Beamline X14A

Camden R. Hubbard, PRT Spokesperson
Metals and Ceramics Division, ORNL

Jianming Bai, Beamline Scientist
University of Tennessee

31 January 2005

Outline

- **X14A PRT Operations**
  - **Members**
  - **Research focus**
  - **Financial and management**
- **Beamline status and upgrades**
- **Examples of research**
- **Metrics**
  - **User statistics**
  - **Publications**
- **Safety**
- **Issues and Vision**
- **Summary**

Current X14A Beamline PRT Members

- **PRT Spokesperson**
  - **C. R. Hubbard (ORNL-M&C)**
- **PRT Local Contact/Beamline Scientist**
  - **J. Bai - Local contact (Univ. of Tennessee)**
- **PRT Members**
  - **J. Biernacki (Tennessee Tech Univ. - New PRT member 2004)**
  - **T.R. Watkins (ORNL-M&C)**
  - **E.A. Payzant (ORNL-M&C)**
  - **C.J. Rawn (ORNL-M&C & Univ. of Tennessee)**
- **PRT Collaborators/Frequent General Users**
  - **P. Dutta (Northwestern)**
  - **S. Moss (U. of Houston)**
  - **T. Tyson (NJIT)**

X14A continues to be a productive beamline for materials science and x-ray scattering

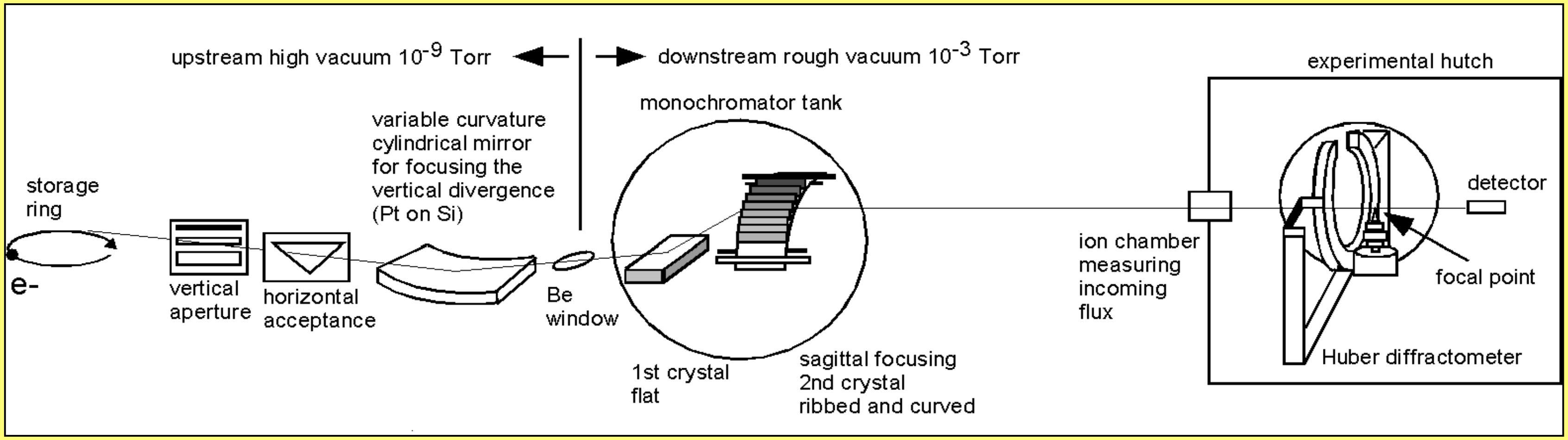
- Historically, basic science research
  - Beamline device development
  - Reciprocal space mapping (alloy ordering, diffuse scattering)
  - Resonant scattering
  - Combined diffraction and spectroscopy methods
- Increasingly adding more materials science
  - Powder diffraction (*in situ*, phase equilibria, kinetics, QXRD, trace phase detection, line broadening analysis)
  - Residual stress (GIXD, curved surfaces, high temp)
  - Crystal structure analysis by Rietveld methods- RT, HT
  - Resonant x-ray reflectometry

Financial and Management Commitments

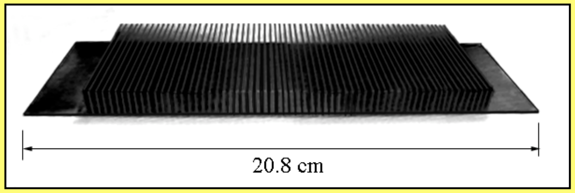
- **Funding**
  - **ORNL/M&C/Diffraction and Themophysical Properties Group**
    - **Crystal Chemistry and Diffraction Programs (ORNL)** **$70K/yr**
    - **Residual Stress Programs (ORNL)** **$50K/yr**
    - **ORNL Indirect funding (ORNL staff time, travel, matls, service)** **> $60K/yr**
  - **Tennessee Technical University**
    - **Concrete and cement research (TTU)** **$20K/yr**
  - ***ORNL programs are primarily funded by DOE-EE-OTT-OFCVT's High Temperature Materials Laboratory User Program and supplemented via a number of other DOE programs led within the Group and the Metals & Ceramics Division***
  - ***TTU's research is sponsored by NSF***
- **Staff**
  - **PRT Spokesperson: Camden R. Hubbard, Group Leader, M&C Div., ORNL**
  - **Beamline scientist: Jianming Bai, U. of Tennessee**
  - **Lab Safety Manager: Thomas R. Watkins, ORNL**
  - **Crystal Chemistry and Diffraction Team Leader: E. Andrew Payzant, ORNL**
- **One additional PRT member desired**
  - **Medium size, regional University? (challenging goal)** **$60K/yr**

Beamline Status

1999 upgrades continue to provide superior optics, excellent flux and improved operation!

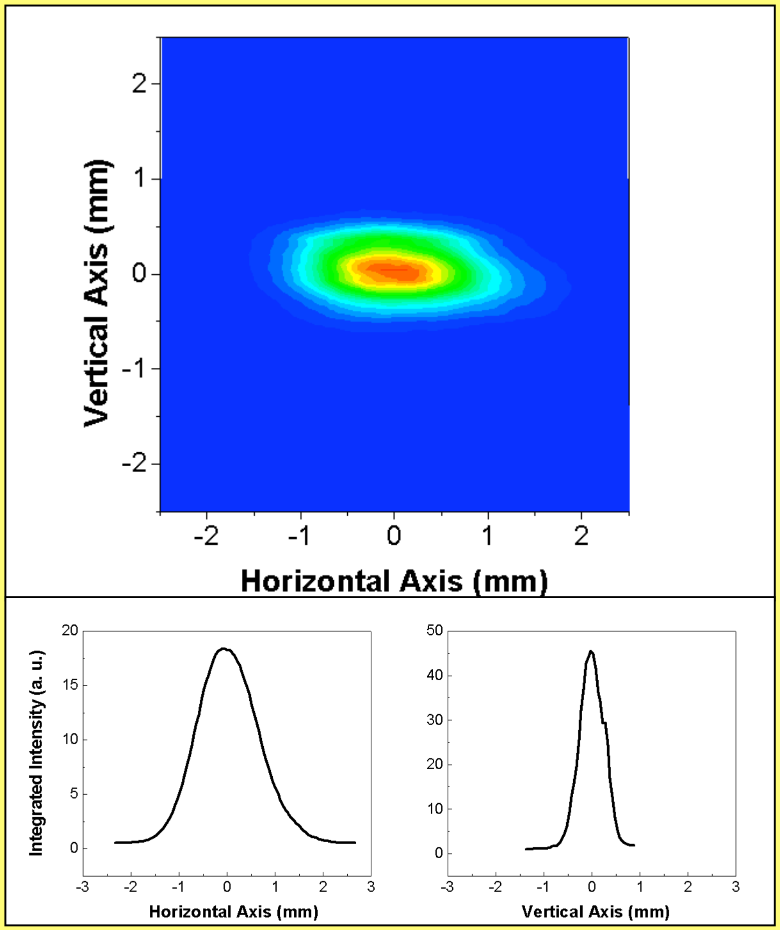


- **High performance grazing incidence mirror**
- **Flat Si (111) monochromator (H_2O cooled)**
- **Sagital focussing Si (111) monochromator**



- **Energy range with mirror 5.5 – 26 keV**
- **Beam divergence V<0.03°, H=0 to 0.6°**
- **Energy resolution with mono. < 3 eV**
- ***Flux approaching NSLS insertion devices***

New optics provides a focused beam ideally suited to wide range of materials studies including in situ powder diffraction



- **Downstream view of focused spot size at 8 keV with 10 mrad horizontal acceptance**
- **The widths (2σ) are 1.24 mm horizontally and 0.52 mm vertically**

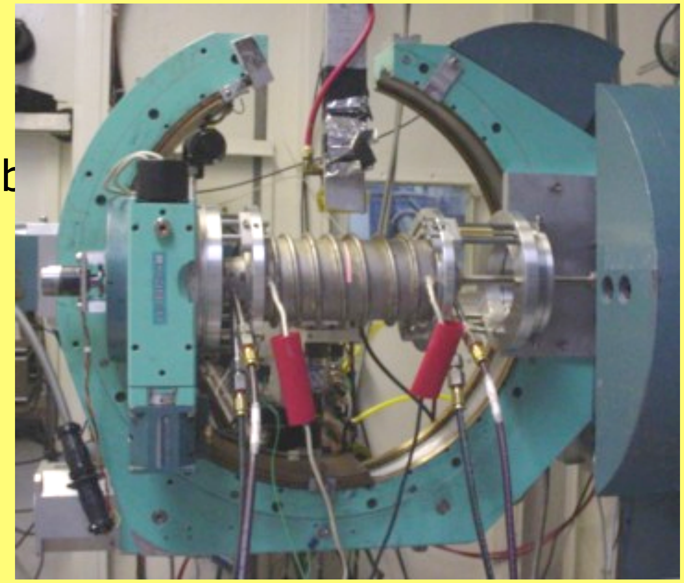
NSLS at 2.8 GeV

X14A's Six-Circle Huber Goniometer and Accessories Provide Excellent Flexibility

Accessories at X14A

- **Capillary furnace (FY01)**
  - Rotating specimen
  - Gas flow option
  - Uniform heating
- **HT Buehler stage**
  - 1500°C in 1 atm
  - ~2400°C in vacuum
- **Be dome hot stage**
  - 700°C in vacuum
- **Displex closed cycle cryostat**
- **Ge & graphite analyzer crystals**
- **Remote collaboration tools**
  http://www.ornl.gov/doe2k/hfir/

2001-2004 Major Additions and Upgrades



- **Capillary furnace added for in situ diffraction**
  - ➢ Designed and built for X14A by Matt Kramer, Ames Lab
  - ➢ Uniformly heats sample up to 1500°C
  - ➢ Gas flow system
  - ➢ Rotating capillary

- **Upgrades**
  - ➢ Software: SPEC, Jade, Shadow, GSAS ...
  - ➢ Database: ICDD-PDF (yearly update)
  - ➢ UNIX Workstation, Motor controller, vacuum pumps, …
  - ➢ Electronic notebook and video presence

- **Development Efforts**
  - ➢ Collaborated with NSLS on Banana Detector
  - ➢ Proposal to DOE (led by P. Stephens)
  - ➢ Speaker at several NSLS Workshops (5/2003, 1/2005)

Selected Examples of Research at X14A

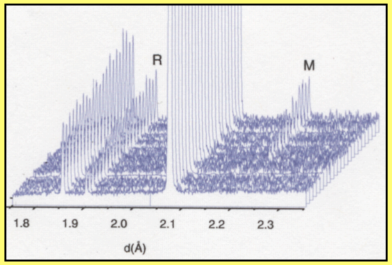
- HT $SrZrO_3$ structure determination
- Crystallite size of Pt catalysts
- Residual stress bond coat at elevated temperature
- GIXD for structure at surfaces
- High resolution x-ray emission - electronic state of Mn
- Reciprocal space mapping - order parameters
- Resonant x-ray scattering to characterize liquid crystal layers
- In situ diffraction of organic-template-directed nucleation

