

## Matias Bargheer

# Examples of Ultrafast X-ray Diffraction Experiments: Synchrotron vs. Laser-Plasma Sources

- Some details of the setup: BESSYII + Plasma  $\Rightarrow$  VSR
- Ultrafast heat transport on nm length scale
- Inhomogeneous lattice dynamics in ferroelectric
  - $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$
  - $\text{BiFeO}_3$

# Team

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**PostDocs and PhD students  
University of Potsdam  
+ HZB:**

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André Bojahr

Lena Maerten

Steffen Mitzscherling

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Dr. Roman Shayduk

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Yevgeni Goldshteyn



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Students**

Alexander von Reppert

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Felix Stete

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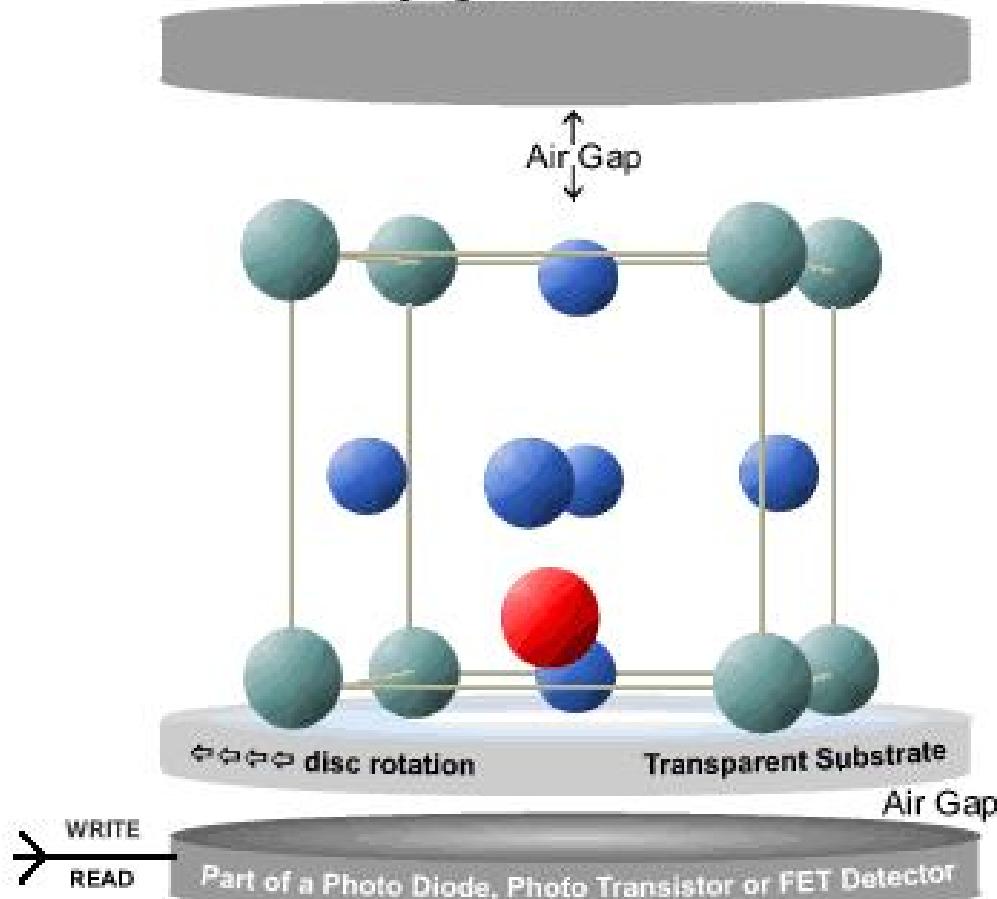
# Ultrafast and Ultrasmall Data Processing



## Schematics Atomic Switch\*

Flying Read/Write Head

\* simplified schematics,  
showing the function  
of one molecule



## Perovskite:

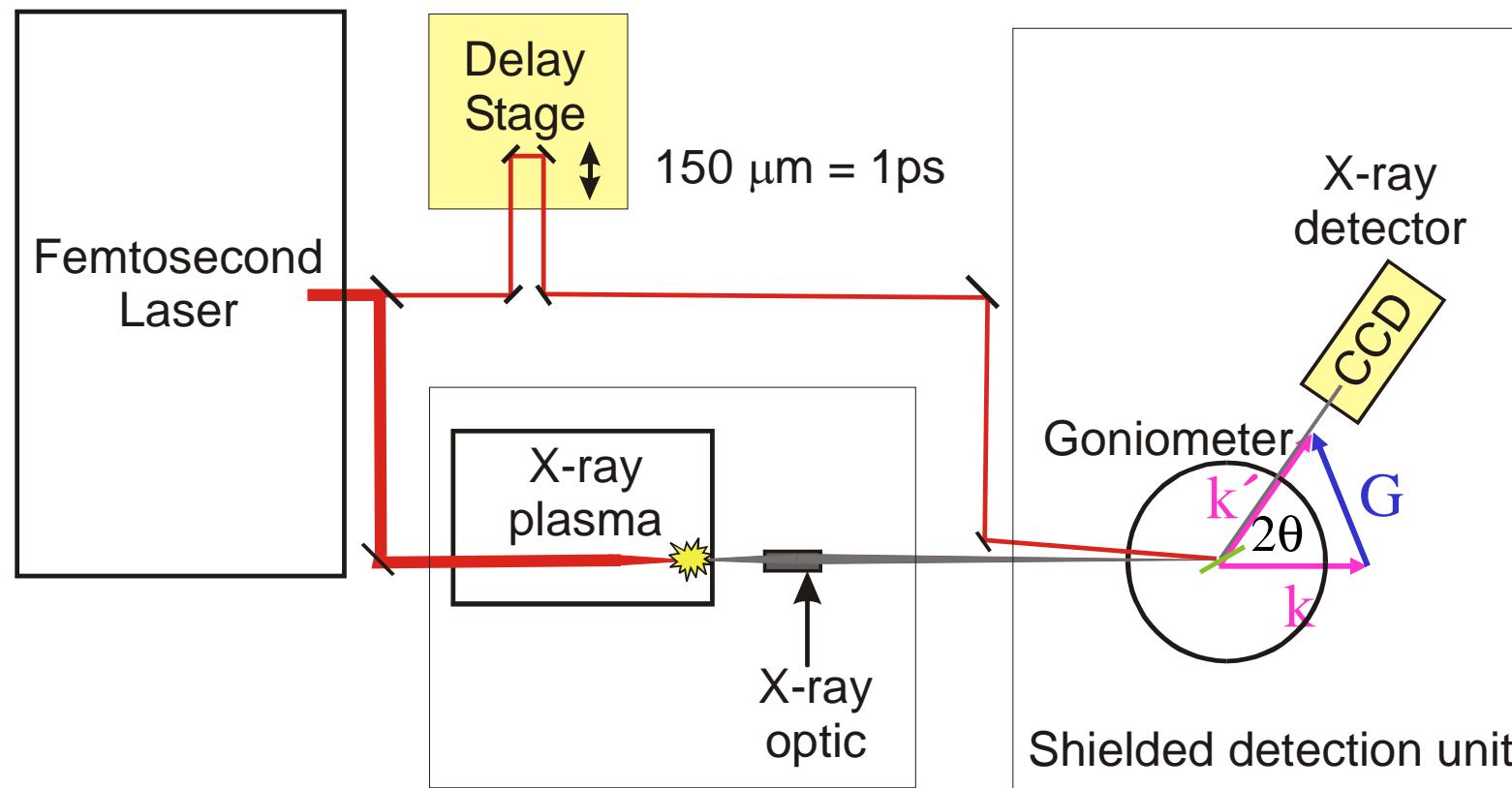
- Store data in the position of the central ion
- Optical excitation + Electric field



