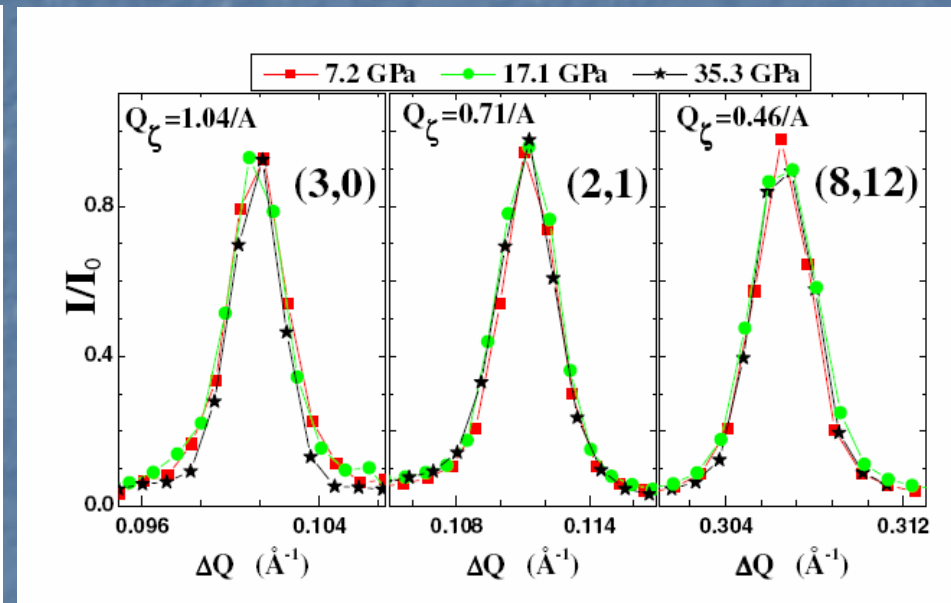
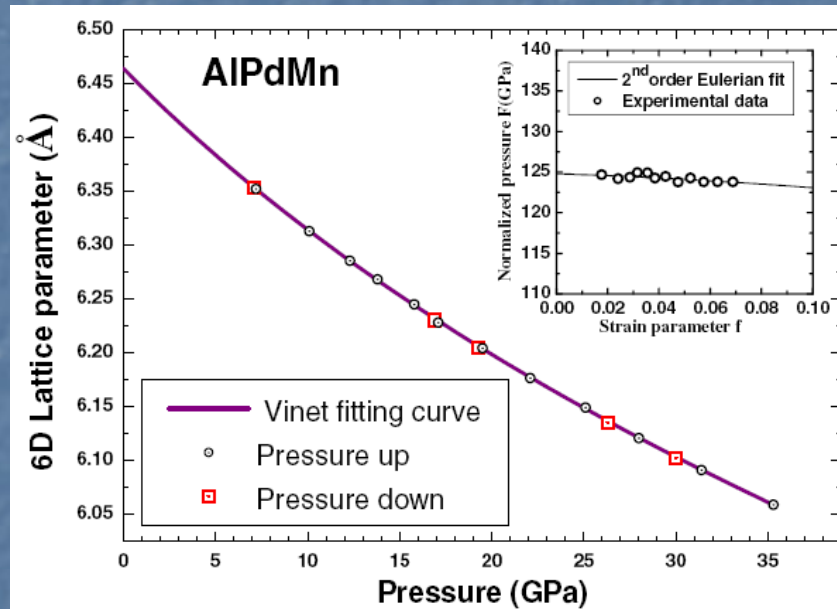


Quasicristaux (i_AlPdMn)

- ✓ Stabilité
- ✓ Amorphisation
- ✓ changement d'entropie...



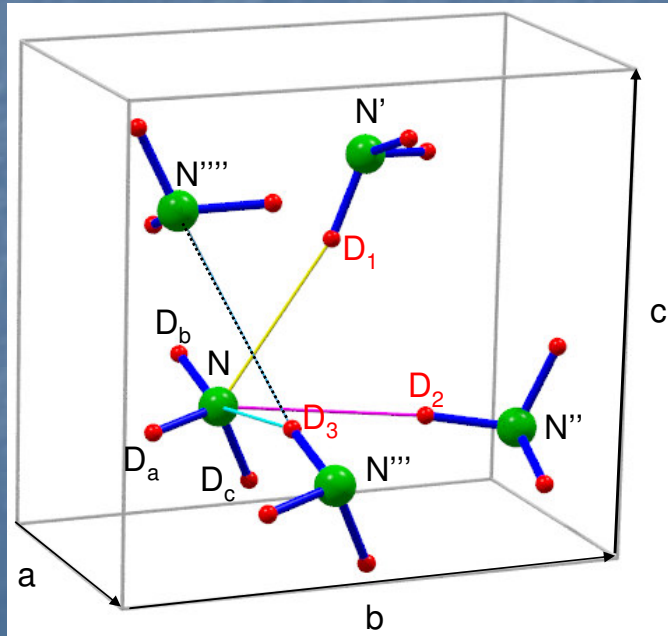
Quasicristaux (i_AIPdMn)