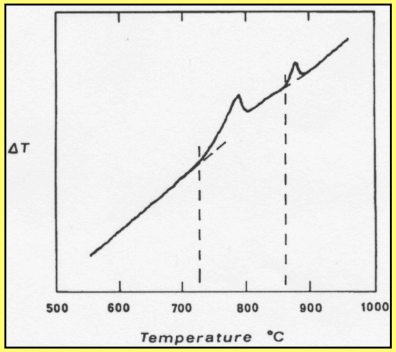
The Transition Path of $SrZrO_3$

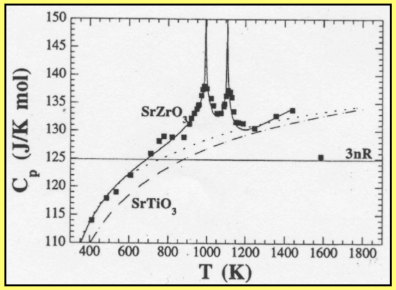
S. Speakman, E.A. Payzant, & J. Bai (ORNL, UT)

- The phase transitions of $SrZrO_3$ have been studied by:
  - High-temperature X-ray and neutron diffraction
    - Carlsson, 1967; Ahtee et al. 1978; de Ligny and Richet, 1996; Kennedy et al., 1999; Howard et al., 2000; Payzant et al., 2000
  - Differential thermal analysis (Carlsson, 1967)
  - Drop calorimetry (de Ligny and Richet, 1996)
- There are four distinct phases:

Phase	T_C (°C) by de Ligny and Richet	Reported T_C's (°C)
Orthorhombic Pnma		
Orthorhombic Cmcm or (metrically tetragonal) Imma	727±5	700 to 750
Tetragonal I4/mcm	832±5	747 to 860
Cubic Pm3m	1167±25	1070 to 1170



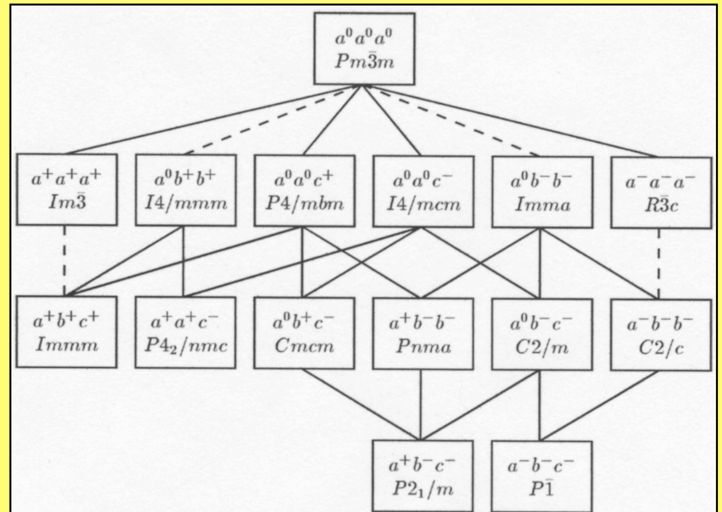


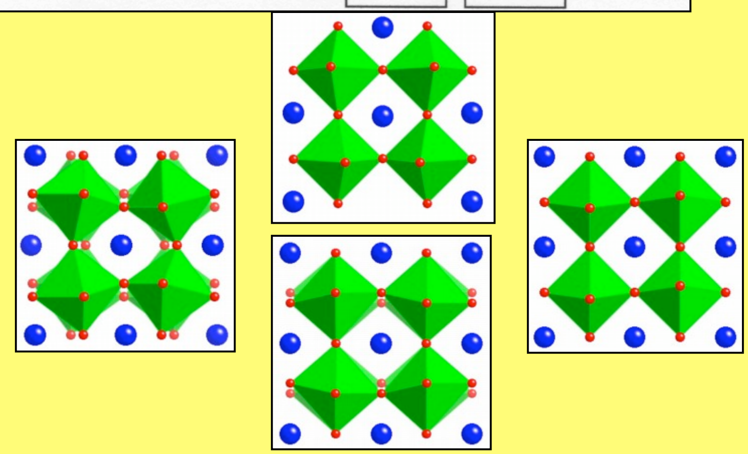


Howard et al. recently proposed a revised transition path for $SrZrO_3$

- **Revised transition path based on:**
  - ➢ **neutron powder diffraction at HRPD (ISIS)**
  - ➢ **group theory analysis (Howard and Stokes)**

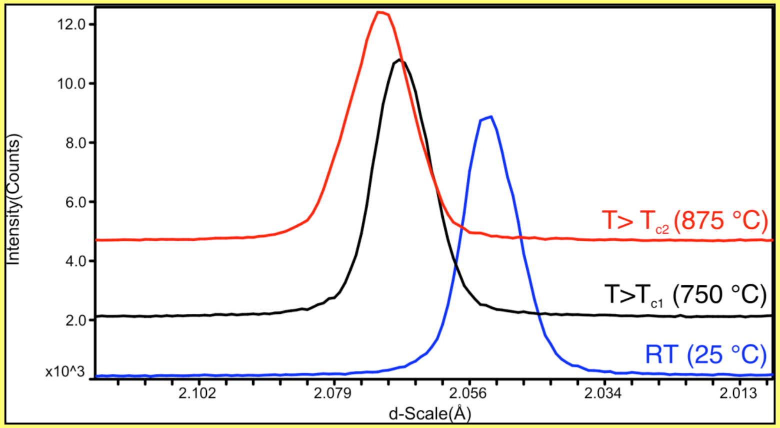
- **Comparison between the two paths**
  - ➢ **old path: Pnma⇒Cmcm⇒I4/mcm⇒Pm3m**
  - ➢ **new path: Pnma⇒Imma⇒I4/mcm⇒Pm3m**
    - **old path: $a^+b^-b^- \Rightarrow a^ob^+c^- \Rightarrow a^oa^oc^- \Rightarrow a^oa^oa^o$**
    - **new path: $a^+b^-b^- \Rightarrow a^ob^-b^- \Rightarrow a^oa^oc^- \Rightarrow a^oa^oa^o$**
    - **In the old path, the first and second transitions are discontinuous**
    - **In the new transition path, the first transformation is continuous**
    - **Howard constrained the Imma unit cell to have a=c (???)**

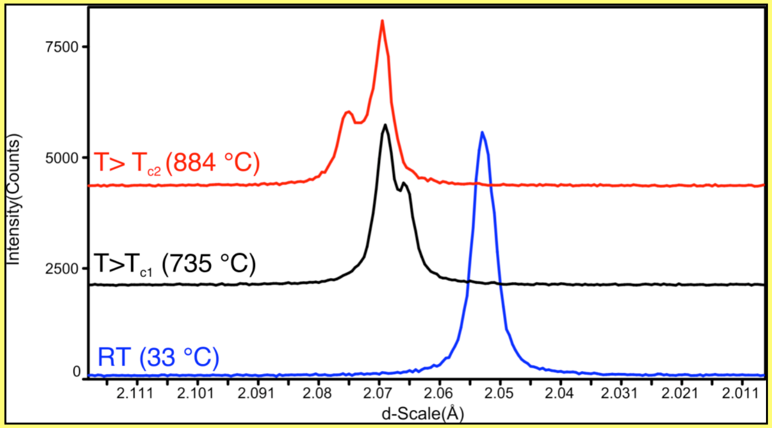




High-resolution in-situ synchrotron data from X14A resolve ambiguities in in-situ laboratory XRD data

- **With in-situ laboratory X-ray data a number of peaks can not be resolved**
  - **For example, the {220} and {004} (below, left)**
  - **This ambiguity leads to multiple erroneous indexing solutions**
- **With in-situ synchrotron data many overlaped peaks are resolved (below, right)**
  - **Structural variations not visible with laboratory facilities become observable with SXRD**

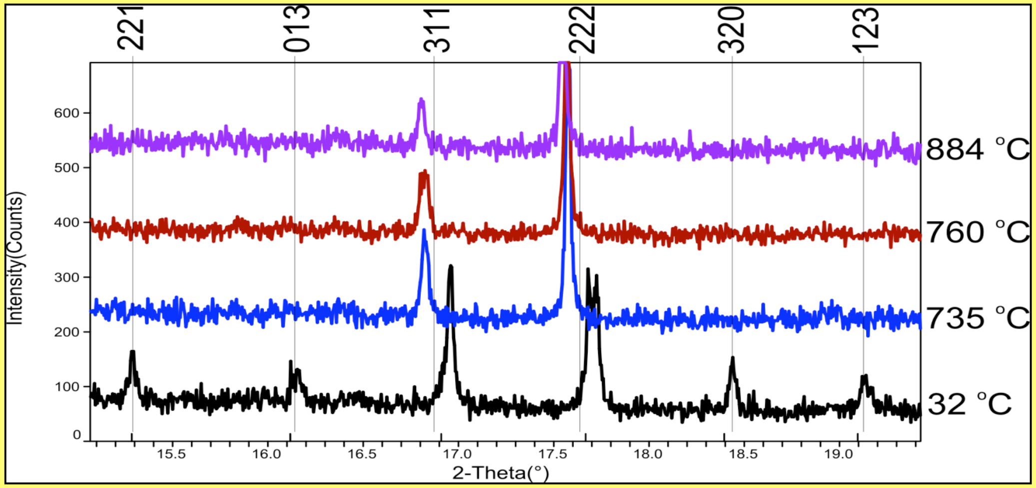




Three phases of $SrZrO_3$ observed with laboratory X-ray data (left) and synchrotron data (right)

Superlattice reflections in X14A diffraction patterns differentiate between in-phase and antiphase octahedral tilting

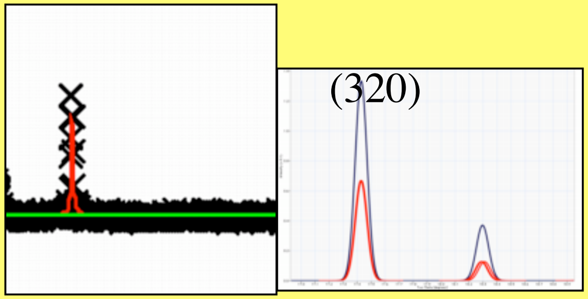
- **Superlattice peaks were indexed using a doubled cubic perovskite cell**
  - **Antiphase tilts produce peaks with all odd Miller indices.**
  - **In-phase tilts produce peaks with two odd and one even Miller indices**
- **At all temperatures (32, 735, 760, and 884 °C) antiphase tilts are present**
  - **At 32 °C, in-phase tilts are present**
  - **At 735 and 760 °C, *only antiphase tilts are present***
    - **Consistent with the Imma ($a^0b^-b^-$) space group, but not with Cmcm ($a^0b^+c^-$)**
    - **Consistent with the neutron diffraction data of Howard et al.**



Computer simulation in the Imma space group confirms assignment of Space Group

- **Empirical potential models used to simulate the $SrZrO_3$ crystal structures**
  - **GULP code of J. Gale, Imperial College**

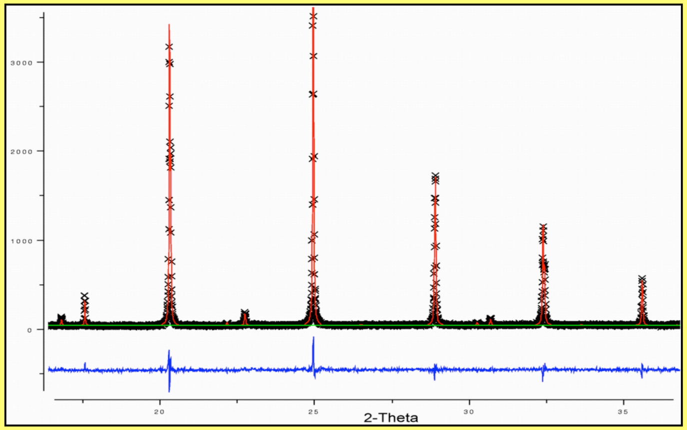
- **Simulation of the Imma crystal structure of $SrZrO_3$**
  - **Produces an a/c ratio of 1.00012**
  - **Compares favorably with the a/c value of 1.0002 from Rietveld refinement**
  - **The ratio a/c is very nearly unity because of balancing interatomic forces**
  - **The unit cell parameters are nearly equal because of nearly equivalent interatomic forces in those directions**
  - **Simulation of the Cmcm space group shows that the intensity of peaks from in-phase tilting are not negligible**



Comparison of calculated diffraction patterns from computer simulation results. On the left is experimental data (black) and the calculated pattern for Imma (red). On the right is the calculated pattern for Cmcm- note the relatively strong (320) peak that is not observed in the experimental data.