# UXRD using Plasma Source



Resolution ~150 fs  
~  $10^6$  photons /s on sample

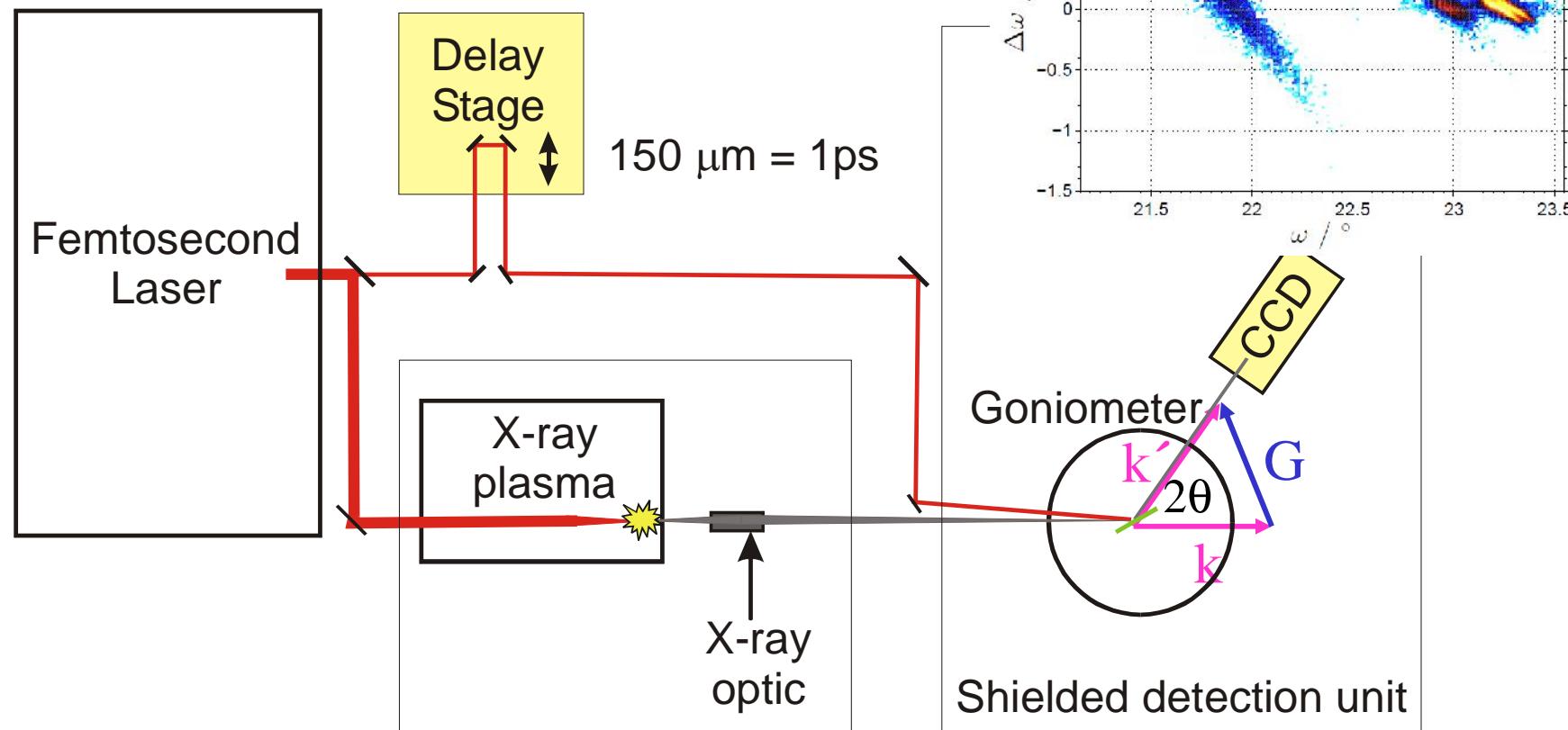




# UXRD using Plasma Source



Resolution ~150 fs  
 $\sim 10^6$  photons /s on sam



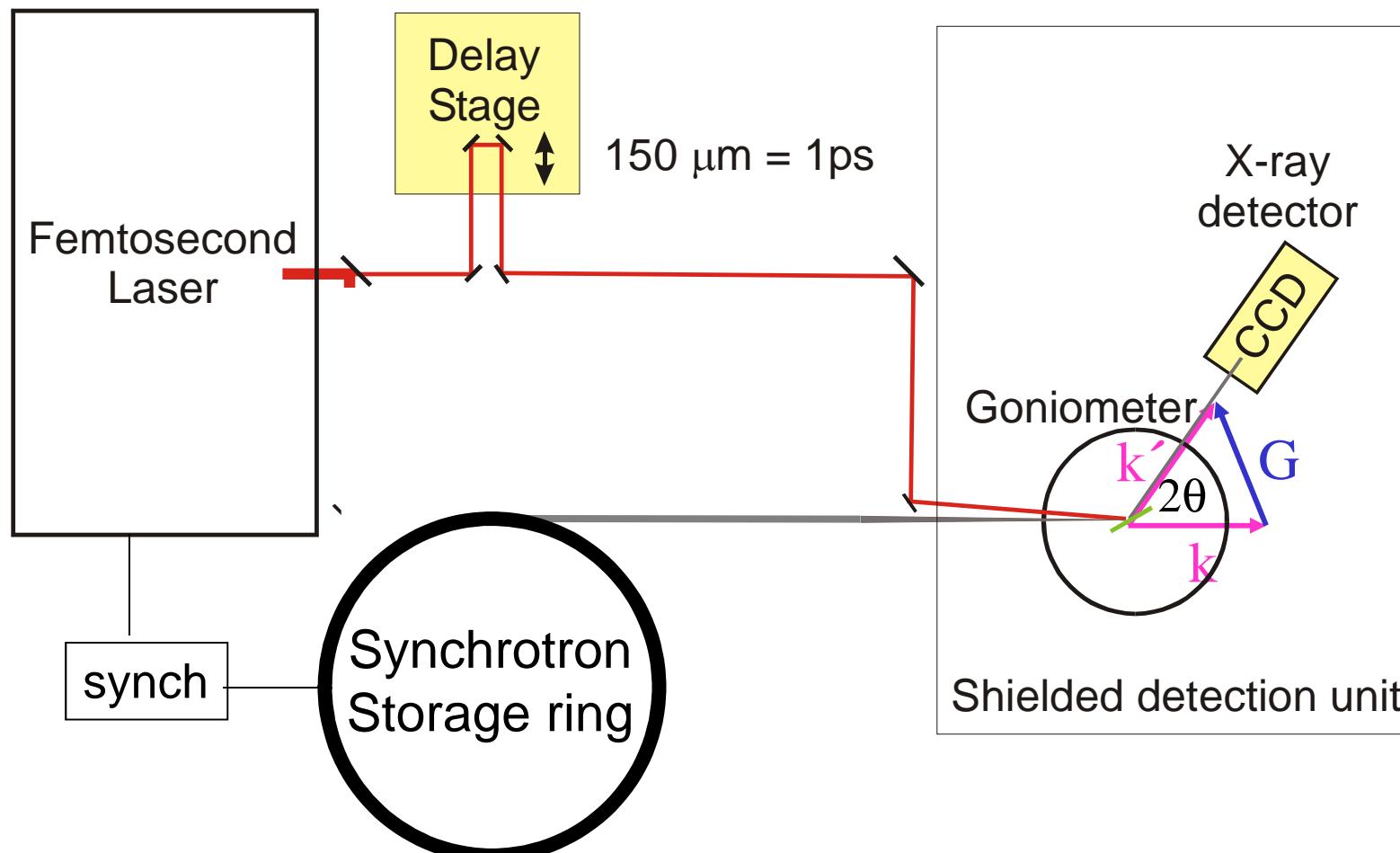


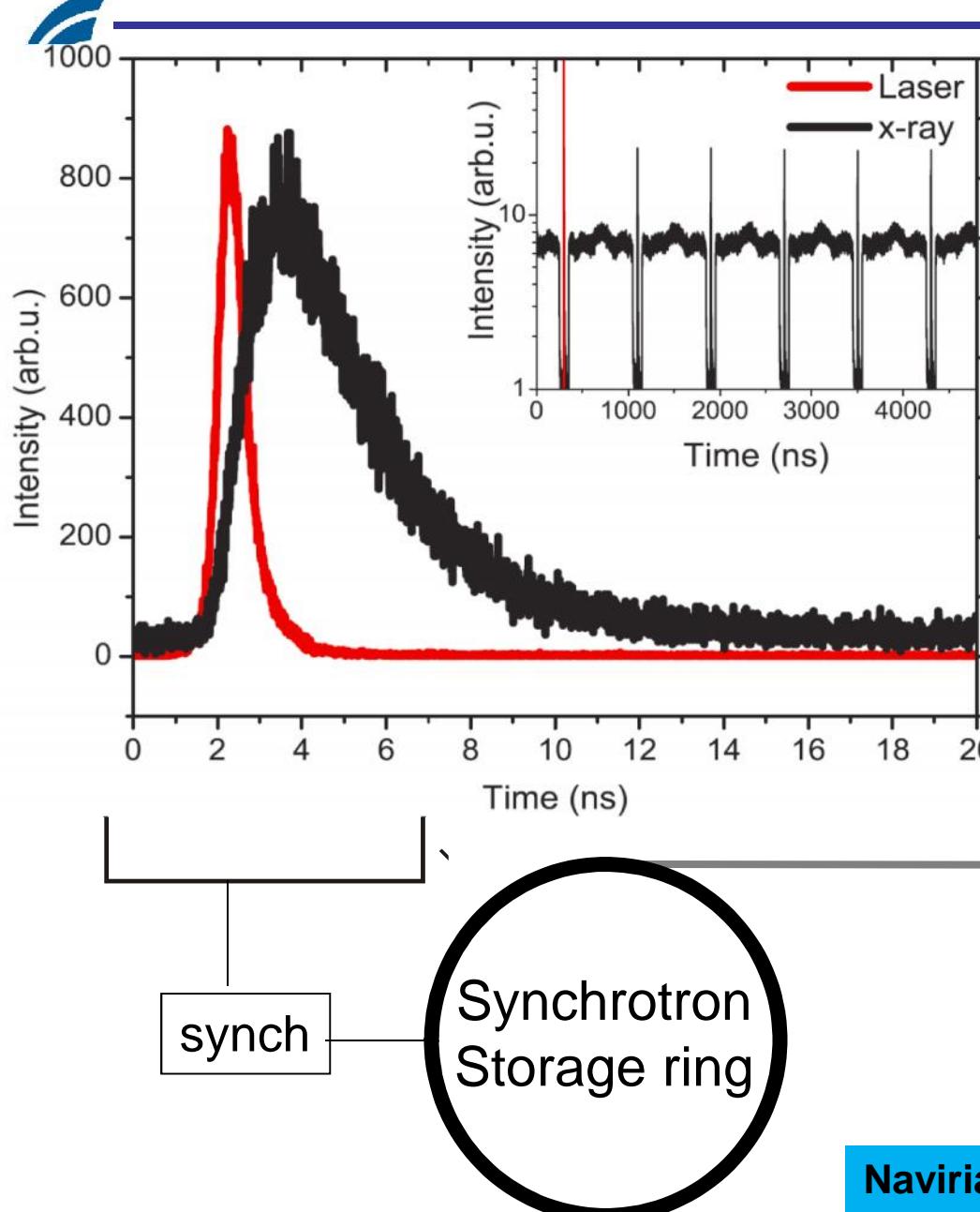
# UXRD at Synchrotrons



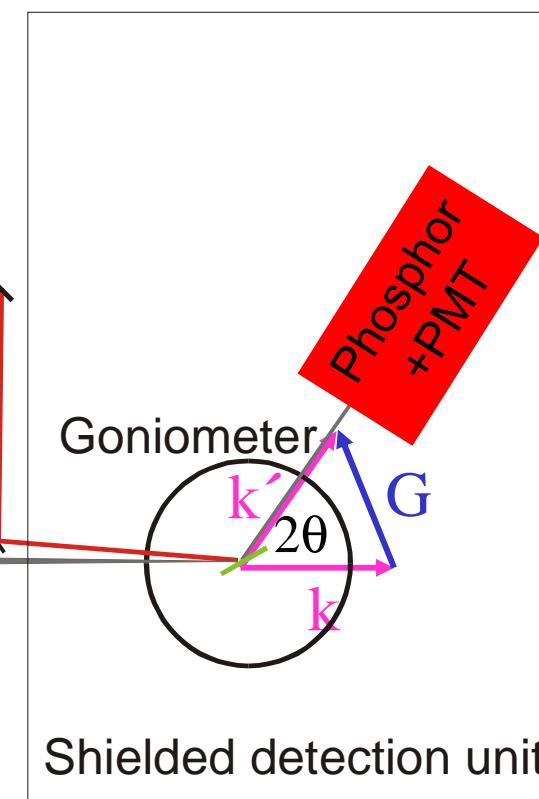
Time resolution  $\sim 100$  ps  $\rightarrow$  **0.3 - 10 ps**

Repetition rate: 208 kHz , 1.25 MHz  
 $\sim 10^5 - 10^9$  photons /s on sample





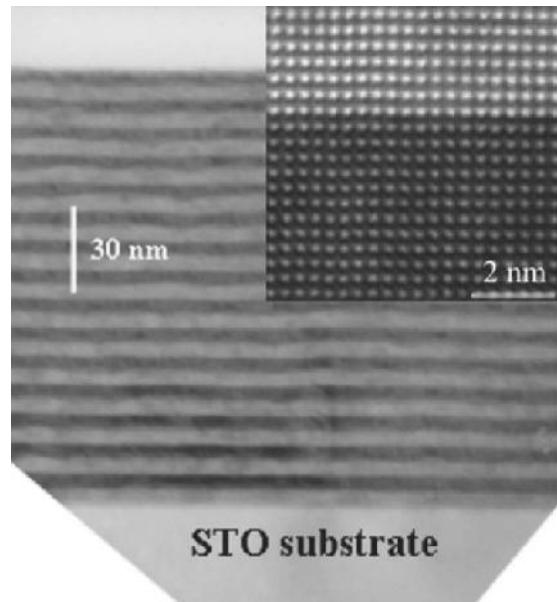
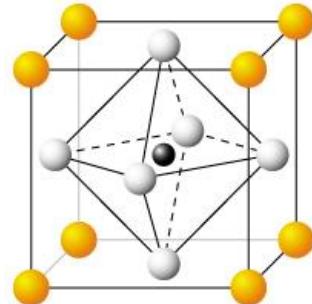
Fast X-ray Detector:  
Record 1 ns – 5 ms data for free  
Pump-Probe: 50 ps time resolution



# Oxide Nanolayers



Peroxskite structure



Vrejoiu et al., APL **92**, 152506 (2008).



## Ferromagnetic metals:

**SRO:**  $\text{SrRuO}_3$   
 $T_c \approx 160 \text{ K}$  (bulk)

**LSMO:**  $(\text{La}_{0.7}\text{Sr}_{0.3})\text{MnO}_3$   
 $T_c \approx 370 \text{ K}$  (bulk)

## Insulators:

**STO:**  $\text{SrTiO}_3$   
dielectric

**PZT:**  $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$   
ferroelectric below  $T_c \approx 750 \text{ K}$

## Other perovskite oxides:

Superconducting, giant magnetoresistance,..  
Rich phase diagrams

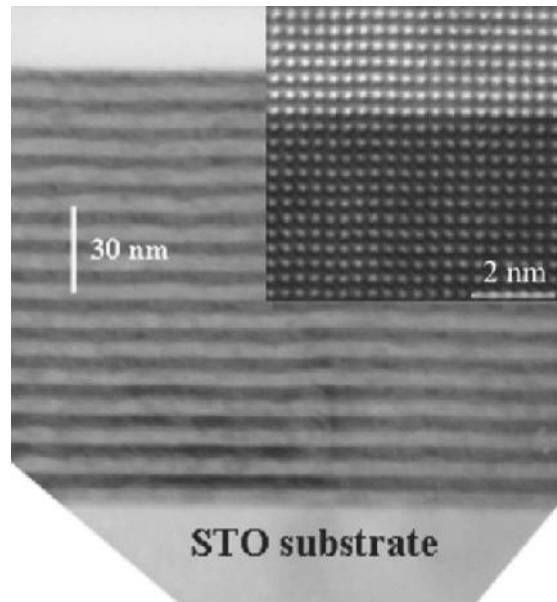
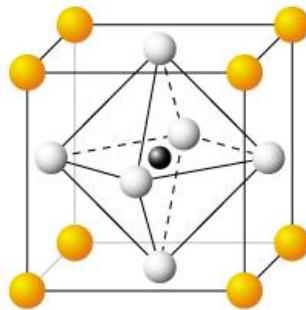
-> Grown by Pulsed Laser Deposition