Parfaitement stable

Liaison hydrogène : NH₃

- ✓ symétrisation liaison Hydrogène
- ✓ perte du caractère moléculaire
- ✓ règles de la glace
- ✓ phase superionique



NH₃-IV

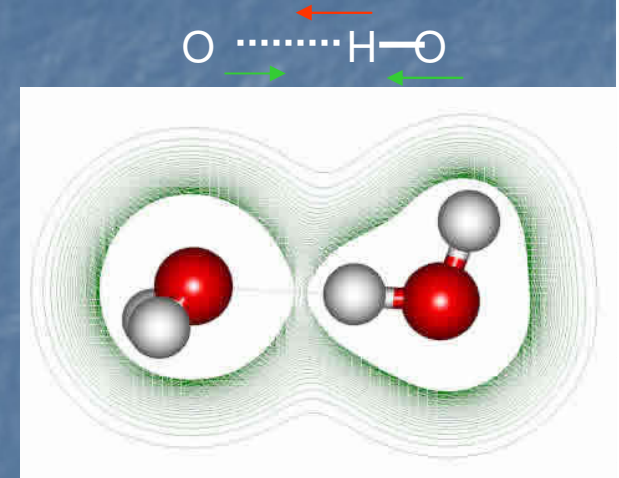
Orthorhombique P212121

Réseau N quasi HCP

Liaisons H "distordues":

longueurs(2.196-2.338 Å)

angles (149°-172°)



Liaison hydrogène : NH_3

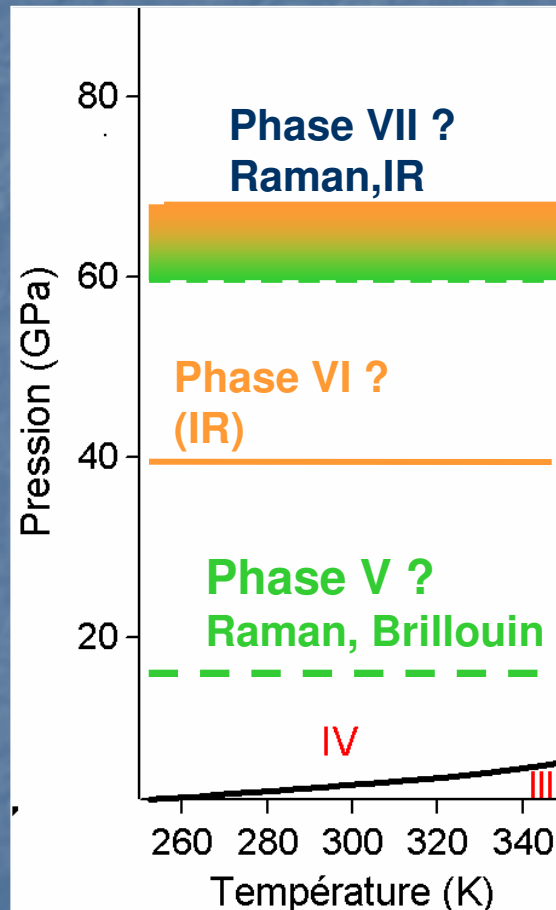
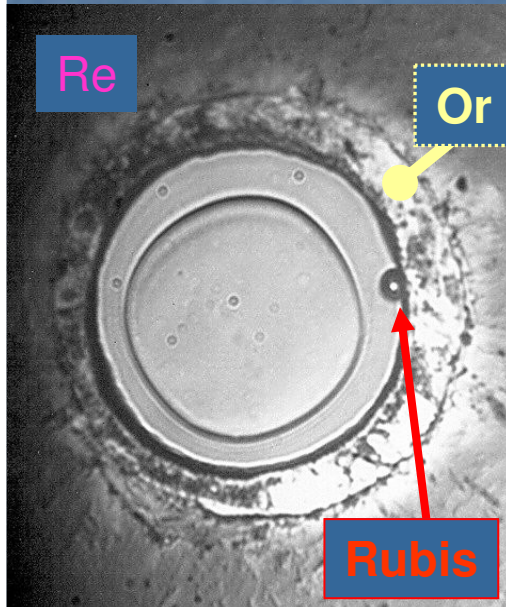


Diagramme de phase très controversé...