Refinement of the Crystal Structure of $SrZrO_3$ at 735 °C in the Imma Space Group is Good

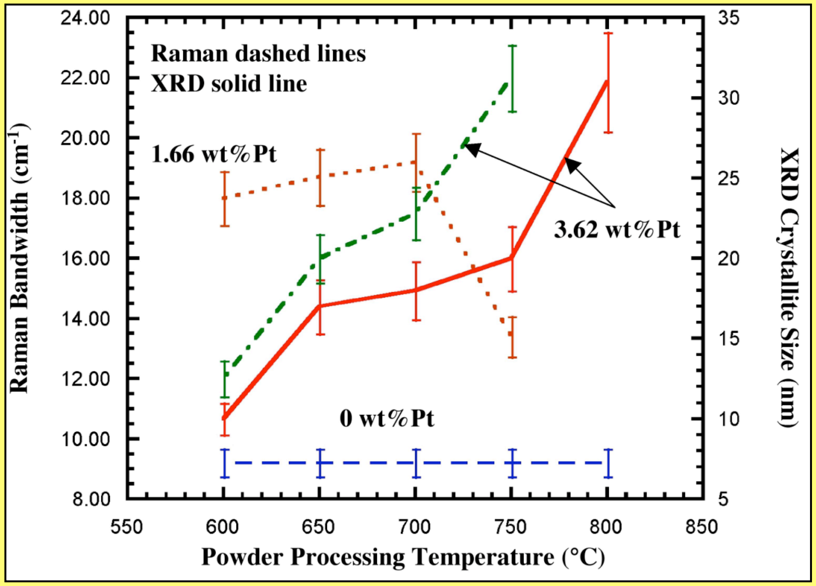
- **Rietveld refinement of the diffraction pattern collected at 735 °C in Imma**
  - ➢ LP's 5.8536(2) x 8.26292(6) x 5.8525(2) Å
  - ➢ X^2 = 1.63, wRp = 14.65%
  - ➢ Not metrically tetragonal (a/c = 1.0002)
  - ➢ Peak profile and lattice parameters are correlated

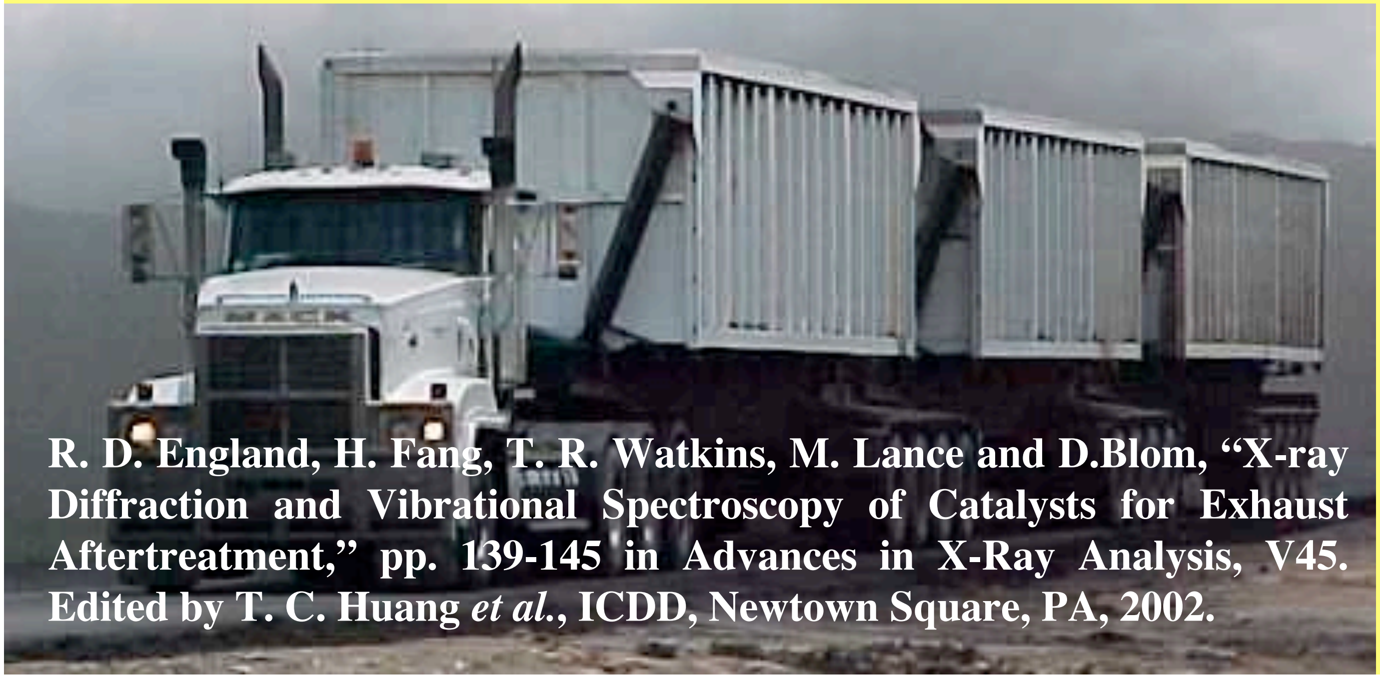


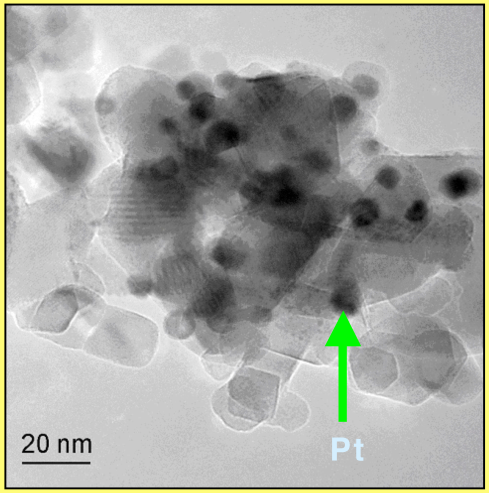
- **Refinement in the Cmcm space group**
  - ➢ X^2 = 1.62 , wRp = 14.59%, ~ equivalent fit
  - ➢ Oxygen atoms move to positions close to those in Imma
- **No other space group (R3c, etc.) satisfactorily describes the diffraction data**

Catalyst Size Characterization - T.R. Watkins (ORNL)

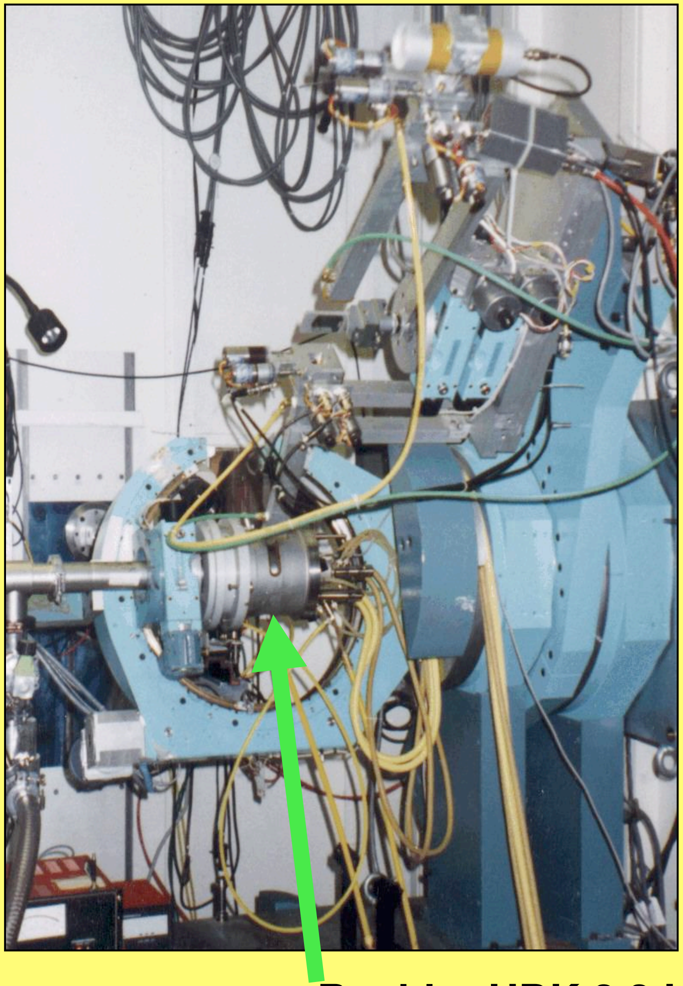
- **Project Goal: To meet 2007 diesel engine emission requirements**
- **Catalytic activity decreases with surface area ⇒ Platinum (Pt) particle size increases**
- **Use X-ray diffraction & TEM techniques to calibrate Raman to track Pt size change**
- **Collaboration: HTML/ORNL & Cummins Engine**







Parallel Beam Optics for Residual Stress Studies
T.R. Watkins (ORNL)

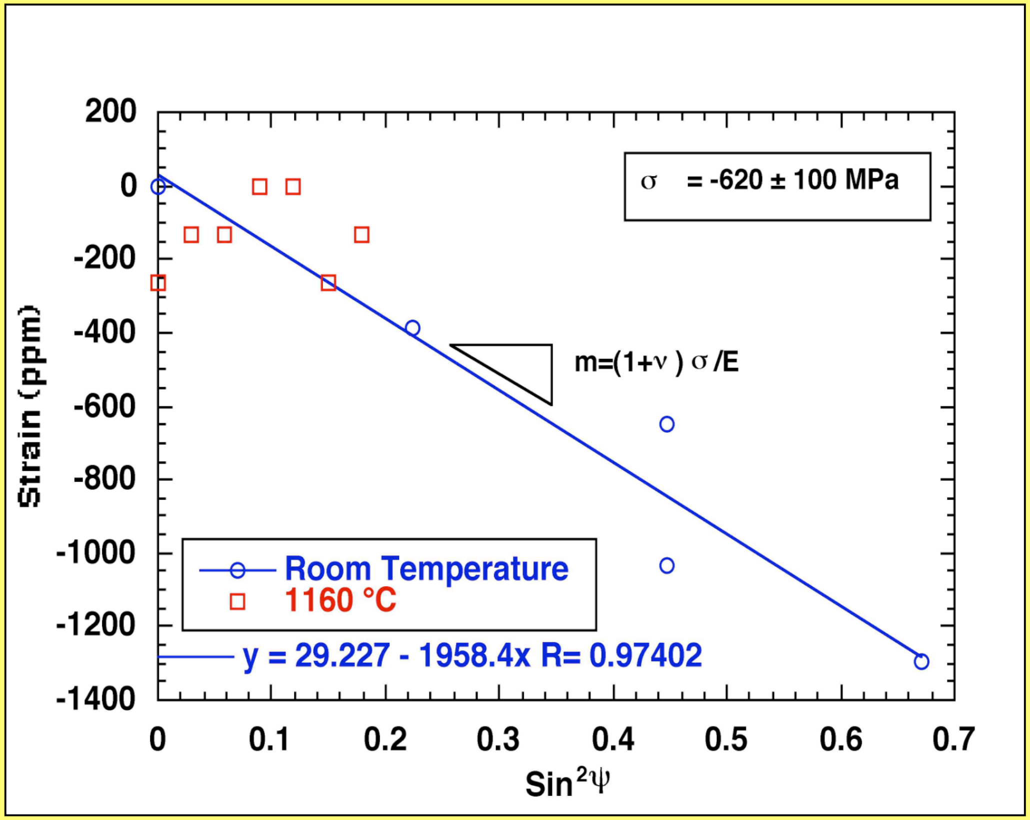


Buehler HDK 2.3 HT stage on X14A

- **Significantly improves the quality of residual stress data by dramatically reducing the sample surface displacement effect on peak position**
  - **Increases confidence in data interpretation**
  - **HTXRD stress (CTE shift eliminated)**
  - **Invaluable for curved surfaces**
- **Example: Thermal barrier coatings (TBCs)**
  - **Prolong the life of metallic components**
  - **TBC failure: spallation of the top coat due to oxide scale growth at the bond coat/top coat interface**
  - **Understanding the residual stresses of the oxide scale growth is critical to enhancing the performance and reliability of TBC systems.**

In-situ Oxidation of Bare Bond Coat

little residual strain present in oxide coating at 1160°C



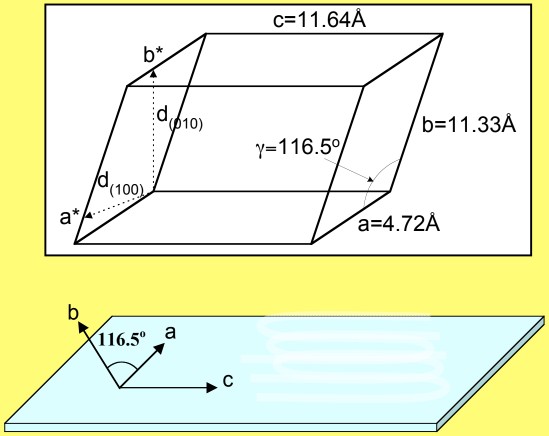
- **X14A synchrotron radiation (λ=1.537 Å)**
- **(300) Al_2O_3, ~67.9°2Θ**
- **HT residual stress similar to others***
- **RT stress is 1/3 in magnitude to those reported due to partial spallation or cracking¥**

* M. Groß et al., Adv. X-Ray Anal., V. 42
¥C. Sarioglu et al., Oxidation of Metals, 1997

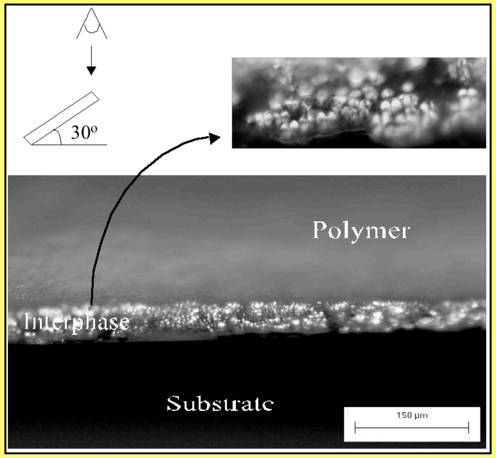
Publication: T. R. Watkins, O. B. Cavin, J. Bai and J. A. Chediak, "Residual Stress Determinations Using Parallel Beam Optics," pp. 119-129 in Advances in X-Ray Analysis, Vol. 46. Edited by T. C. Huang *et al.*, ICDD, Newtown Square, PA, 2003.