MPI Halle: D. Hesse, M. Alexe, I. Vrejoiu

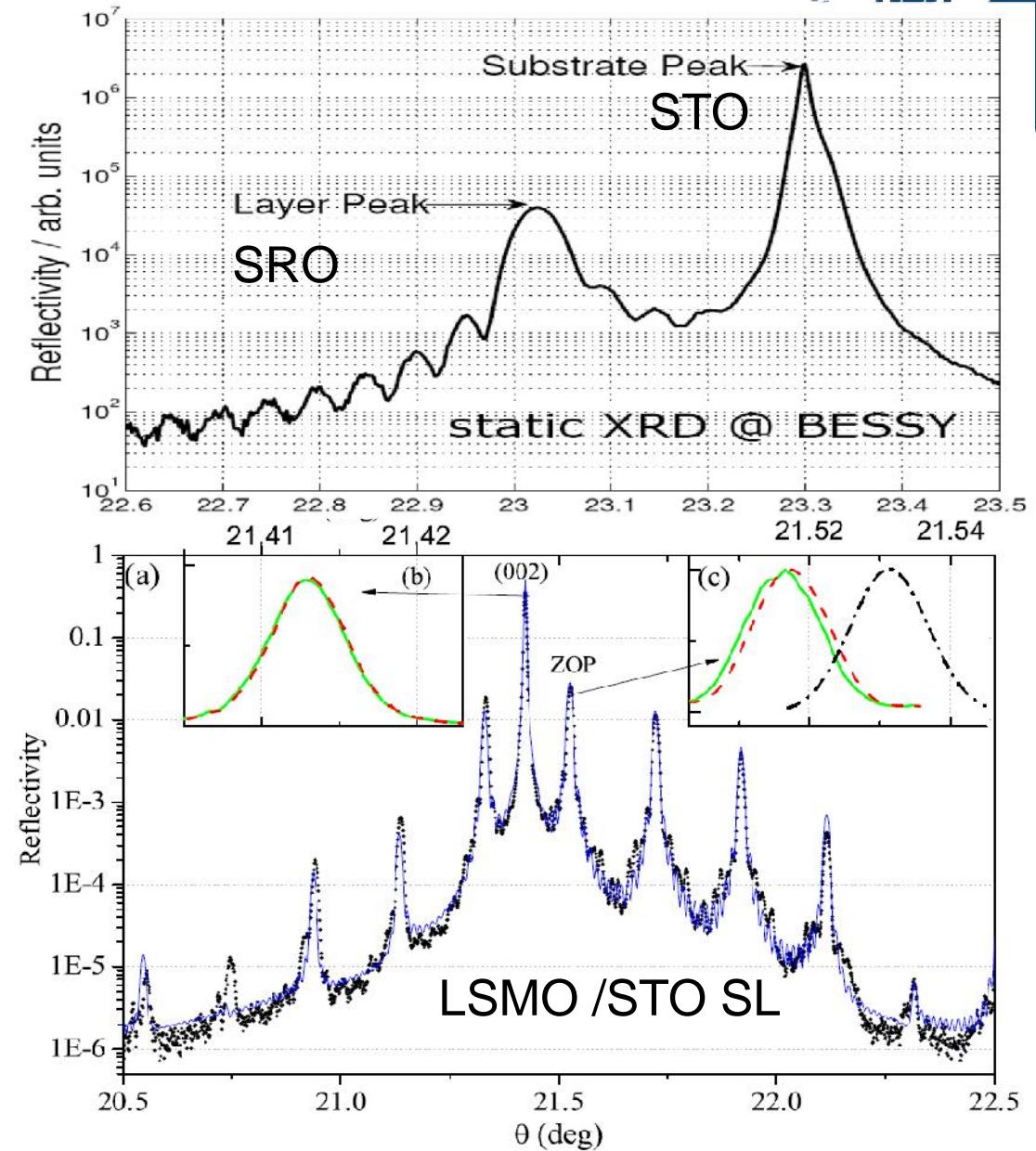
# Oxide Nanolayers



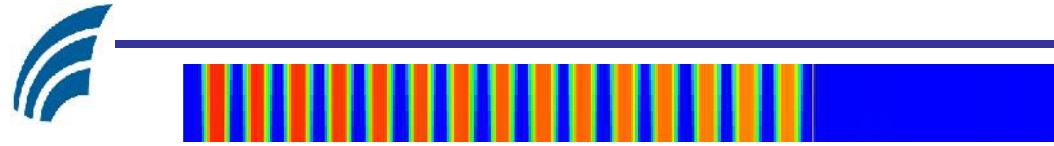
Peroxskite structure



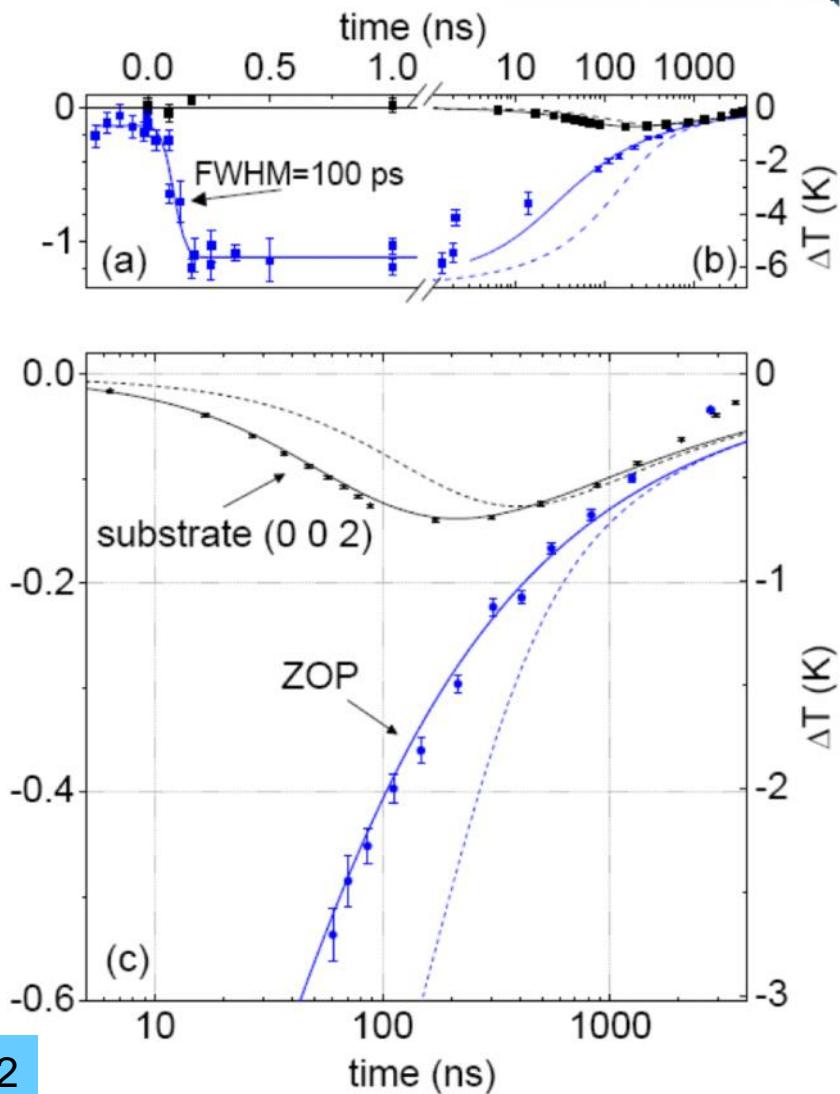
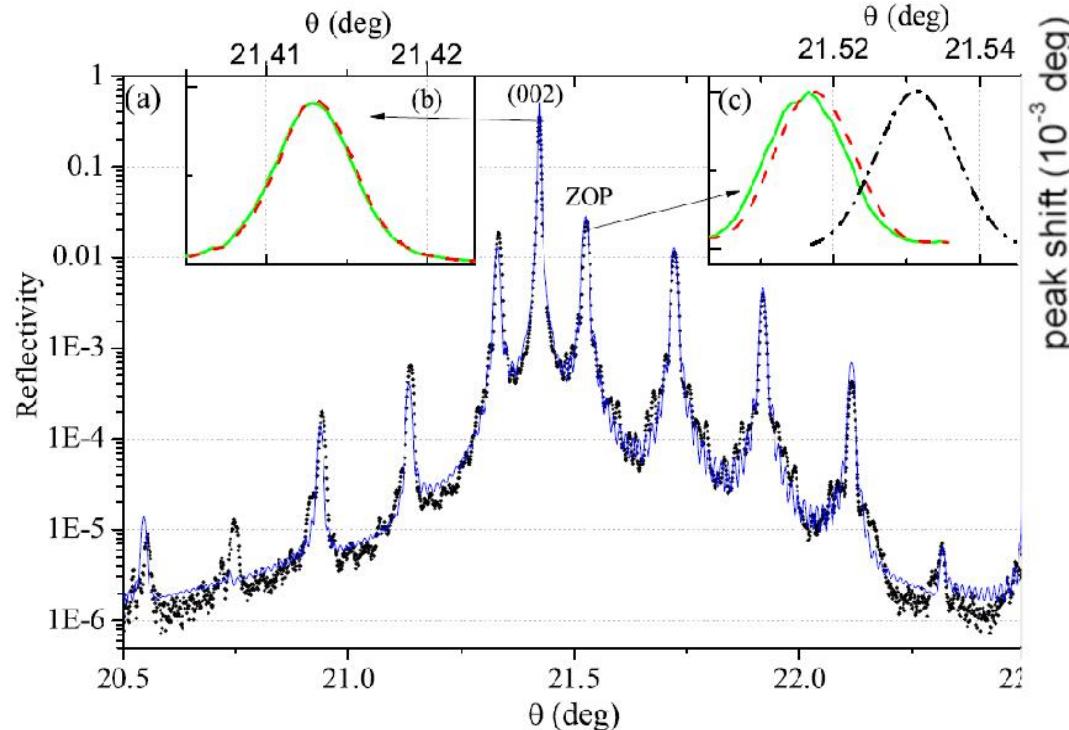
Vrejoiu et al., APL 92, 152506 (2008).



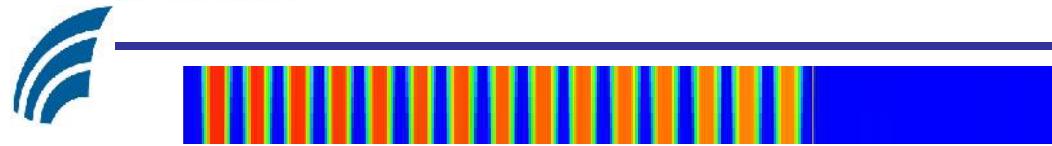
# Heat Diffusion from SL into Substrate



Example: LSMO/STO SL (9+14nm) on STO  
Heat equilibrated within SL after ~ 10 ps!!  
Heat flow to substrate ~ 100 ns