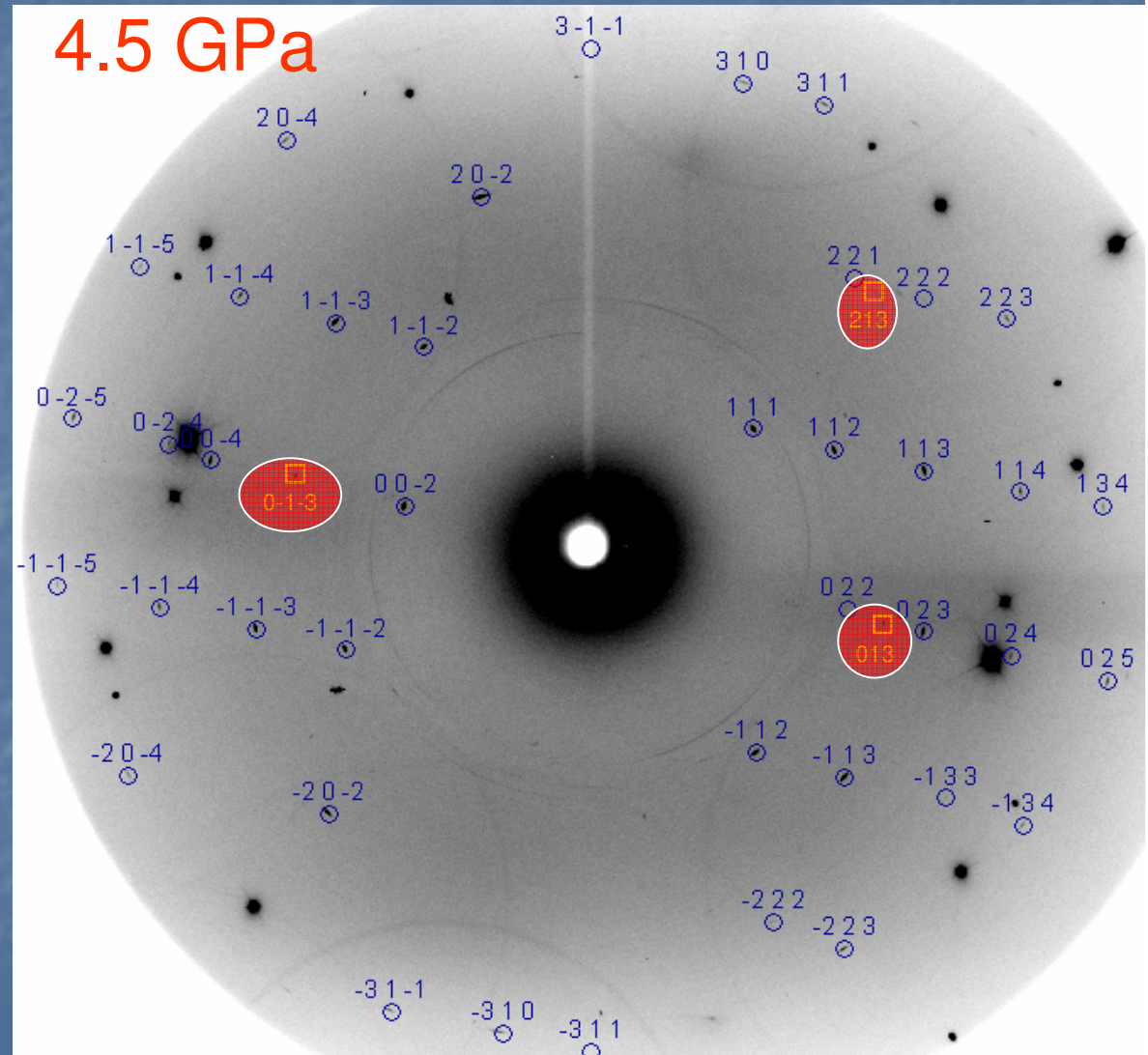
- ✓ Peux t-on confirmer la structure de la phase IV ?
- ✓ Y-a-t-il vraiment des nouvelles phases au dessus de 4 GPa ?
- ✓ Y-a-t-il symmétrisation des liaisons hydrogène ?
- ✓ Si oui, comment ?