Grazing Incidence X-ray Diffraction Studies on the Structures of Polyurethane Films and Their Effects on Adhesion to Al Substrates

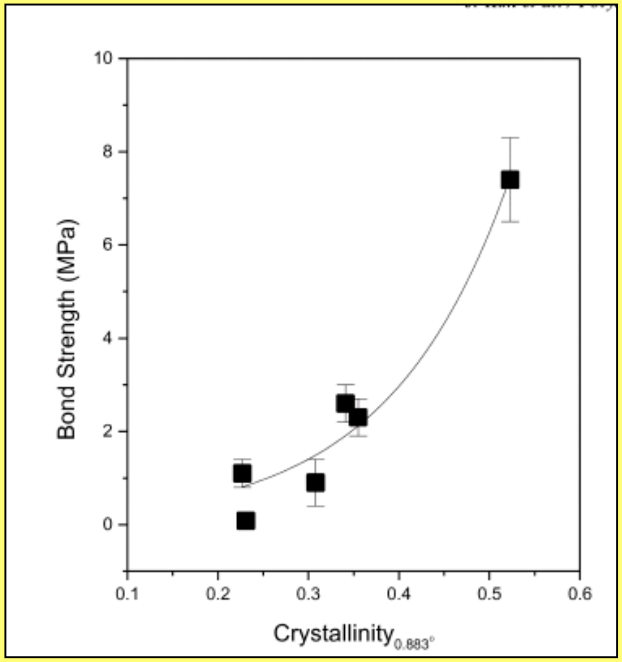
Jangsoon Kim and Earle R. Ryba (The Pennsylvania State University)



Monoclinic unit cell of polyurethane-urea



Optical micrographs of the APU-375



The bond strength of the polyurethane film to the aluminum was found to be exponentially proportional to the crystallinity including the crystalline interphase formed near the substrate. It is also found that the polymer film contained more (100) planes and provided higher bond strength. Aging led to the improvement of bulk crystallinity of all the samples and dramatically increase the bond strength.

Publication: J. Kim et al., Polymer 44 (2003) 6663–6674
Studies of related polymer film adhesion - 3 more publications

Observation of a Strain Induced High-Spin to Low-Spin Transition in Thin Manganite Films

NJIT

Q. Qian, T. A. Tyson (NJIT) , J. Bai (ORNL) and M. DeLeon (NJIT)

In order to understand the observed dramatic reduction in magnetization with decrease in manganite film thickness, high resolution Mn K_b x-ray emission measurements were conducted on films with thickness ranging from 50 to 4000 Å. The high flux available at X14A (10^{12} photons/sec) made this experiments on thin films possible.

This work followed detailed x-ray diffraction studies on a broad range of manganite films. Evidence for strain induced high spin to low spin transition on the Mn sites was found. The resulting violation of the assumed strong Hund's rule coupling on the Mn sites suggest that the existing theoretical models of these correlated systems must be extended.

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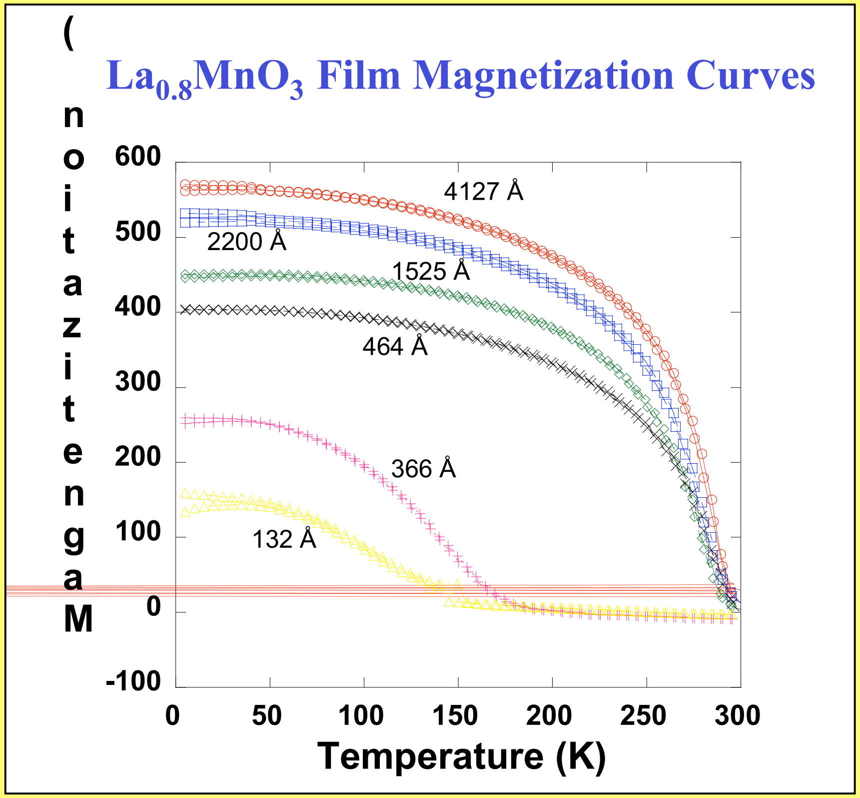

The magnetic moment per moment drops dramatically as the film thickness is reduced. The reduction had been attributed to spin canting or ferromagnetic-antiferromagnetic phase separation.

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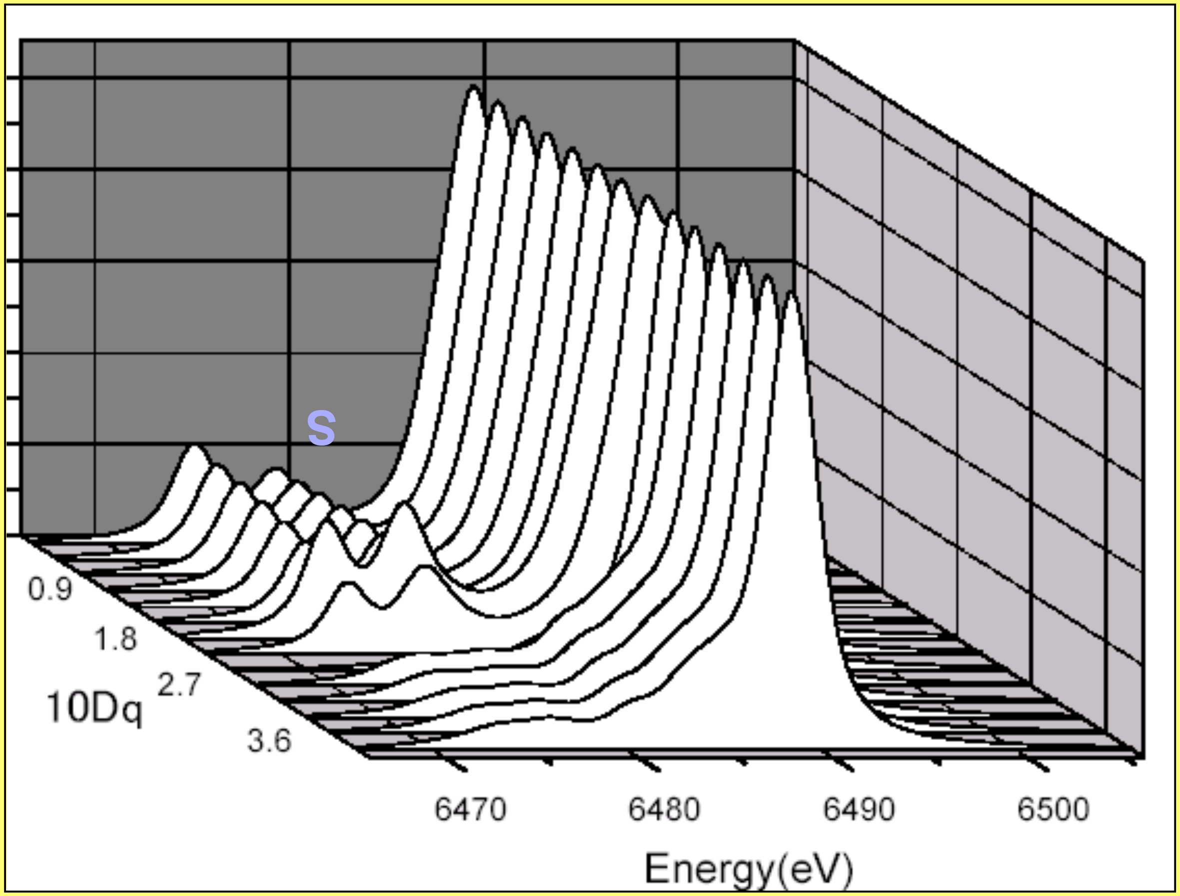
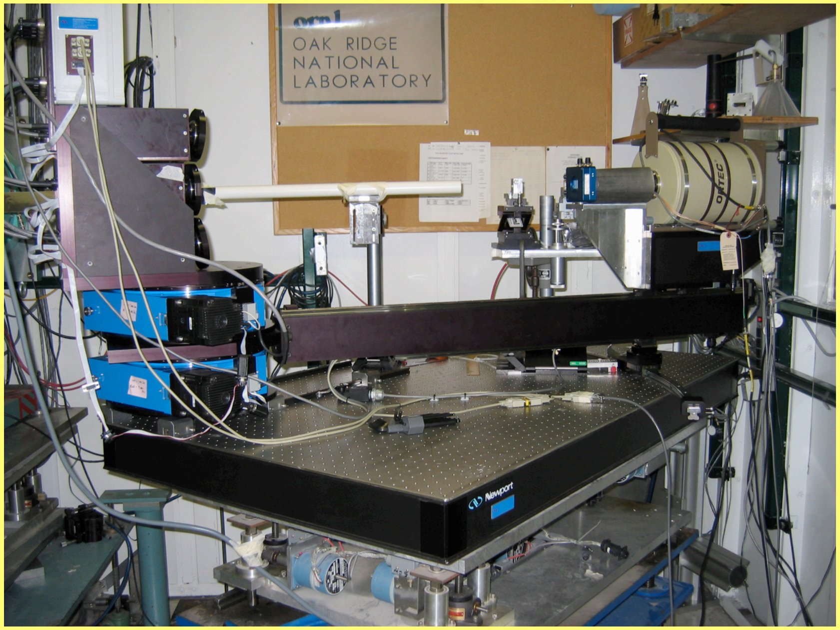
Calculated Mn^{3+} K_β Emission vs. 10Dq

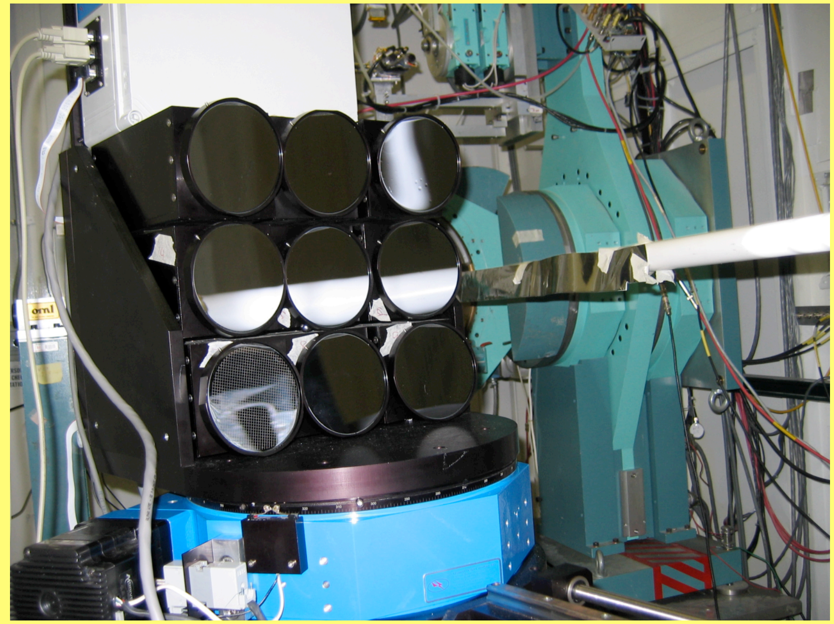


Simulation of Mn^{3+} K_β emission spectrum for varying 10Dq (e_g-t_{2g} splitting). Note the drop in the satellite features (S) for 10Dq above ~2.7 eV signifying the onset of the high-spin to low-spin transition on Mn.