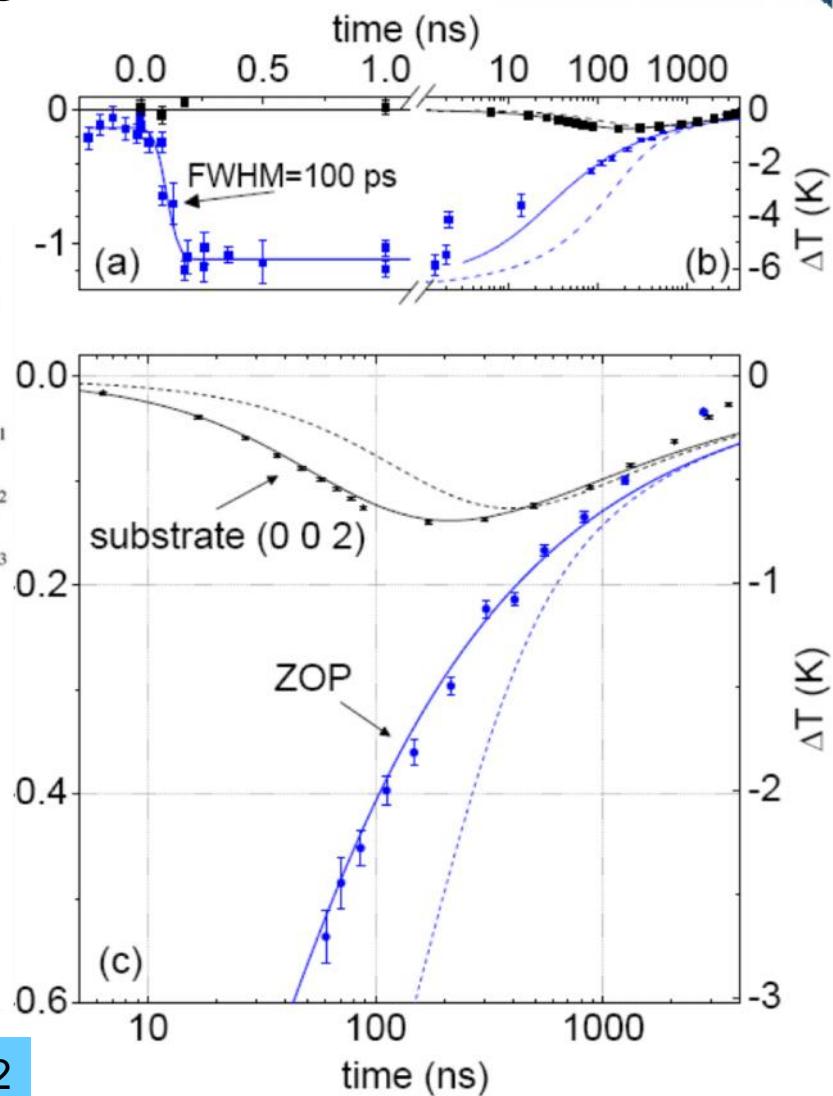
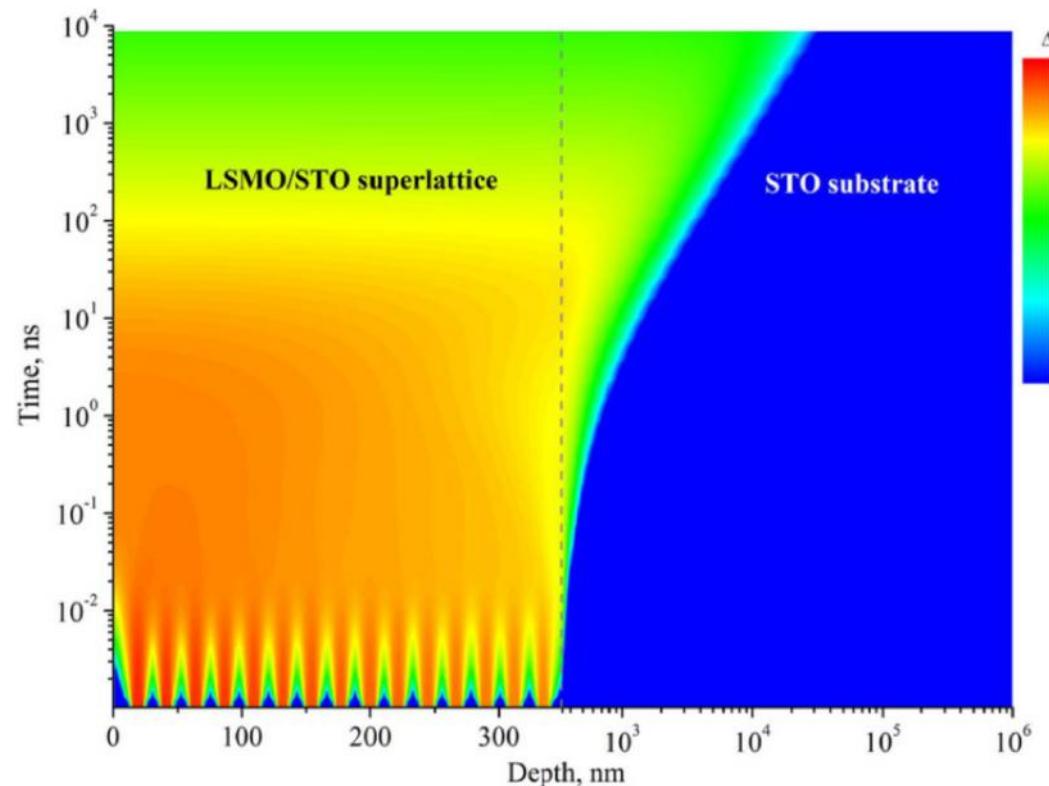
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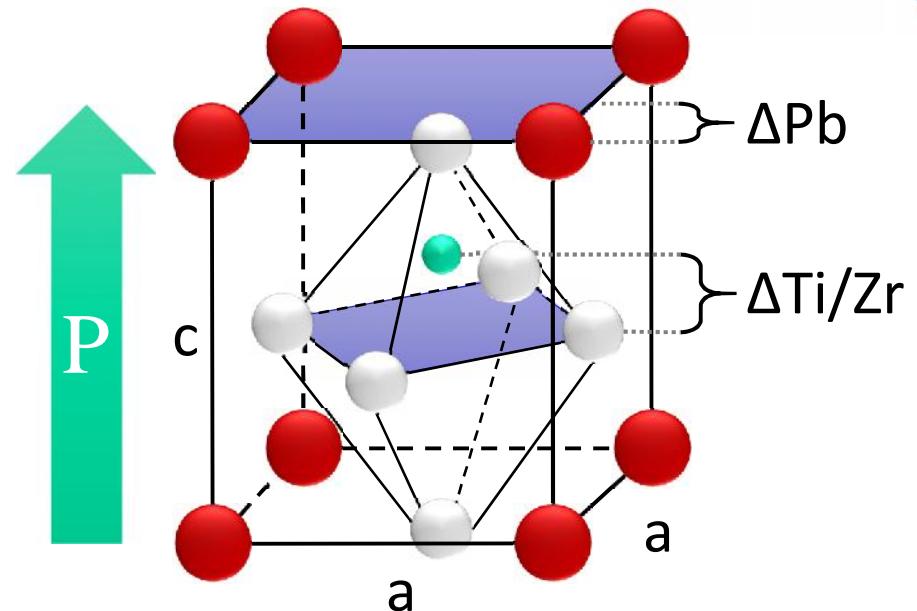
Heat flow to substrate ~ 100 ns



# Ferroelectric Perovskite: $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$

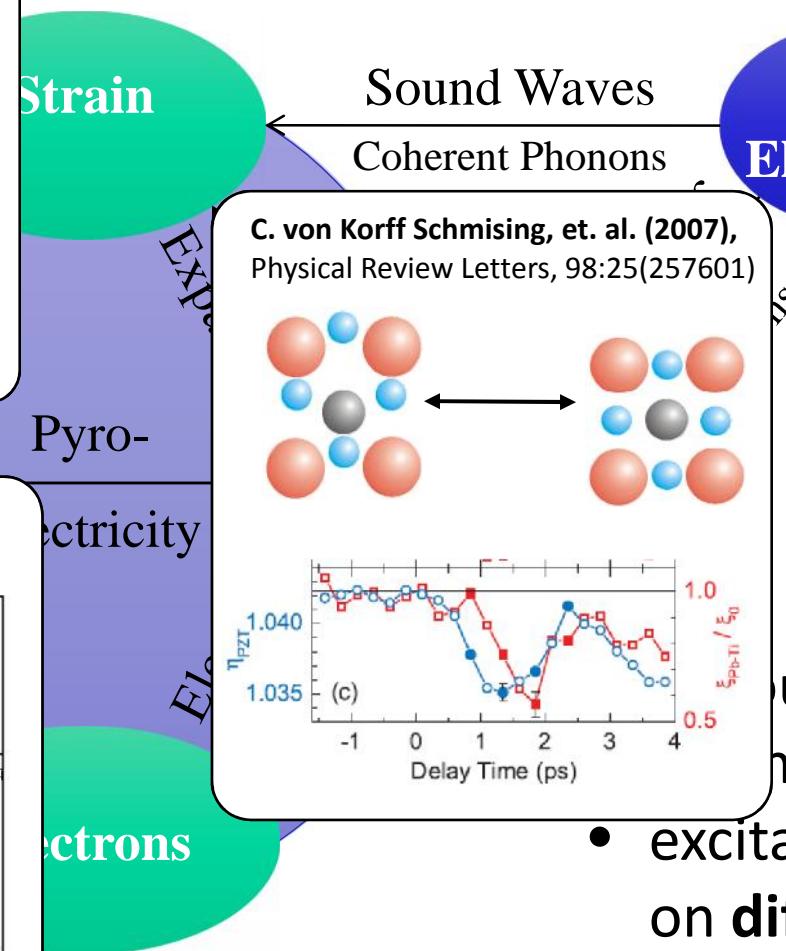
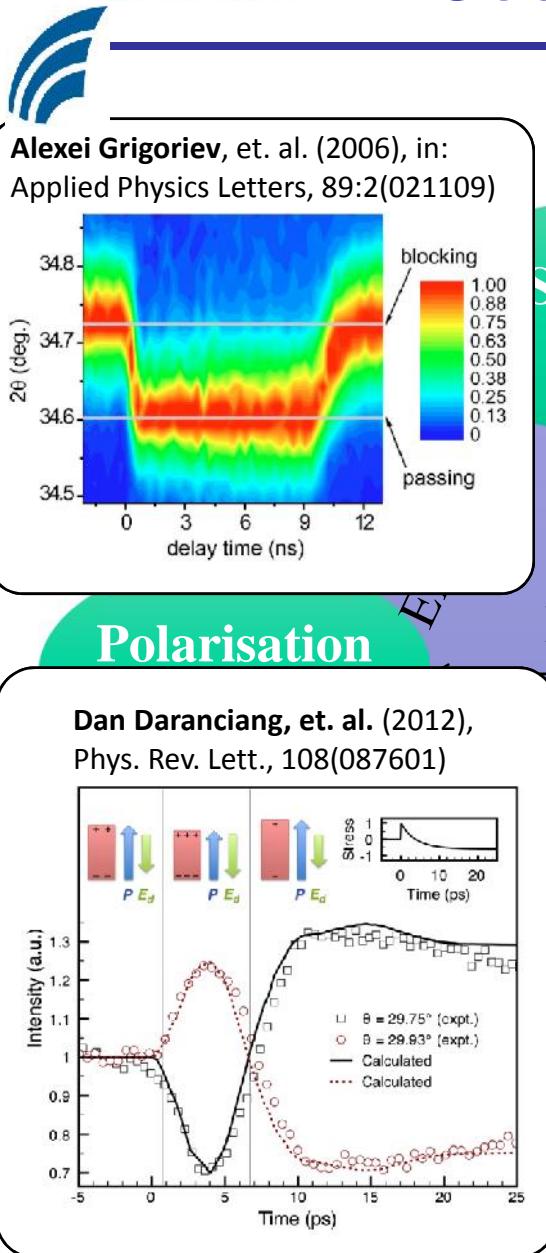


- A-site cation: Pb
- B-site cation: Zr/Ti
- Oxygen



- ferroelectric due to tetragonal distortion of Pb and Zr/Ti below  $T_c \approx 400^\circ\text{C}$
- additional piezo- and pyro-electricity
- various applications in MEMS or FeRAM