Liaison hydrogène : NH₃

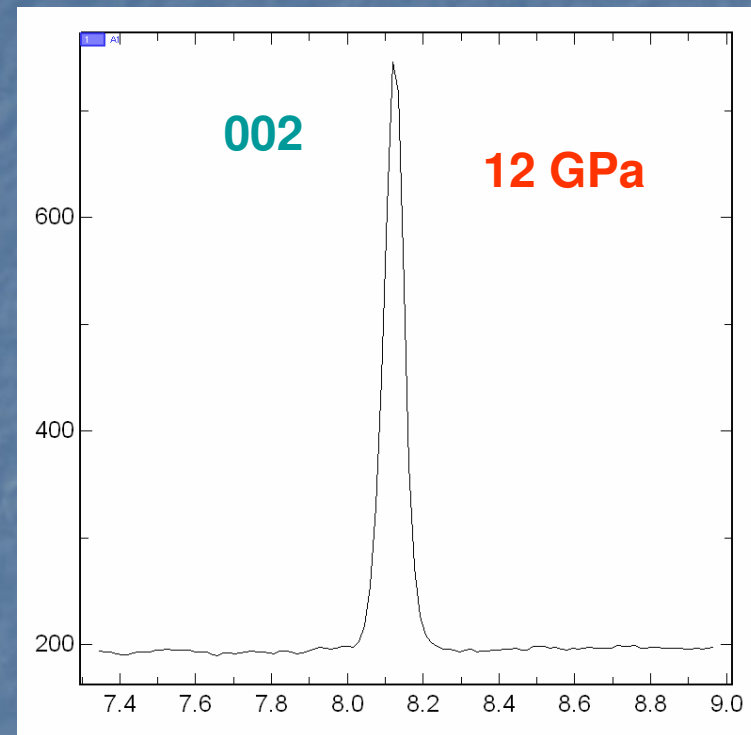
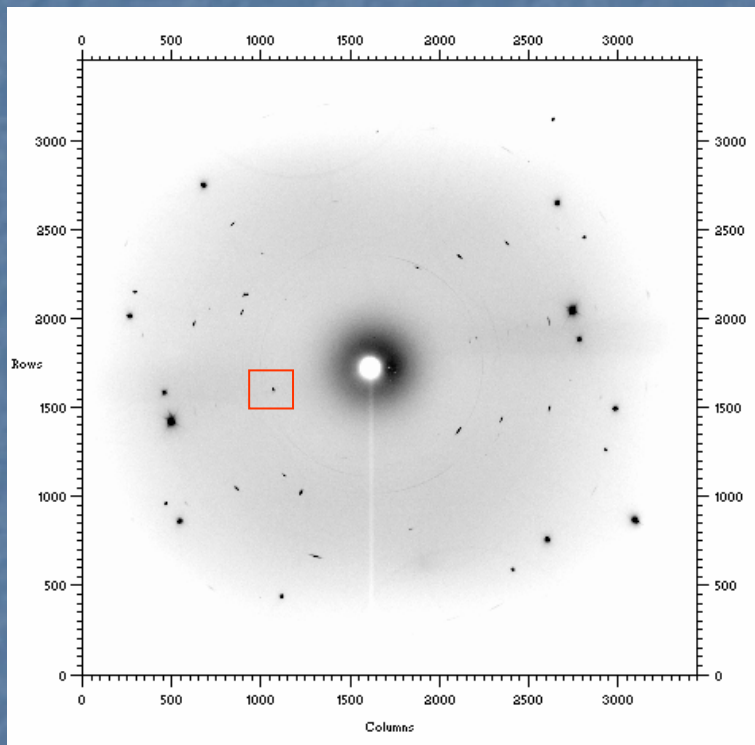


équilibre fluide/solide III
(1 GPa, 295K)