High Resolution X-Ray Spectrometer for Inelastic X-Ray Scattering Set up at X14A

NJIT





A recently developed multi-mirror high-resolution x-ray analyzer system was used to conduct Mn K_β x-ray emission experiments on magnetic oxide films ranging from 52 to 4127Å. On the left we show the full system comprised of a detector, sample support (next to detector) and the nine-element mirror system. The sample, detector and mirrors sit on a Rowland circle. On the right we show a blow-up of the full analyzer array. Each mirror can be adjusted independently in the horizontal and vertical planes with microradian precision. The high flux available at beamline X14A ($\sim 10^{12}$ photons/s in 1 x 1 mm^2) makes possible these low cross-section experiments.

Measured Mn K_β Emission Spectra as a Function of Layer Thickness

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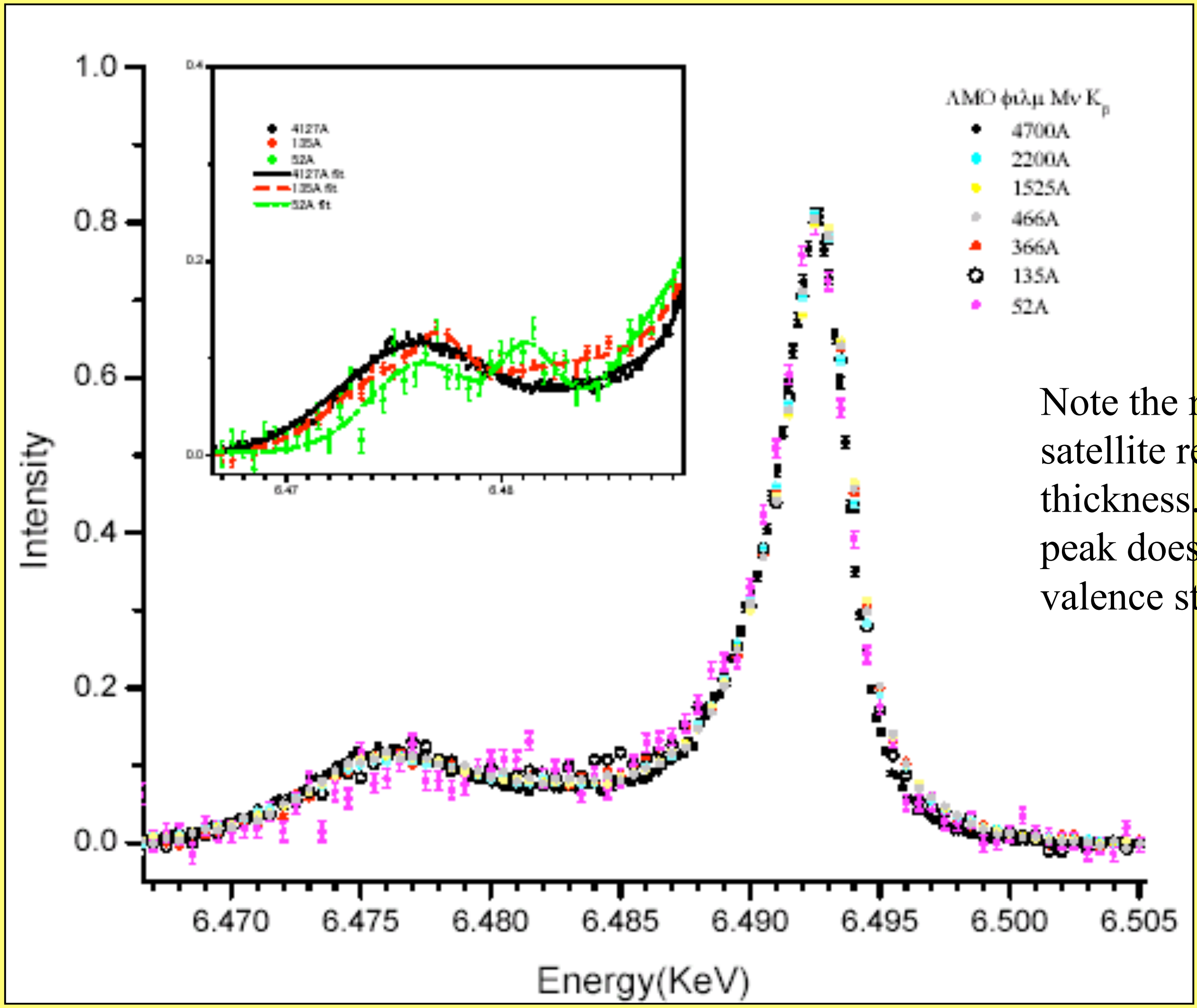

Note the reduction in intensity in the satellite region (inset) with reduced thickness. On the other hand, the main peak does not shift indicating a constant valence state

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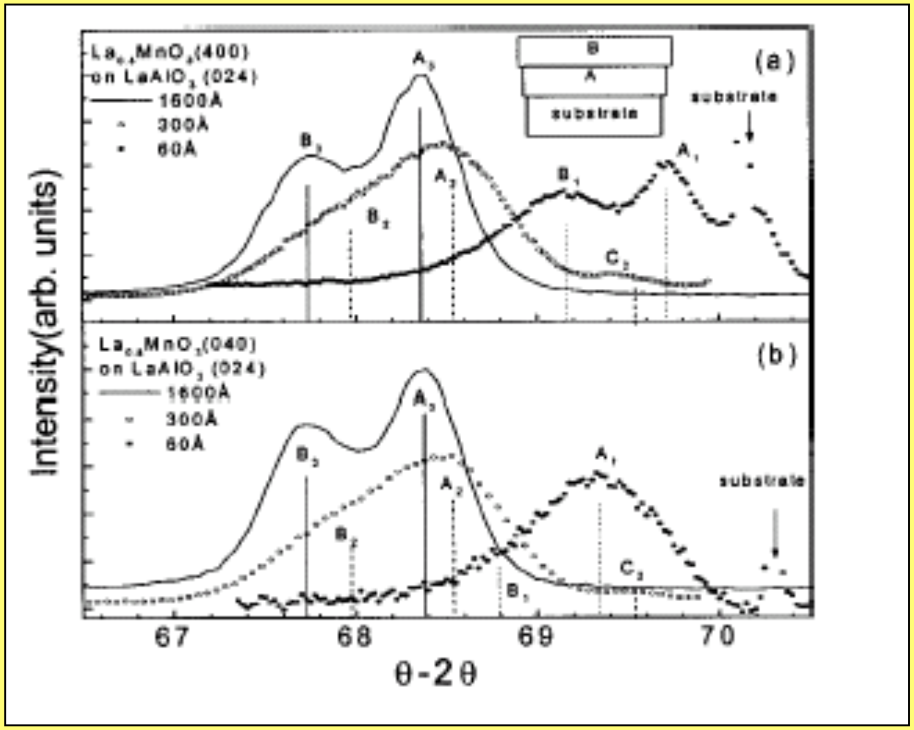
In-Plane XRD Measurements on First Series Films



High Resolution In-plane {(400) and (040)} combined with out-of-plane reflections reveal a heavily strained layer near the substrate and relaxed layers far from the substrate.

NJIT

Summary for Full Range of Films Studied

- Very high strain induced by the substrate results in high-spin to low-spin Mn site transitions in manganite films. (The crystal field energy dominated over the Hund's exchange energy)

- Detailed x-ray diffraction measurements revealed multiple components in these films with a highly strained layer near the substrate.

- Work on both the La_xMnO_3 and the $Nd_{1/2}Sr_{1/2}MnO_3$ series reveals significant in-plane strain persisting beyond 2000 A.

Submitted and Published Work Based on X14A Experiments

Q. Qian, T. A. Tyson, M. Deleon, C.-C. Kao, W. Prellier, J. Bai, A. Frenkel, A. Biswas and R. L. Greene, "Influence of strain on the Local Atomic, Electronic and Magnetic Structure of Manganite Films", Submitted to Phys. Rev. B.

Q. Qian, T. A. Tyson, C. Dubourdieu, A. Bossak, J. P. Senateur, M. Deleon, J. Bai, and G. Bonfait, "Structural studies of annealed ultrathin La0.8MnO3 films", Applied Physics Letters **80**, 2663 (2002).

Q. Qian, T. A. Tyson, C. Dubourdieu, A. Bossak, J. P. Senateur, M. Deleon, J. Bai, G. Bonfait, and J. Maria, "Structural, magnetic, and transport studies of La0.8MnO3 films", Journal of Applied Physics **92**, 4518 (2002).

Q. Qian, T. A. Tyson, C. C. Kao, W. Prellier, J. Bai, A. Biswas, and R. L. Greene, "Strain-induced local distortions and orbital ordering in Nd0.5Sr0.5MnO3 manganite films", Physical Review B: Condensed Matter and Materials Physics **63**, 224424/1 (2001).

NSF Grant DMR-0209243 and NSF IMR Grant DMR-0216858

UH

X-ray Studies of Spontaneous Atomic Ordering in III-V Semiconductor Alloy Films

S. Moss and J.H. Li, Univ. of Houston

Information obtained from quantitative analysis of X14A data

1. Two variants coexistence
2. Order parameter
3. Atomic displacement
4. Anti-phase boundaries
5. Orientational (variant) boundaries
6. Size and spatial distribution of the antiphase and the orientational boundaries

J.H. Li, "X-ray characterization of CuPt-ordered semiconductor alloy films," in *Spontaneous Ordering in Semiconductor Alloys*, ed. A. Mascarenhas (Plenum Press/Kluwer Academic, 2002)

UH

Determination of the Order Parameter

- Traditional method

$$I_{fundamental} \propto |F_{fundamental}|^2$$

$$I_{order} \propto s^2 \cdot |F_{order}|^2$$

$$s \propto I_{order}/I_{fundamental}$$

Problems:

Modulation of the ordering reflection by atomic displacement and possibly also by antiphase domains.

Determination of the intensity of a fundamental reflection is often not easy because the layer is usually lattice matched to the substrate.

In case of co-existence of two variants, one effectively determines the product of the order parameter and the volume fraction of the corresponding variant.