# Couplings Investigated by UXRD

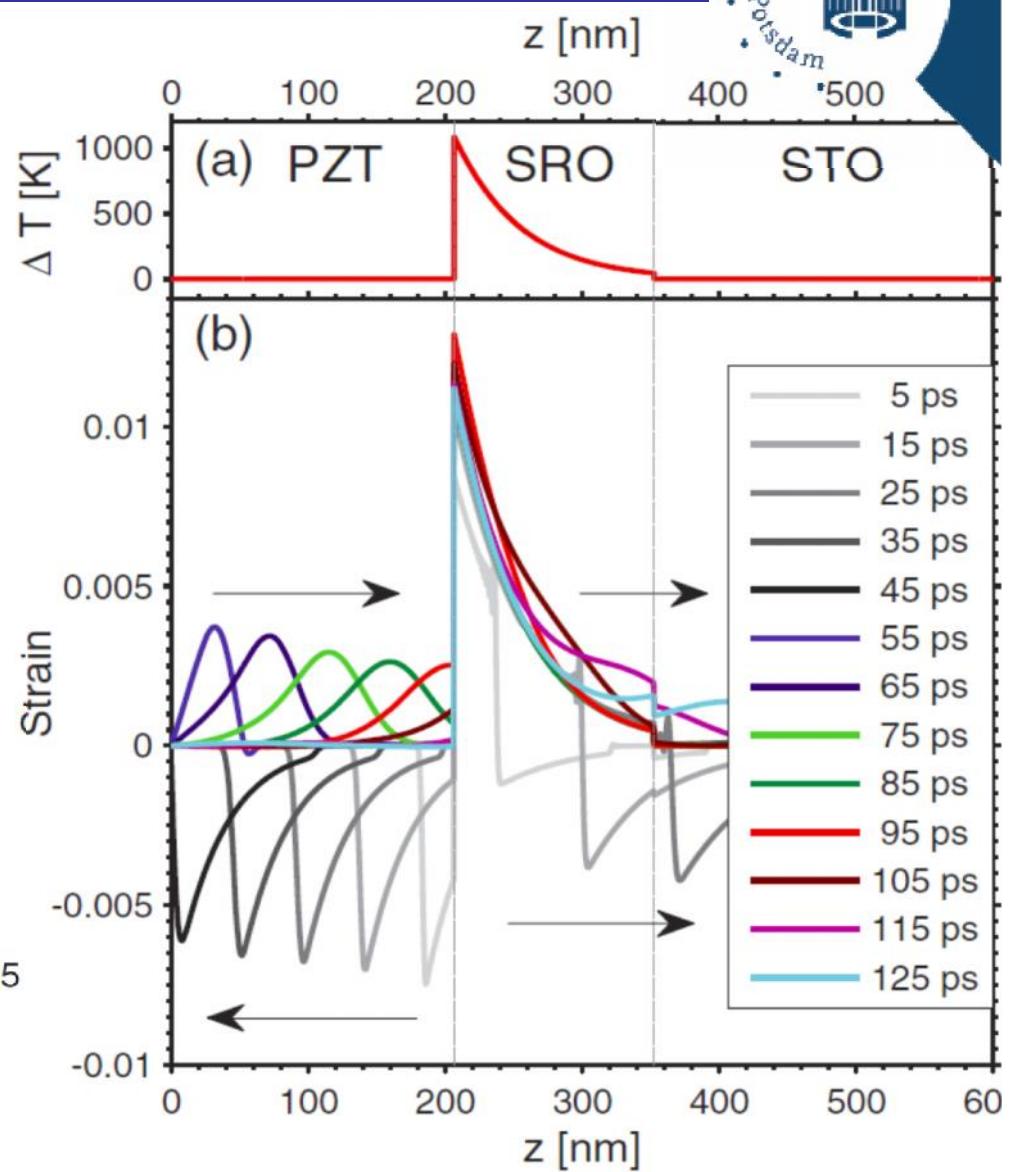
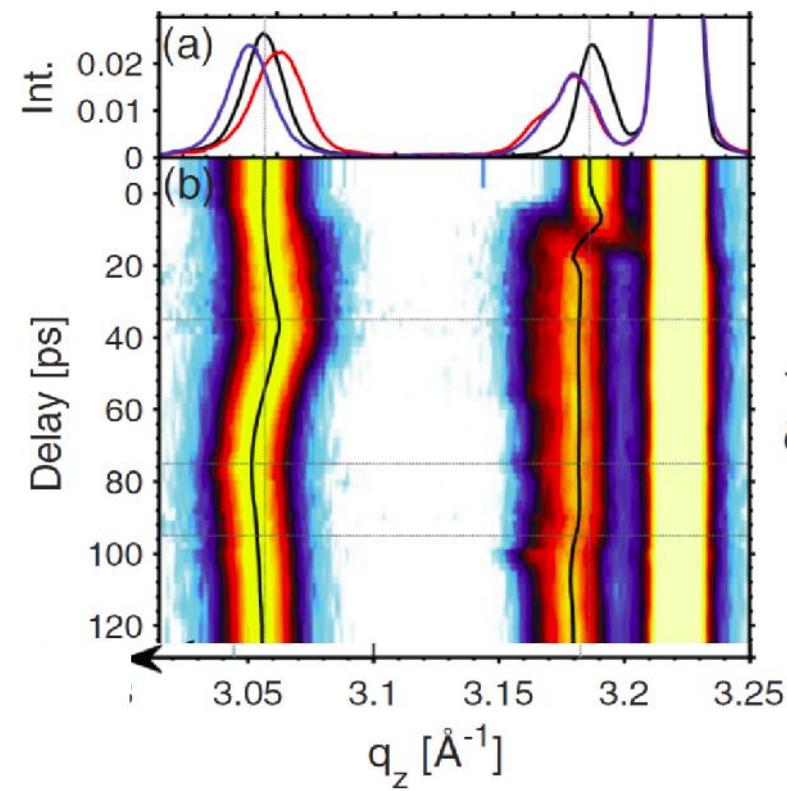
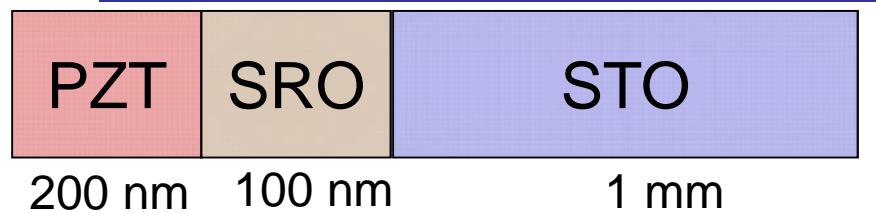
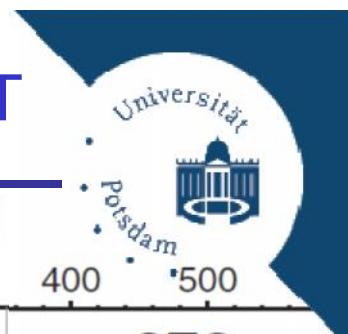


Various excitation mechanisms

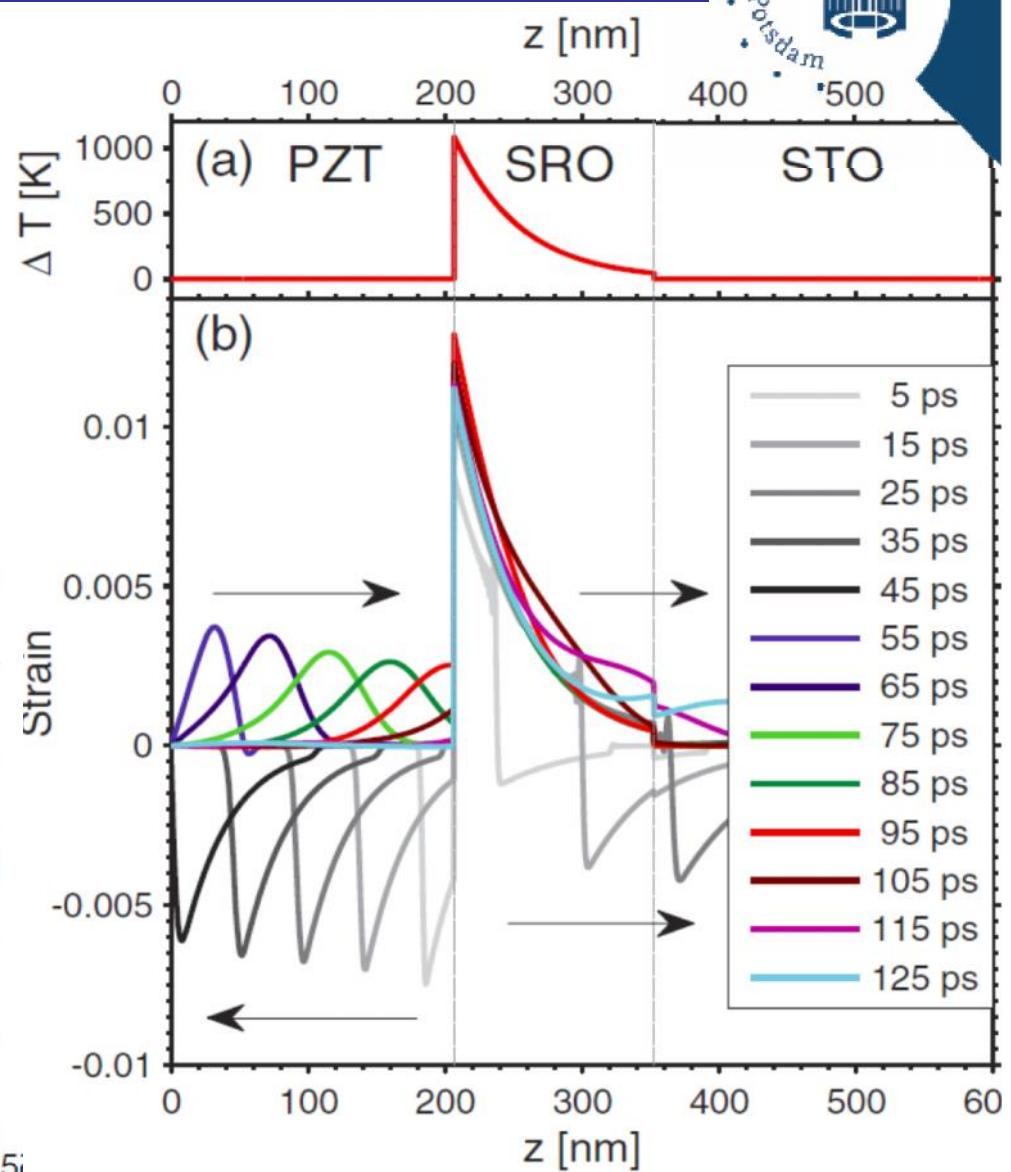
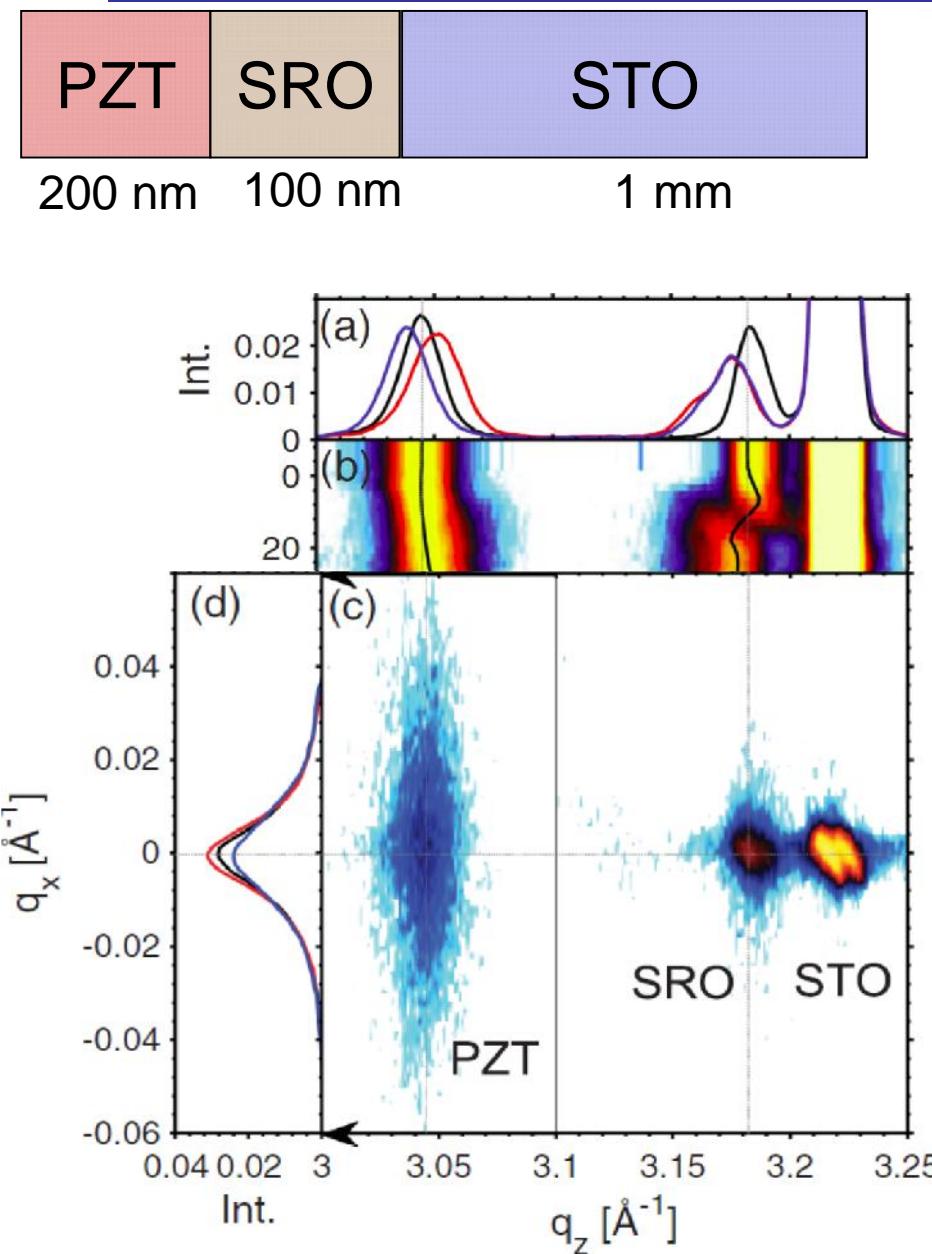
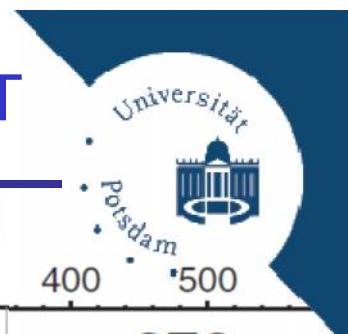
- excitation and coupling on **different time scales**