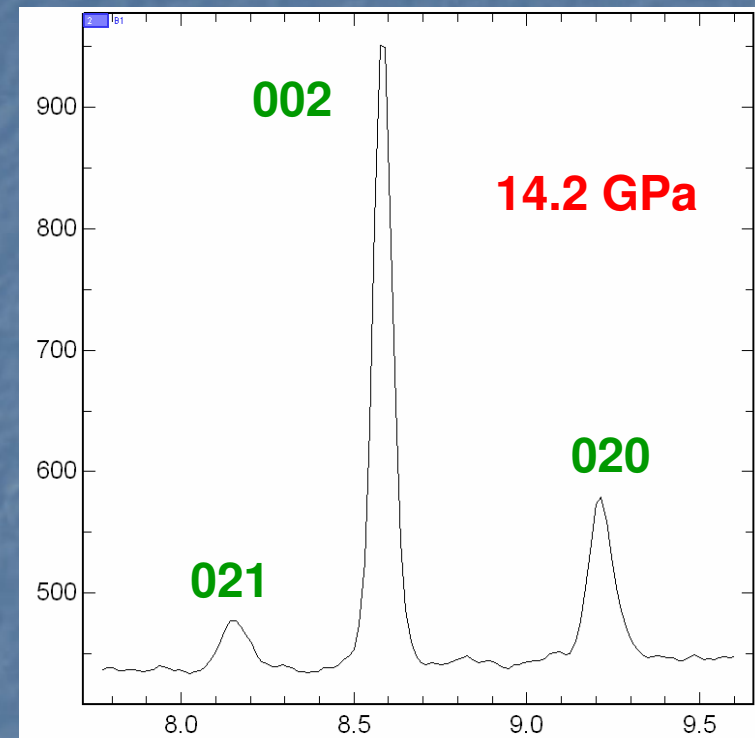
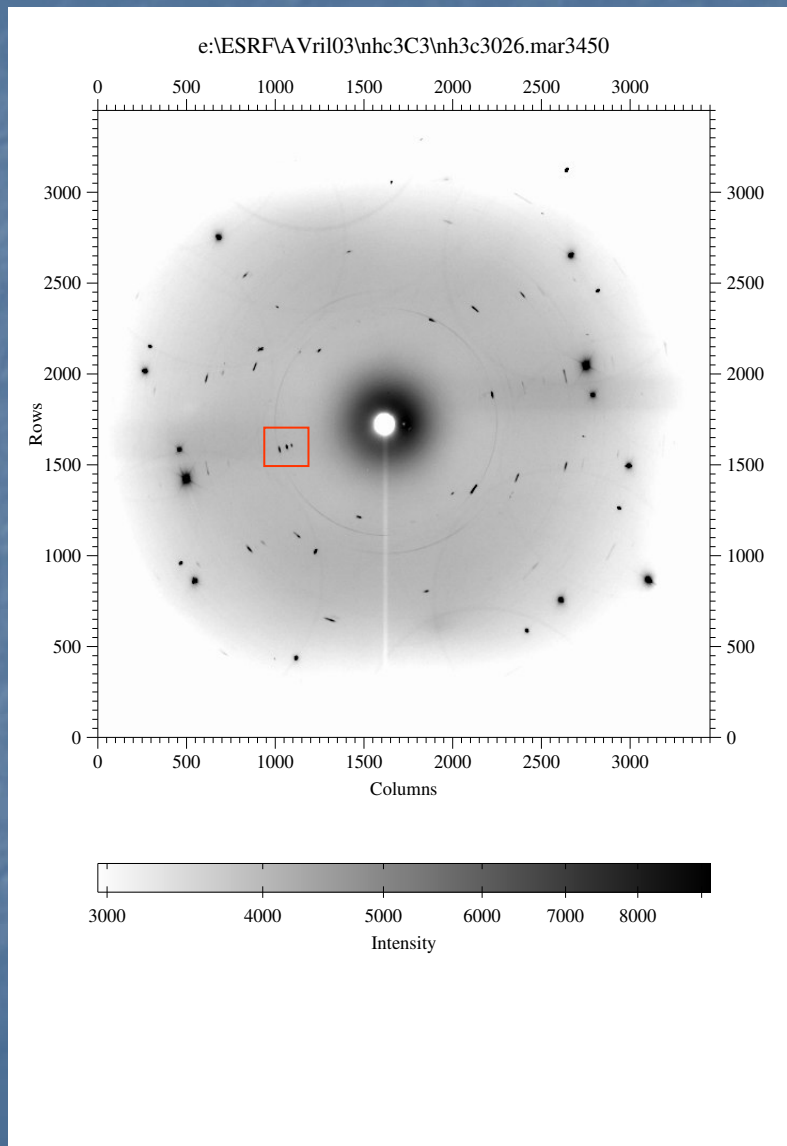
Structure identique à
celle de ND₃ (Loveday et al.)