Determination of the Order Parameter

UH

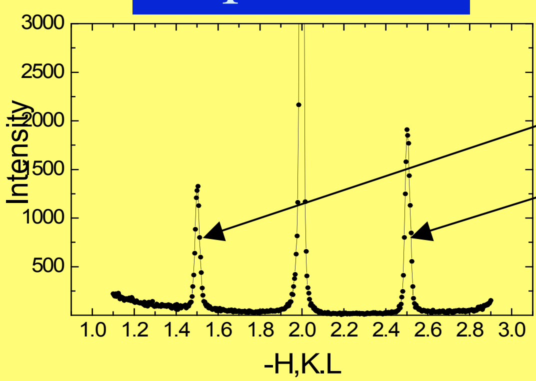
Our Approach

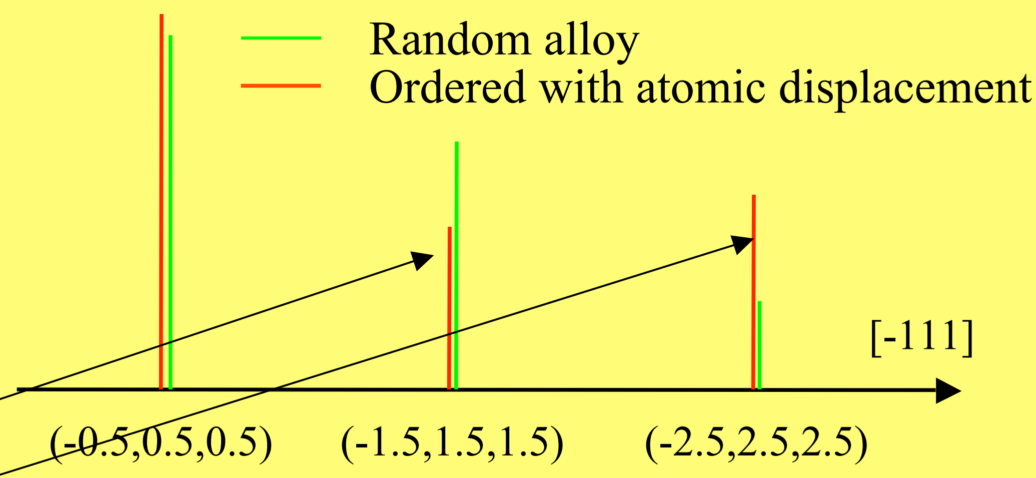
J. H. Li, R. L. Forrest, S. C. Moss , Y. Zhang , A. Mascarenhas, J. Bai, “Determination of the order parameter of CuPt-B ordered $GaInP_2$ films by x-ray diffraction, ” Journal of Applied Physics , Volume 91, Issue 11, pp. 9039-9042, 1 June 2002

Ordering peaks —Modulated by→ Atomic displacement → Order parameter

✓No structural detail is needed
✓Average order parameter for all ordered domains of the same variant

Experiment

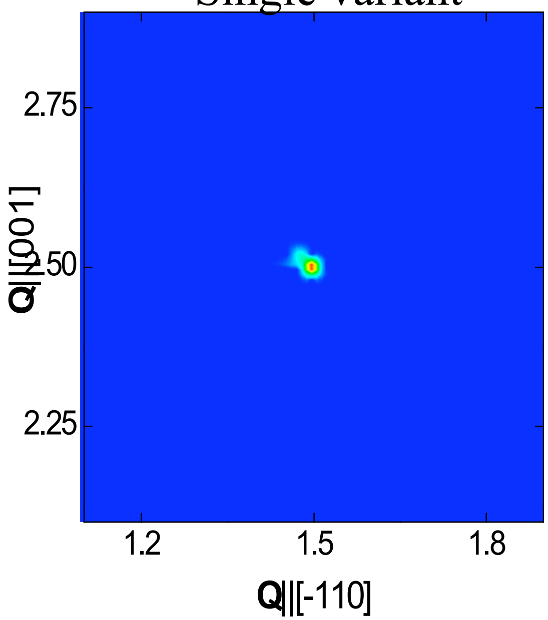




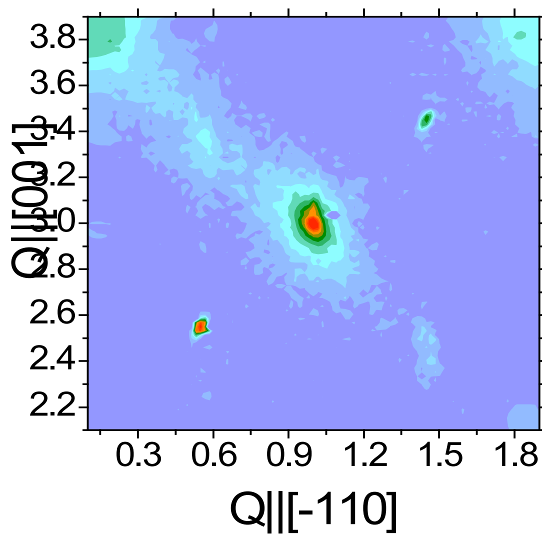
Amplitude of intensity modulation $\propto |\mathbf{Q} \cdot \delta|^2$

X-ray [110] Zone Diffraction - $Ga_{0.5}In_{0.5}P/GaAs$ (001)

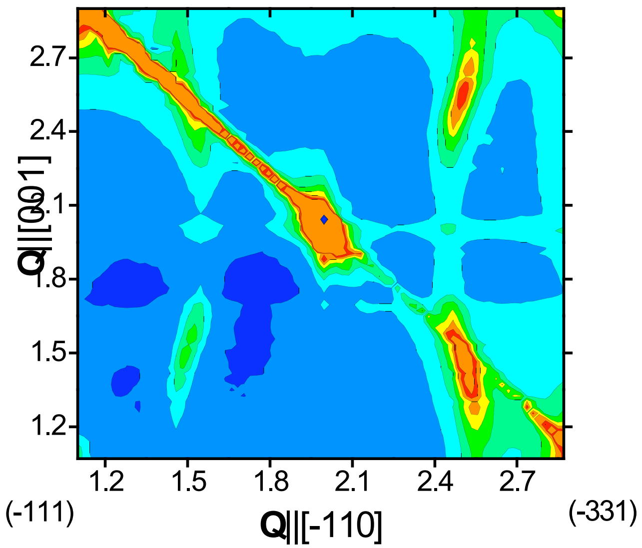
Single variant



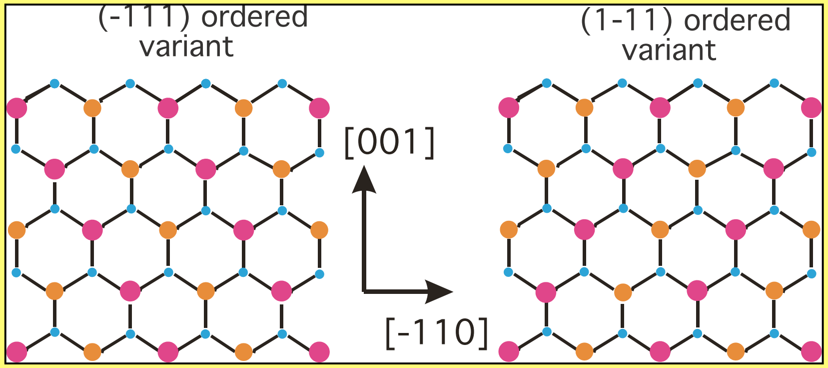
Biased double variants



Double variants



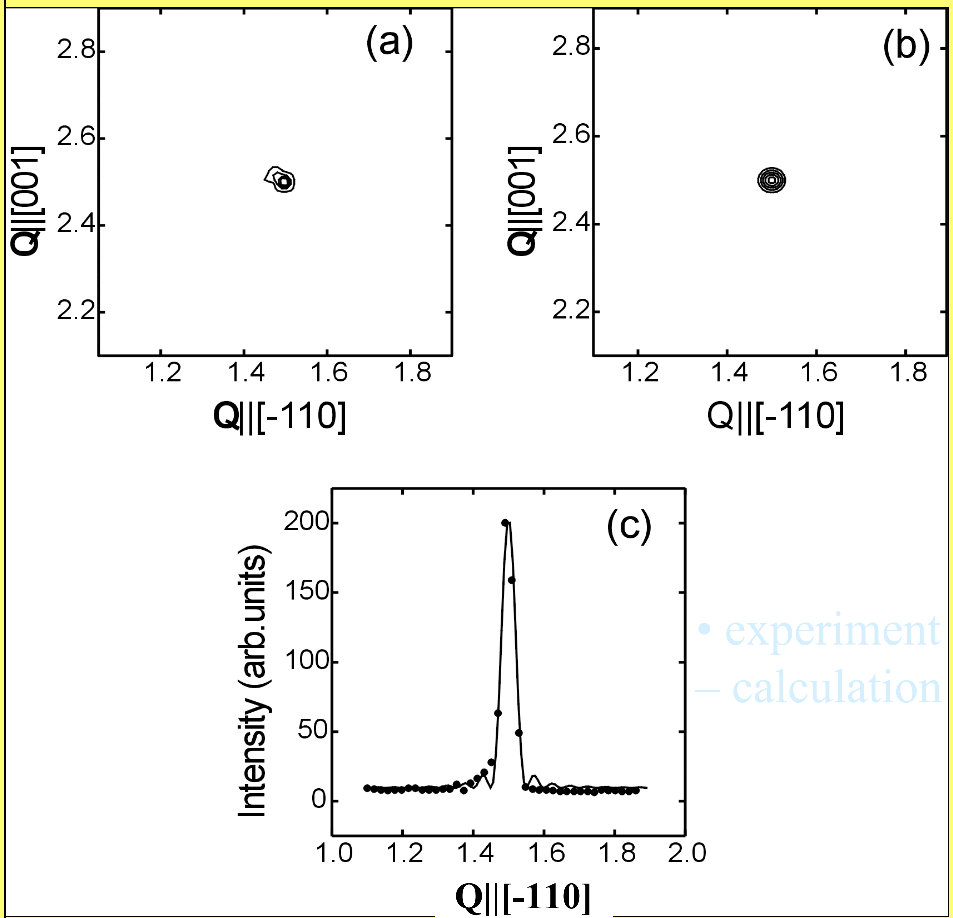
- In-rich
- Ga-rich
- P



UH

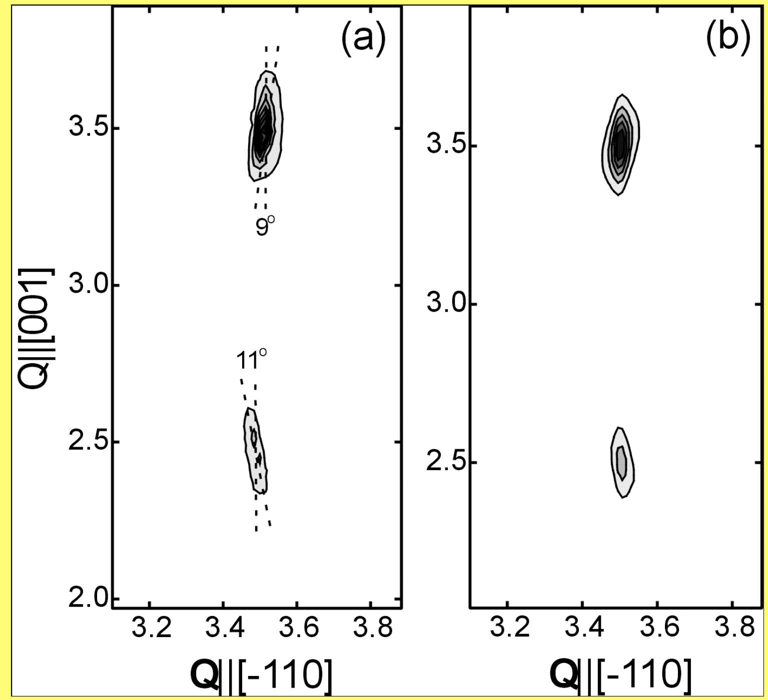
Single variant - $Ga_{0.5}In_{0.5}P$

experiment calculation



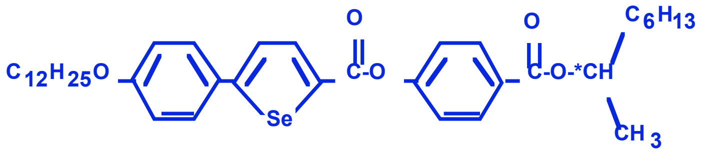
Double-variant $Ga_{0.5}In_{0.5}P$

experiment calculation

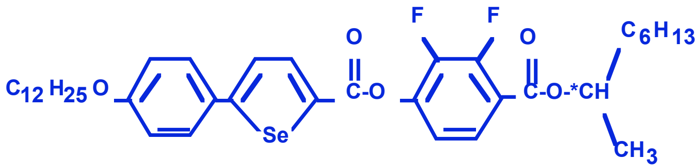


Antiferroelectric (AFE) & Ferroelectric (FE) Liquid Crystals- Helen Gleeson, U. of Manchester

New General User



K 67.7 SmC^*_A 97.8 SmC^*_{FI1} 99.0 SmC* 109.4 SmA 116.6 I
(SmI* 33.3 SmI^*_A 42.2)



K 46.3 SmC^*_A 82.6 SmC^*_{FI1} 83.6 SmC^*_{FI2} 86.3 SmC* 84.3 SmA 93.7 I

- **Synthesised by Goodby (Hull/York University)**
- **Studied via optical and x-ray techniques**
  - **X14A to explore interlayer structure in smectic liquid crystals**