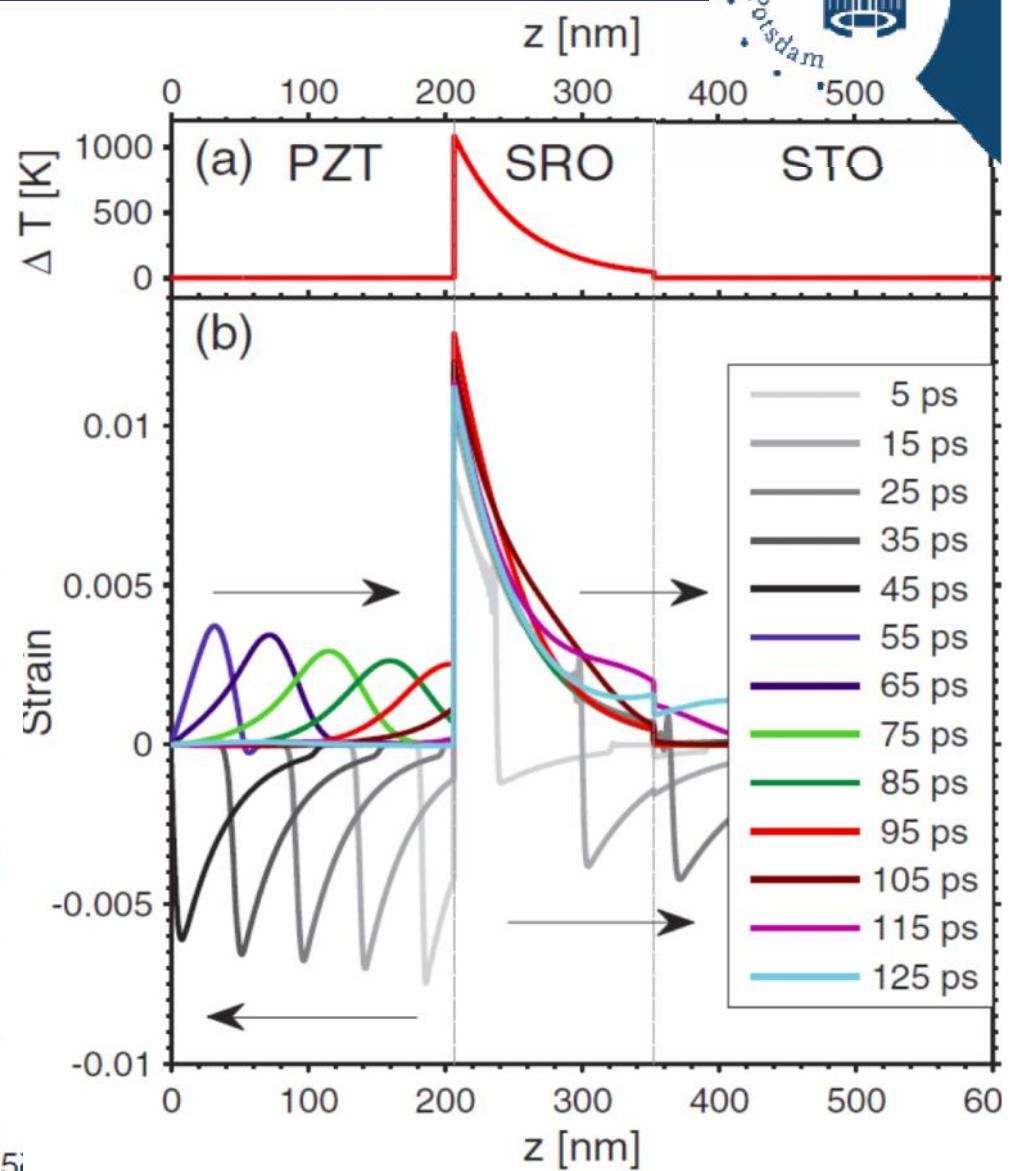
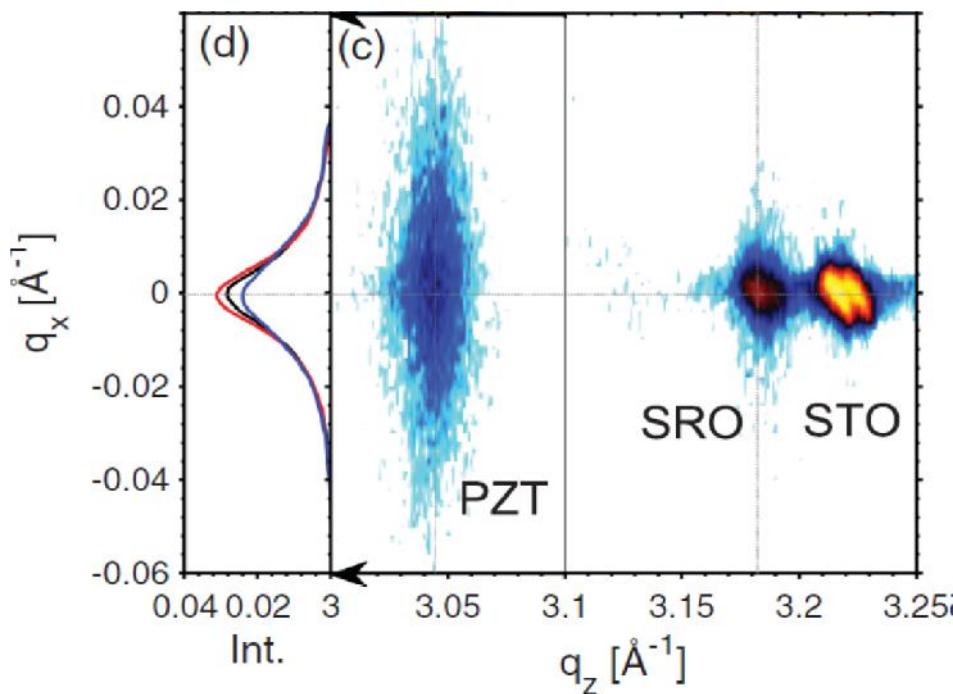
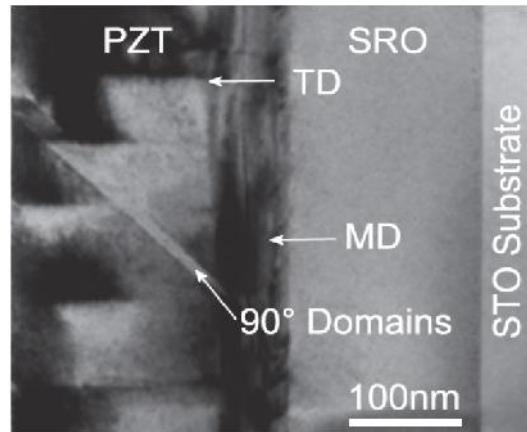
# Inhomogeneous Strain Propagation in PZT