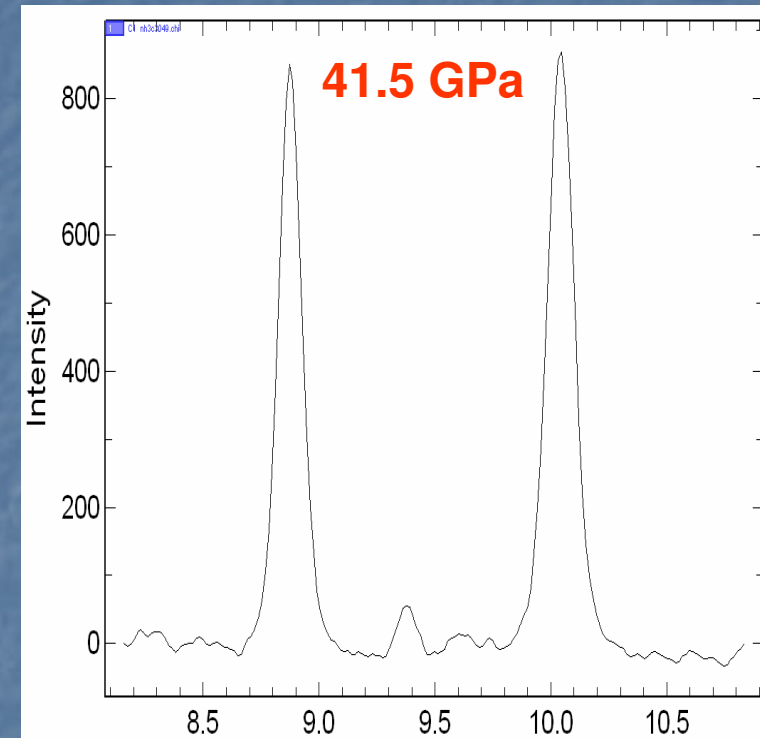
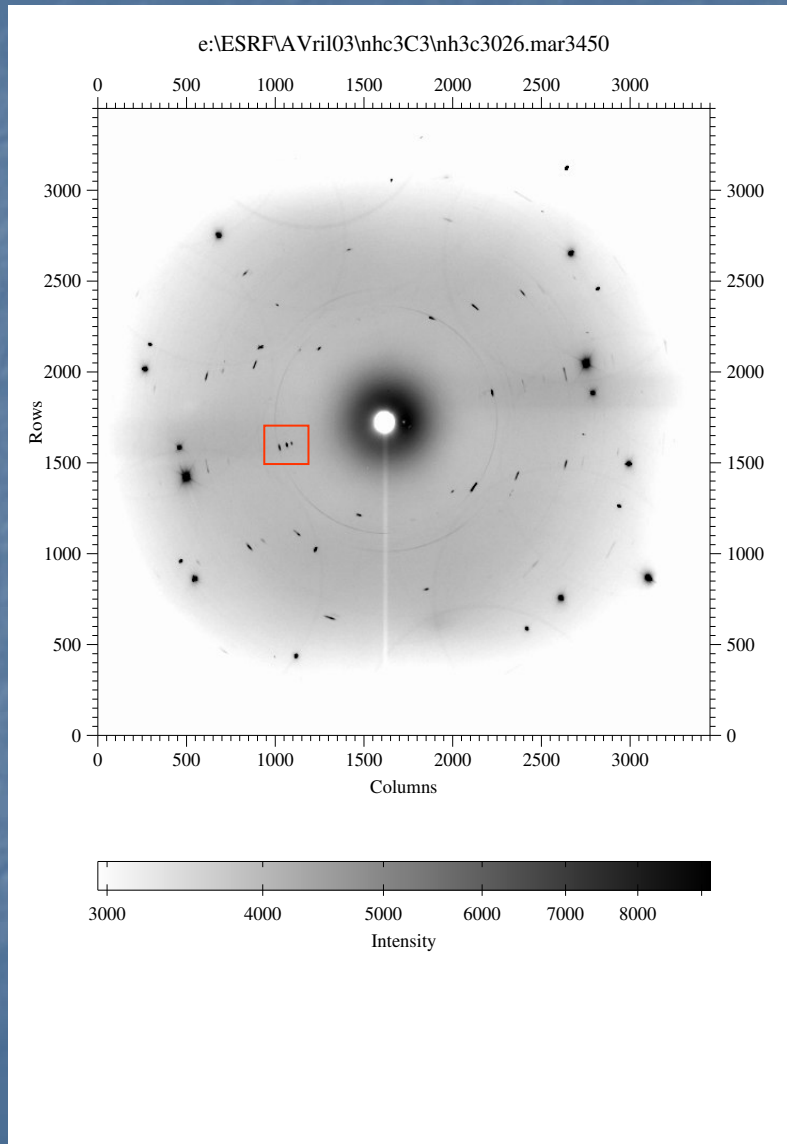
Liaison hydrogène : NH₃