Resonant x-ray scattering

U. Manchester

- **Conventional x-ray scattering gives scalar information, e.g. size & position of layers, but cannot distinguish AFE, FI and FE. Sees (0 0 1), (0 0 2) peaks**

$$Q_z = 2\pi l/d = l\,Q_0$$

- **Scattering at an atomic absorption edge - resonant scattering gives tensor response**
  - **Forbidden reflections occur reflecting interlayer periodicity, e.g. for AFE at (0 0 n+0.5)**

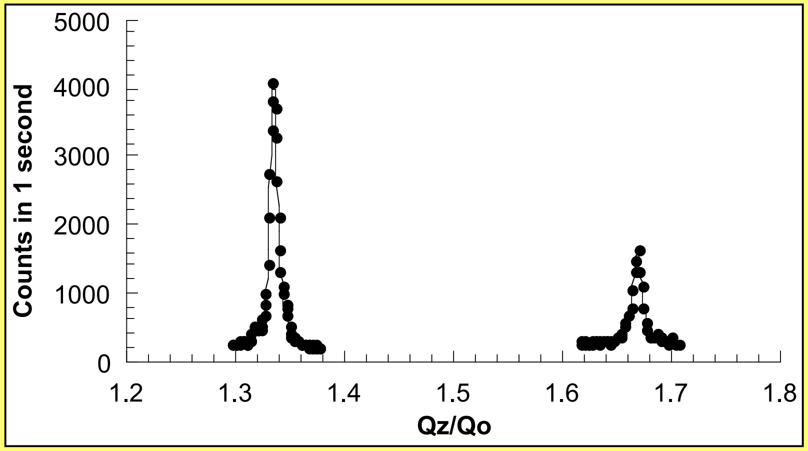
$$\frac{Q_z}{Q_0} = l + m\left(\frac{1}{n} + \frac{d}{p}\right)$$

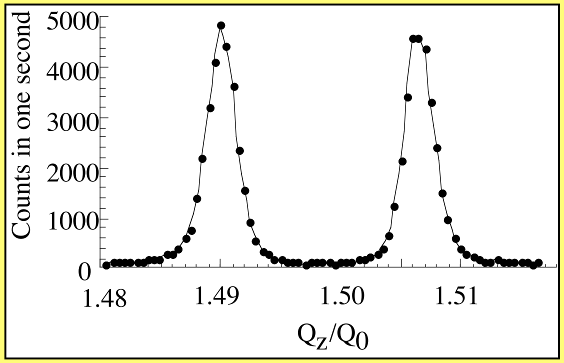
U. Manchester

Resonant signals

Resonant peaks occur at:

Phase	Qz/Qo
AFE	0.5, 1.5, …
3-layer	0.33, 0.67, 1.33, …
4-layer	0.25, 0.5, 0.75, …



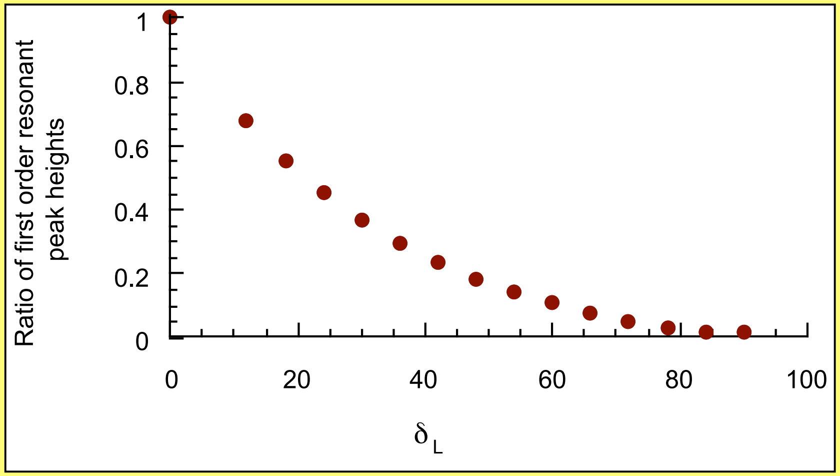


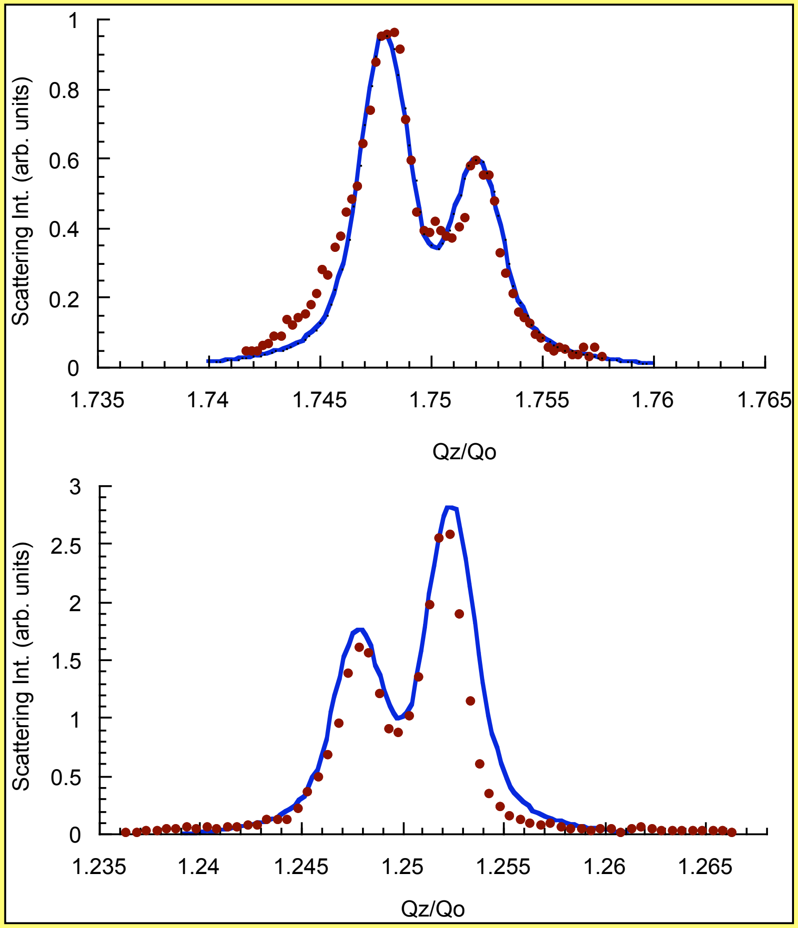
Polarization analysis -
clock model

Peak splitting -
helical superstructure

Biaxial 4-layer phase

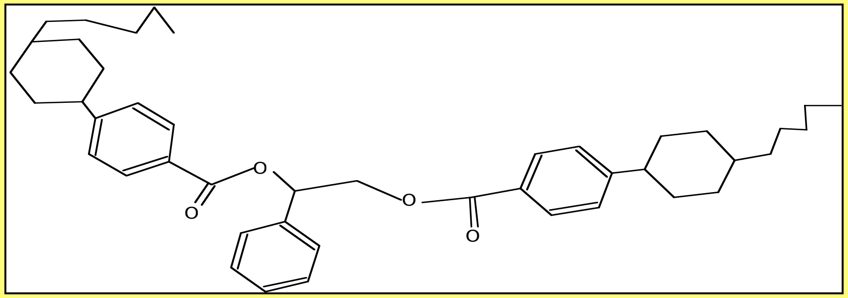
- Distortion angle is ~15˚
- Doesn't appear to be very temperature dependent

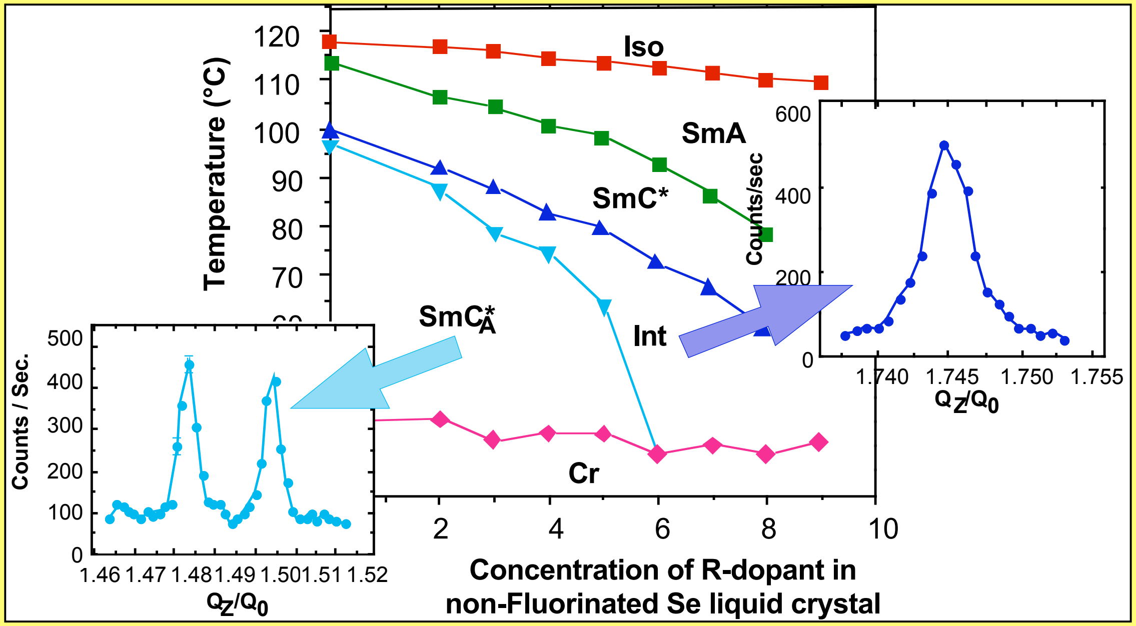




Is the 3-layer phase distorted too?

- Very 'fragile' phase
- Mixtures with chiral dopants increase intermediate phase range to >15 °C
- Tilt decreases with concentration





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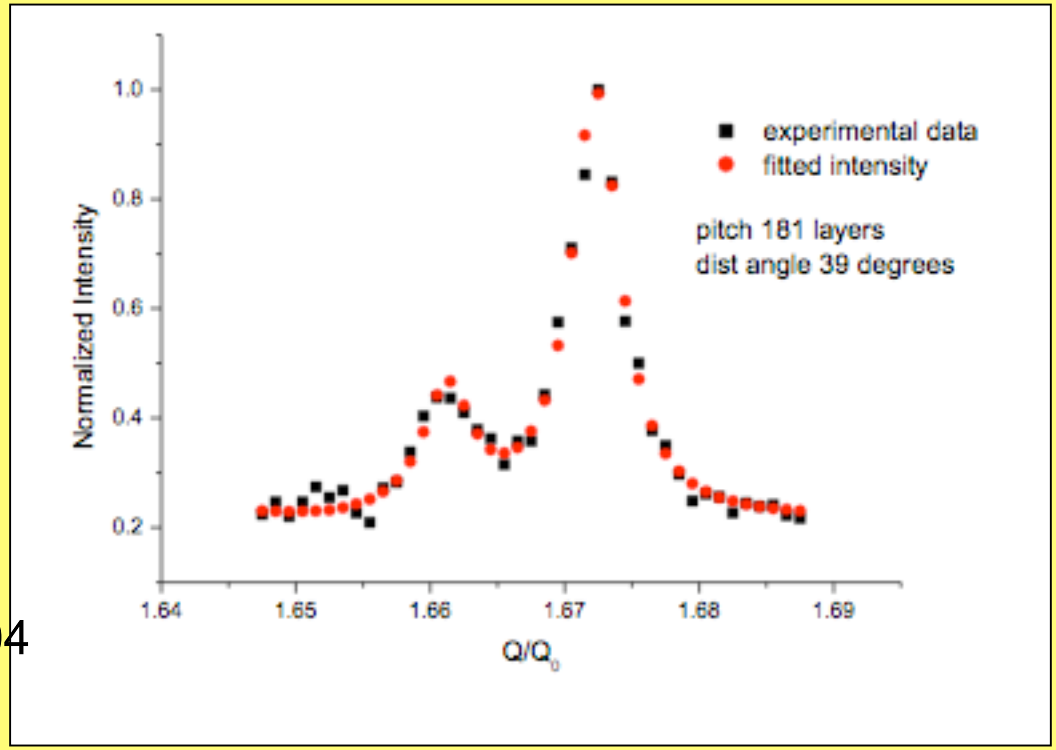
Recent Project (Sept 2004)

- **Very successful measurements on 3-layer phase**
- **Distortion angle is ~40˚**

- Pitch is ~181 layers (550nm)
- Temperature dependence (next proposal)?