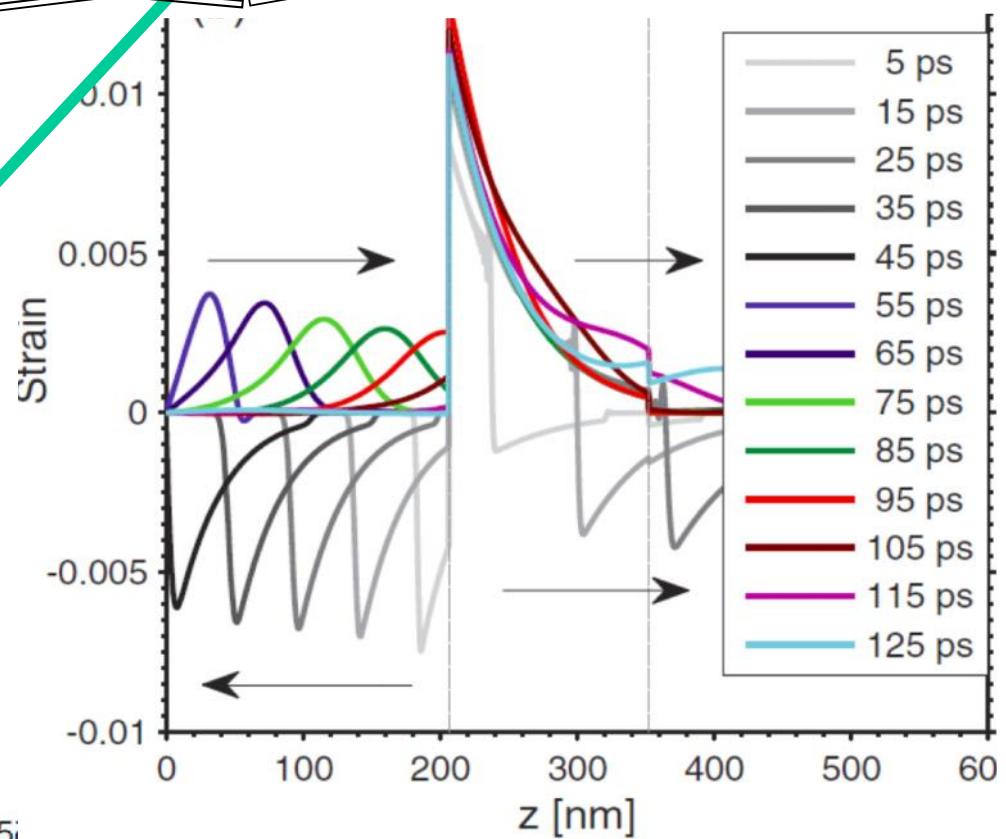
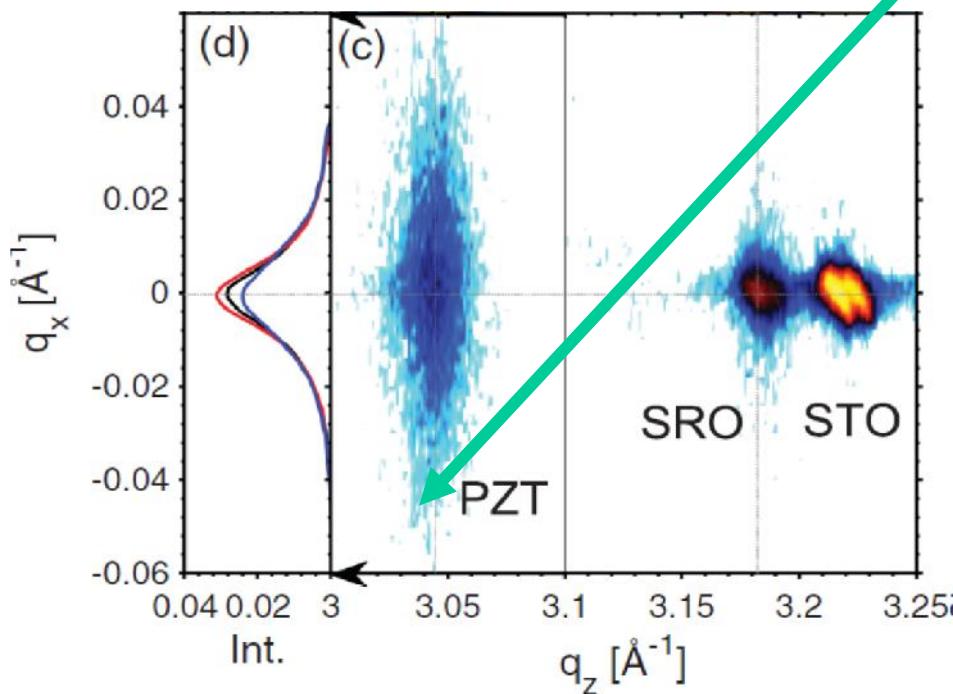
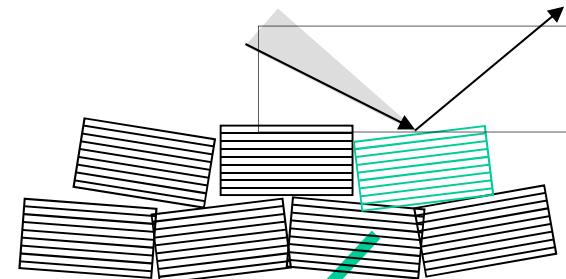
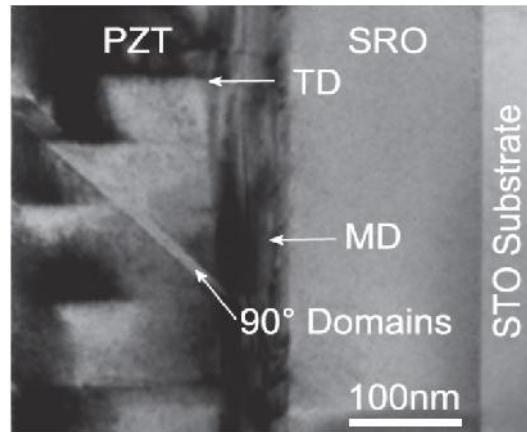
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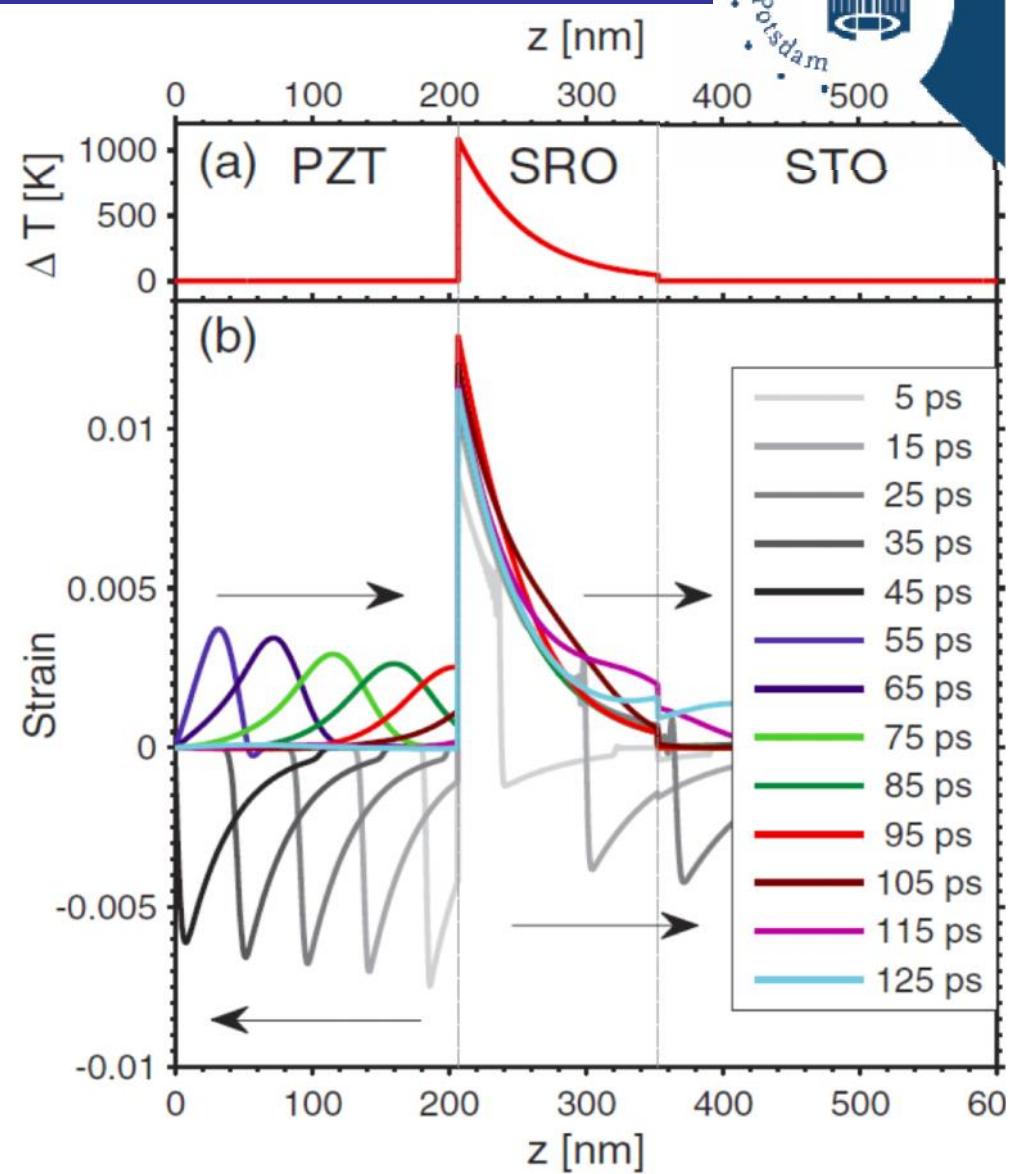
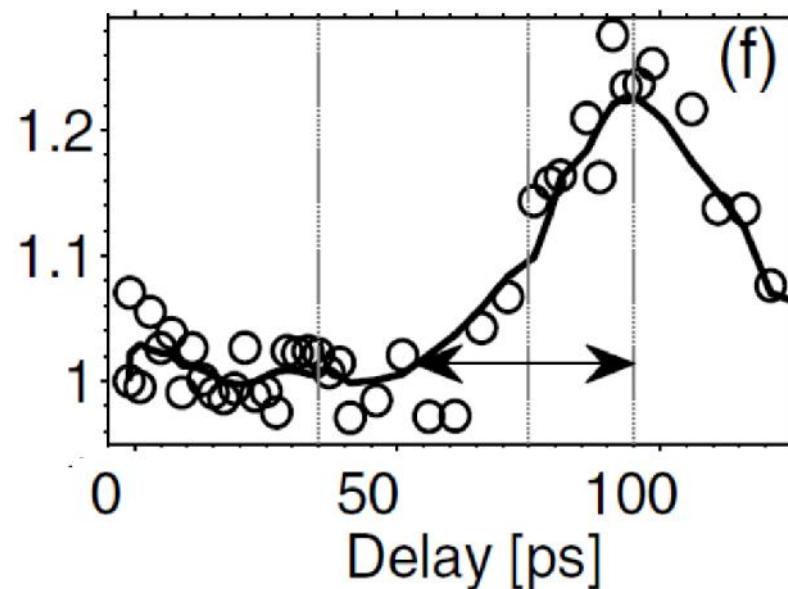
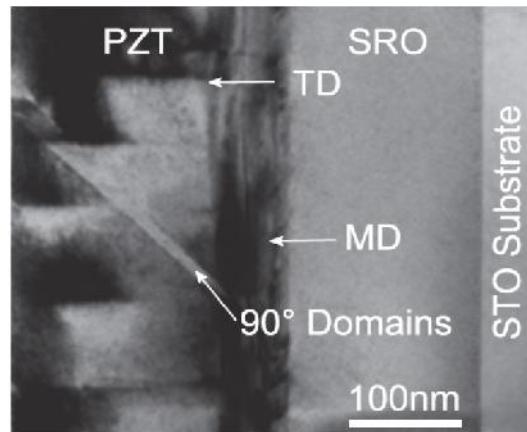
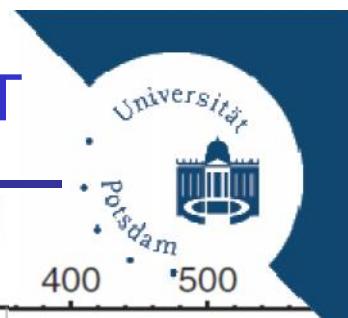
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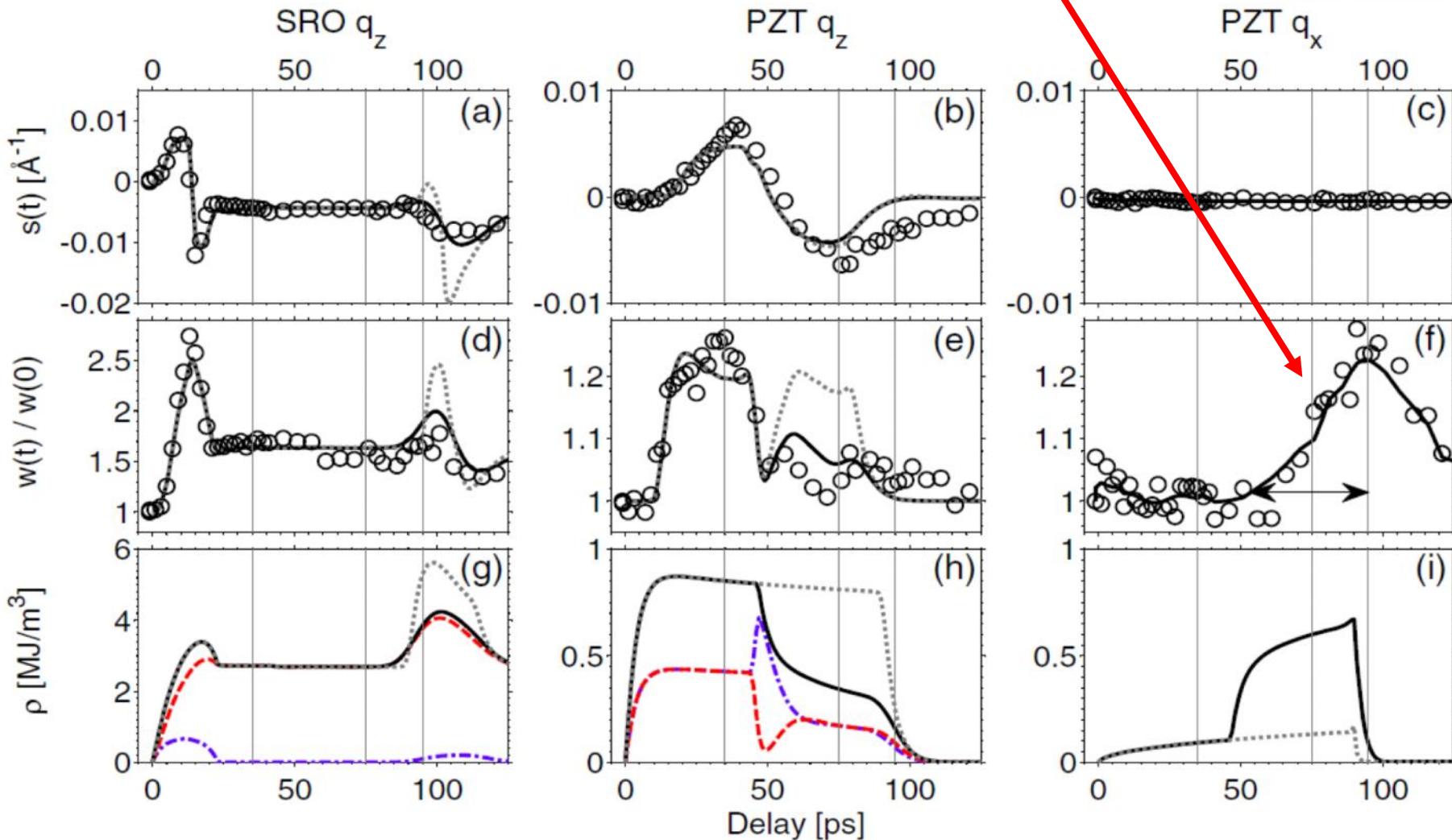
# Inhomogeneous Strain Propagation in PZT



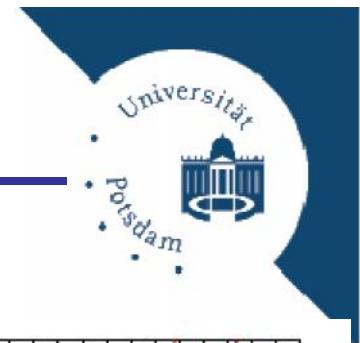
# Inhomogeneous Strain -> Broadening



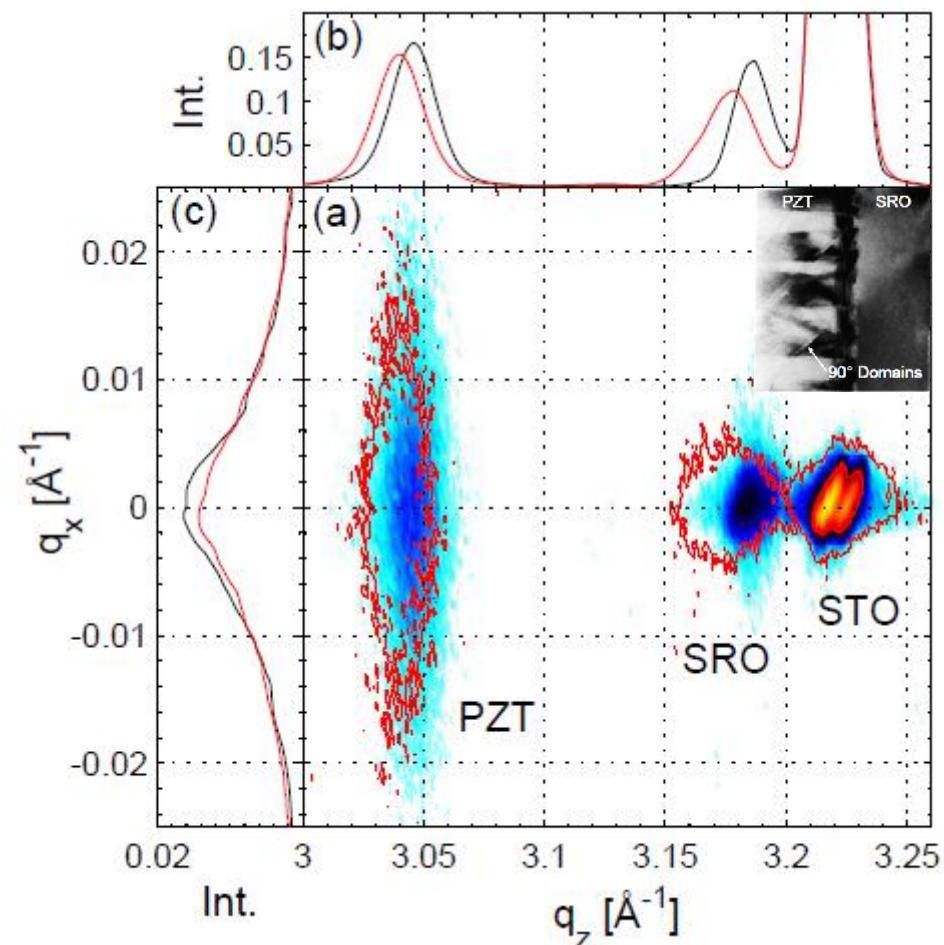
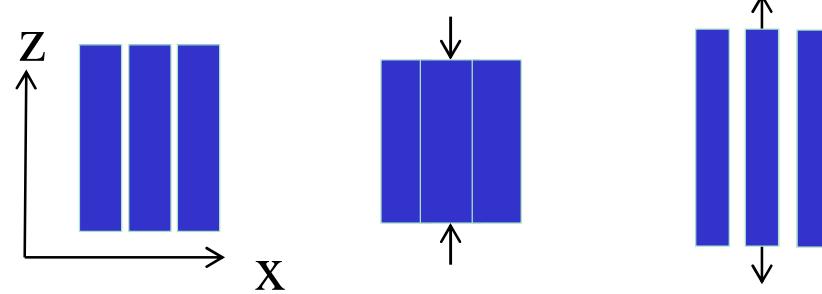
Reciprocal space mapping