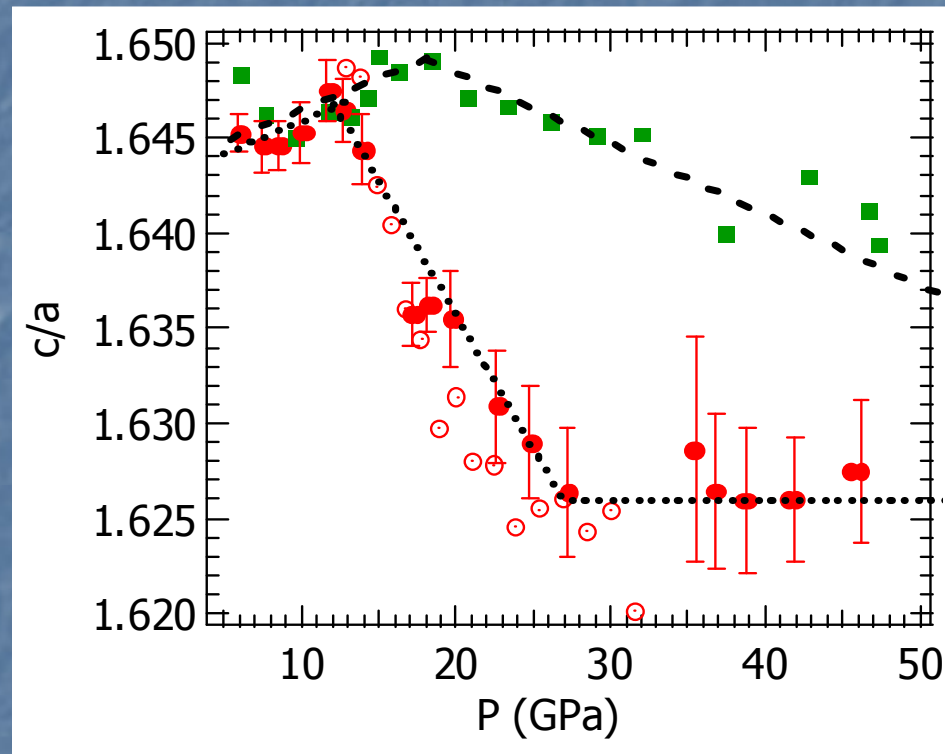
Liaison hydrogène : NH₃



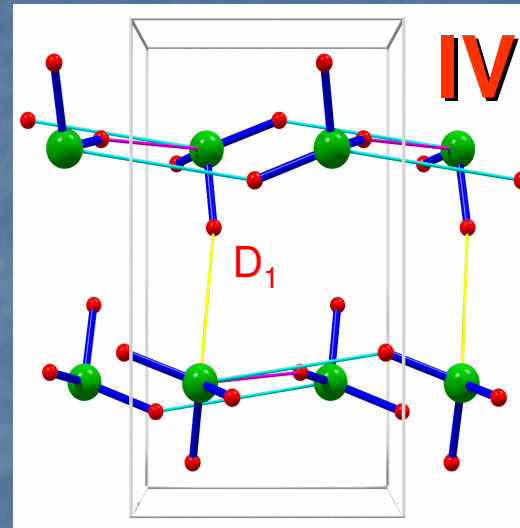
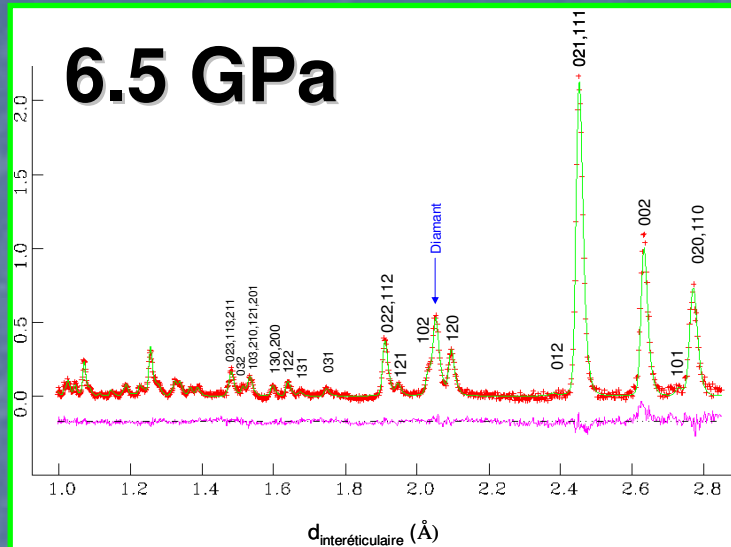
Liaison hydrogène : NH₃



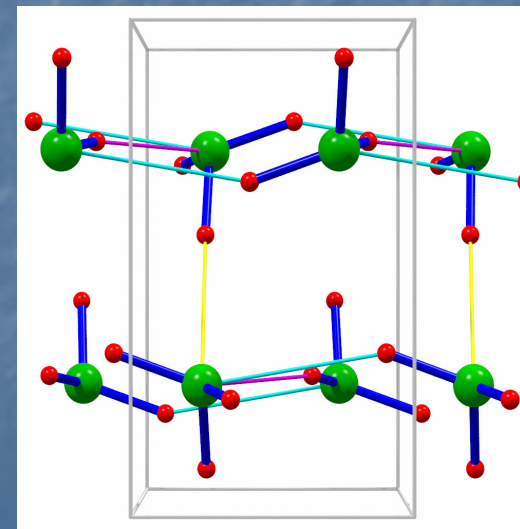
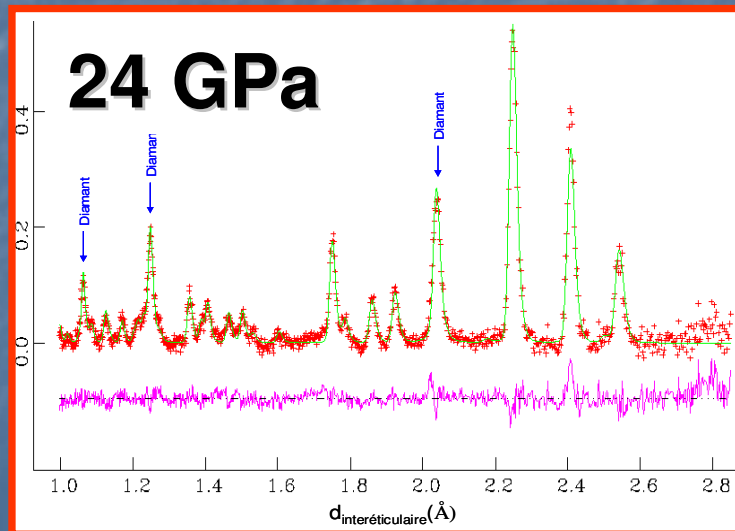
Liaison hydrogène : NH₃