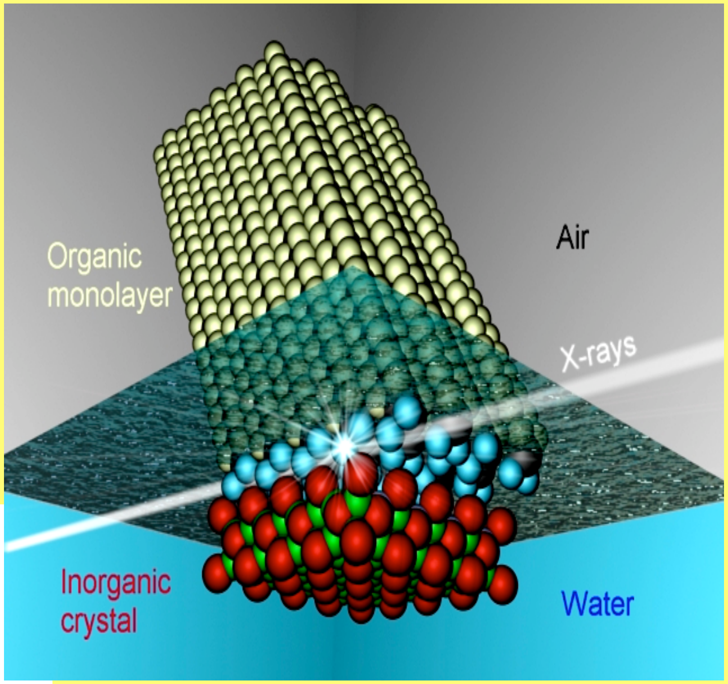
Invited Presentations:

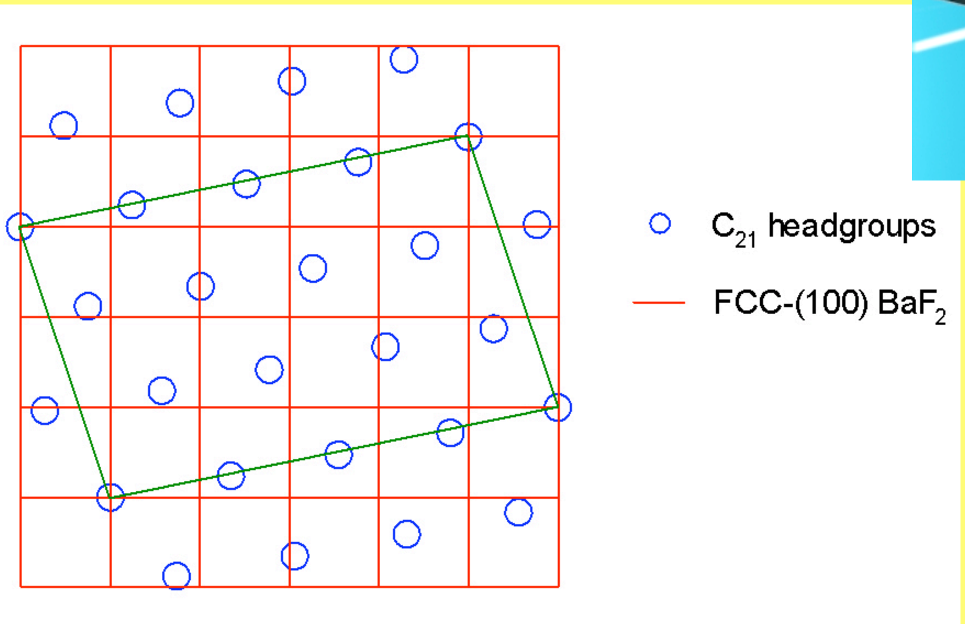
✓ British Liquid Crystal Society, 4/2004
✓ Rank Prize Meeting, 12/2004
✓ 19th Thermo Conference, 5/2005

Publications (in progress)

Commensurate growth of BaF2 under floating (Langmuir) monolayers

Palak Dutta (Nortwestern)

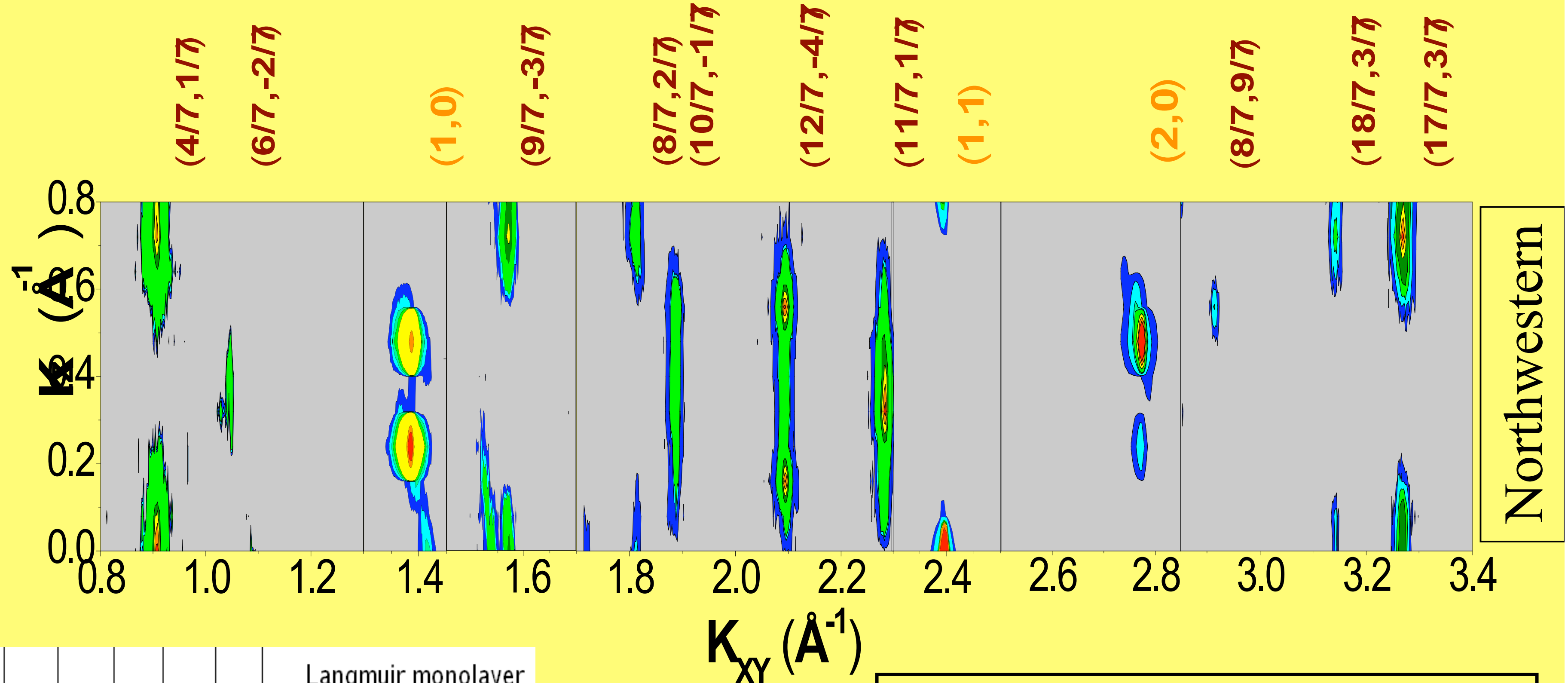


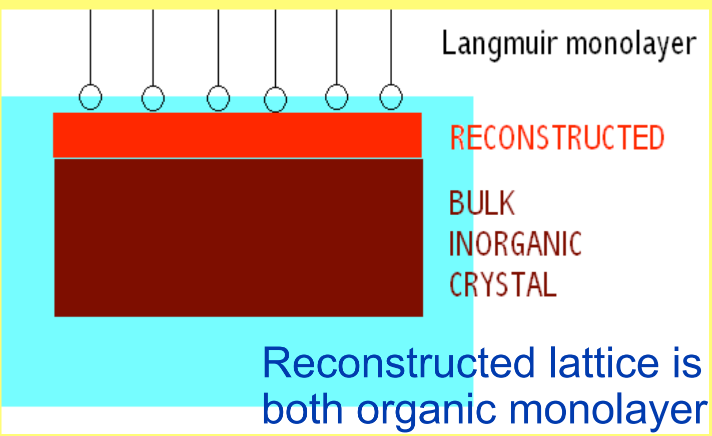


BaF_2 unit cell area:	**33.86 Å**
Fatty acid unit cell area:	**22.59 Å**
Ratio:	**1.50**

Nucleation of $PbCO_3$ under a Langmuir monolayer

(fractional-index peaks are from a √7x√7 reconstructed surface)





Reconstructed lattice is commensurate with both organic monolayer and bulk inorganic crystal

Organic-template-directed nucleation:

New method of thin film growth (No UHV!). Strain, commensurate growth and surface reconstruction are seen

Metrics

User day statistics show an upturn since monochromator upgrades

	1998-2000 3 years		2003-2004 2 years	
Total days	658.5		430.0	
Beamline Upgrades	-155.5		-26.6	
Productive days	503.0	**(166.5/yr)**	403.4	**(201.7/yr)**
General Users' days	136.0	(27%)	128.4	(32%)
PRT Users' days	367.0	(73%)	275.0	(68%)

- ✦ Major beamline upgrades in 1999
- ✦ Highly productive operational time since 2000

10/1/01 to 9/30/04 Publications

- **23 journal publications (5 premier)**
- **2 Ph.D. theses**

Safety at X14A

- We utilize both NSLS and ORNL-M&C safety expertise & systems
- All NSLS-BNL safety requests addressed
  - BLOSA revisions
  - Hazardous equipment assessment and list
  - Beamline Scientist up to date on trainings
- ORNL's direct efforts
  - Research Hazard Analysis and Control (RHAC) reviews
  - Research Safety Summaries and Authorization to Operate
  - M&C ES&H staff member visited X14A and conducted safety review
    - Performed in conjunction with Andrew Ackerman of BNL
    - Continued telephone contact when questions develop
  - PRT's Lab Safety Manager T.R. Watkins made multiple visits to X14A
  - PRT Spokesperson and Beamline Scientist both personally conduct safety assessments yearly

Issues and Vision

- **PRT expanded**
  - ORNL-M&C providing a strong PRT foundation
  - TTU - Biernacki added as PRT member in 2004
  - Additional member being sought
- **PRT collaborators/ General Users / Potential institutions**
  - Hesitant to finance beamlines due to ready access to General User time across the country
- **Targeted upgrades for 2005-2007 -- would make X14A a true world class powder diffraction instrument**
  - NSLS's high speed detector (10 ns deadtiime; P. Sidons)
    - Dynamic range improves reflectometry, epitaxial layer studies, …
  - Linear position sensitive detector for studies of kinetics of solid-solid and gas-solid reactions
    - 50-100x faster data collection possible with new commercial detectors
  - Multi monochromators & detectors to gain speed in high resolution powder diffraction
    - 5 to 10x possible
  - Capital equipment funding source(s) not clear

Opportunities at NSLS to Be World Class
- Diffraction Beam Lines -

- **Collaboratively develop strategic plans for optimizing the various diffraction beamline instruments**
  - **Upgrade detectors for major gains in speed of data collection**
  - **Develop agreement for exchange of time between PRTs that each optimize for one class of measurements yet PRT needs several classes of measurements**

- **Enhance database access at this group of beamlines**
  - **NSLS purchase multi seat license for major crystallographic databases and update yearly (relatively low cost!)**
    - **Cambridge Structure Database**
    - **Powder Diffraction File (PDF4 Full File & PDF4 Organics)**
    - **Inorganic Crystal Structure Database**
  - **Assure users access and provide training in their use (workshop?)**

Summary

- **X14A PRT research focus and capabilities continues to evolve**
  - **Broader ORNL research basis (EERE, BES, FE)**
  - **More materials R&D relevant to energy and industry**
  - **Increased breadth of user activity by U.S. institutions**
    - **High Temperature Materials Laboratory User Program**
    - **ORNL based research programs**
    - **New NSF sponsored research on cement materials at TTU**
  - **Continued fundamental science**
- **Added capillary furnace accessory which enables advanced in situ materials research and crystal structure analysis**
- **Strong scientific output by PRT and General Users**
- **Dedicated to achieve world class safety record**
- **Anxious to work with NSLS and other PRTs toward world class powder diffraction capabilities**

Questions?