Liaison hydrogène : NH₃

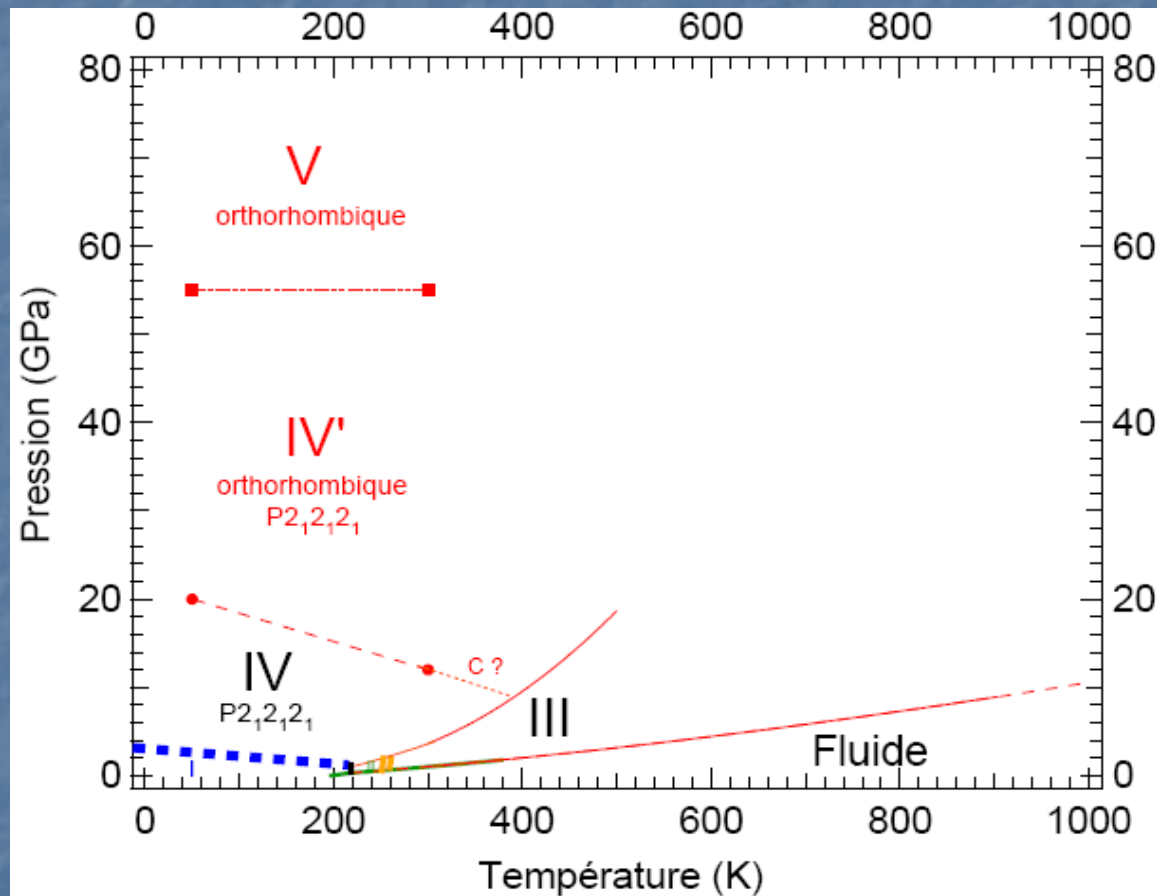


Structure identique à celle de Loveday et al.



Quasi-linéarisation de N-D₁...N à 24 GPa

Liaison hydrogène : NH_3



Conclusions

- ✓ Indispensable (contraintes, statistique, intensité, ...)
- ✓ Performant (manips simples, temps,...)
- ✓ Fiable (EOS, symétrie NH₃ par exemple,...)
- ✓ Extraction des positions atomiques : Pb en cours
- ✓ Offre software sur les grands instruments....
- ✓ ...

Collaborations - Remerciements

- ✓ F. Datchi, F. Decremps, S. Ninet, A. Polian,...(IMPMC).
- ✓ J. Loveday, R. Nelmes,... (ISIS)
- ✓ J.P.Itié (LURE)
- ✓ M. Hanfland, D. Hauserman, M. Mezouar, W. Crichton,... (ESRF, Id09 ,Id27, Id30)
- ✓ E. Iakovenko, (IHPPT, Troïtsk) ...