# Dynamic stress relaxation at inhomogeneities

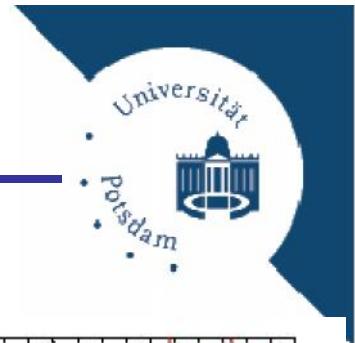


- coupling of **out-of-plane** into **in-plane lattice dynamics** for expansion wave due to **defects**
- not for **compression wave** or **laterally perfect structures**



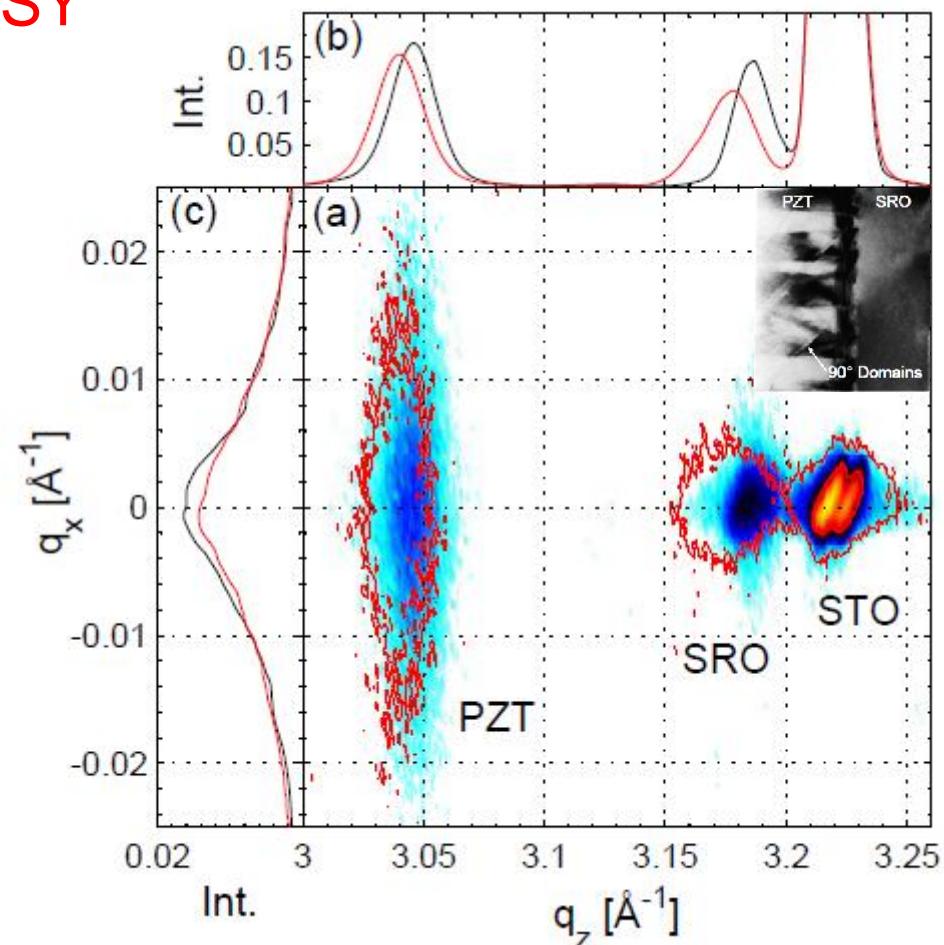
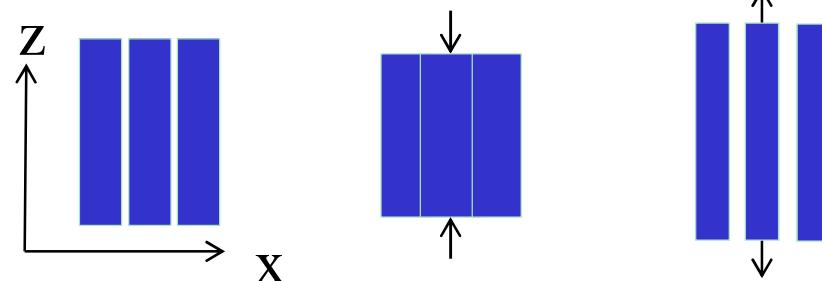


# Dynamic stress relaxation at inhomogeneities

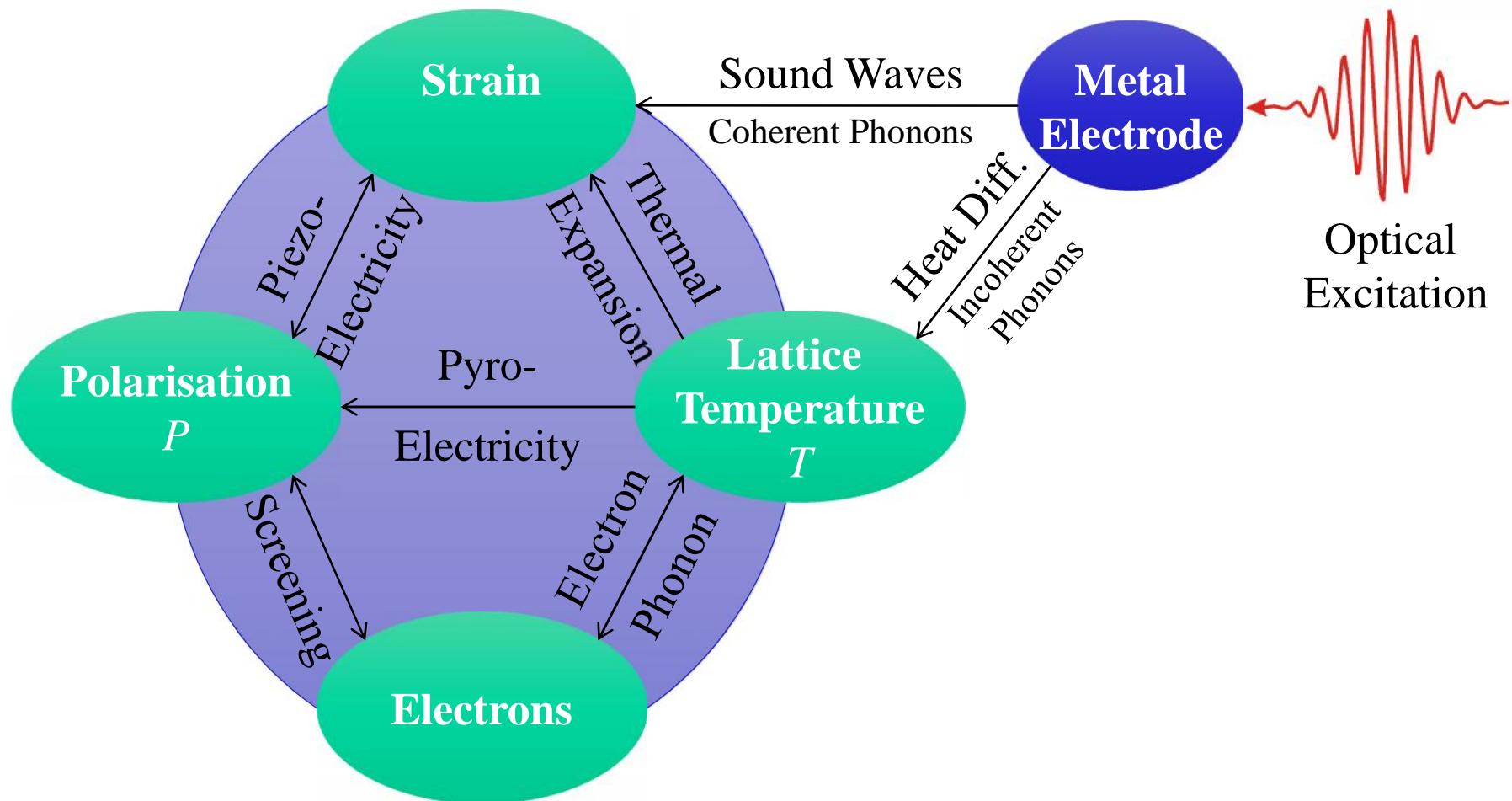


Need VSR to do this at BESSY

- coupling of **out-of-plane** into **in-plane lattice dynamics** for expansion wave due to **defects**
- not for **compression wave** or **laterally perfect structures**



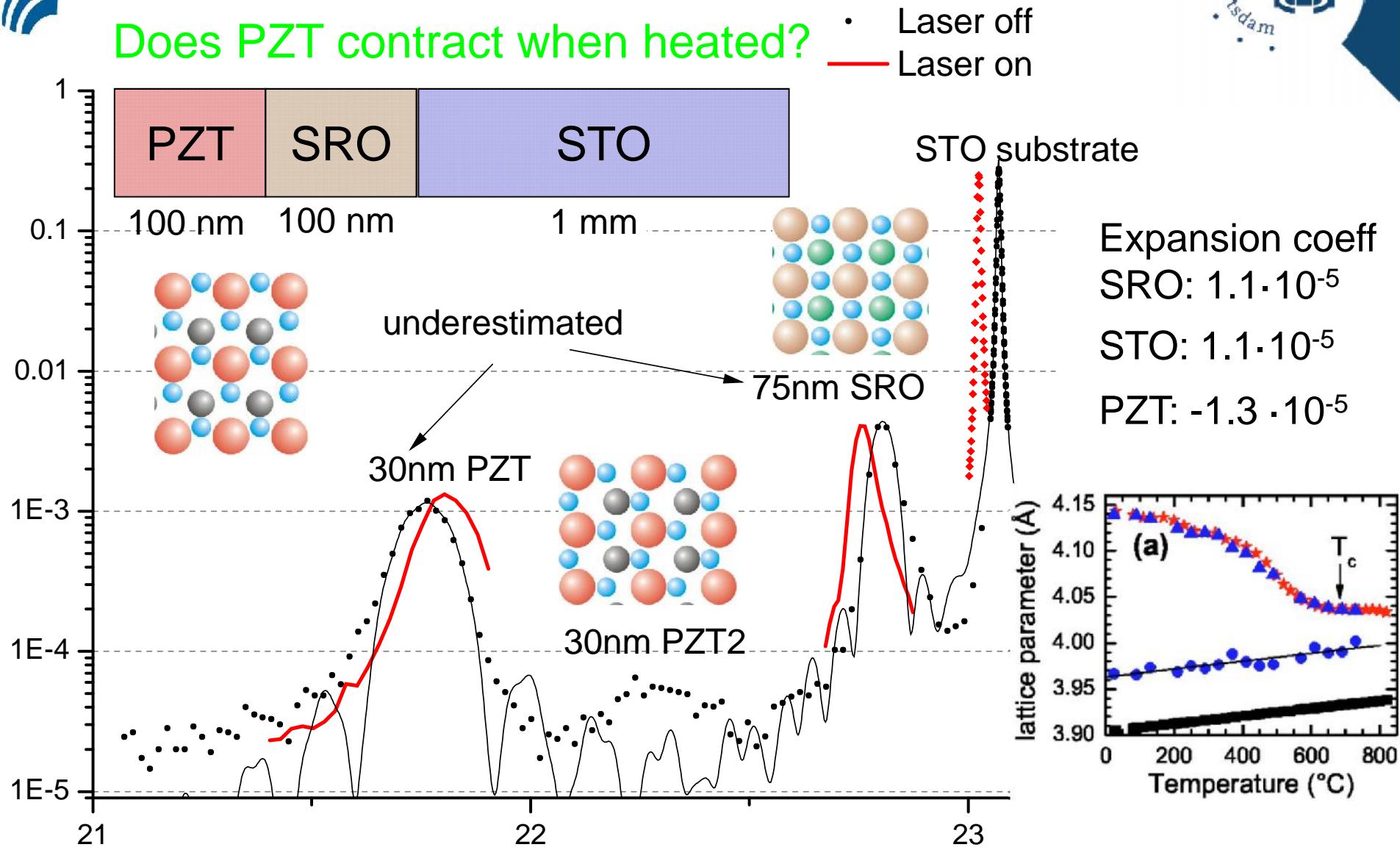
# Couplings Investigated by UXRD



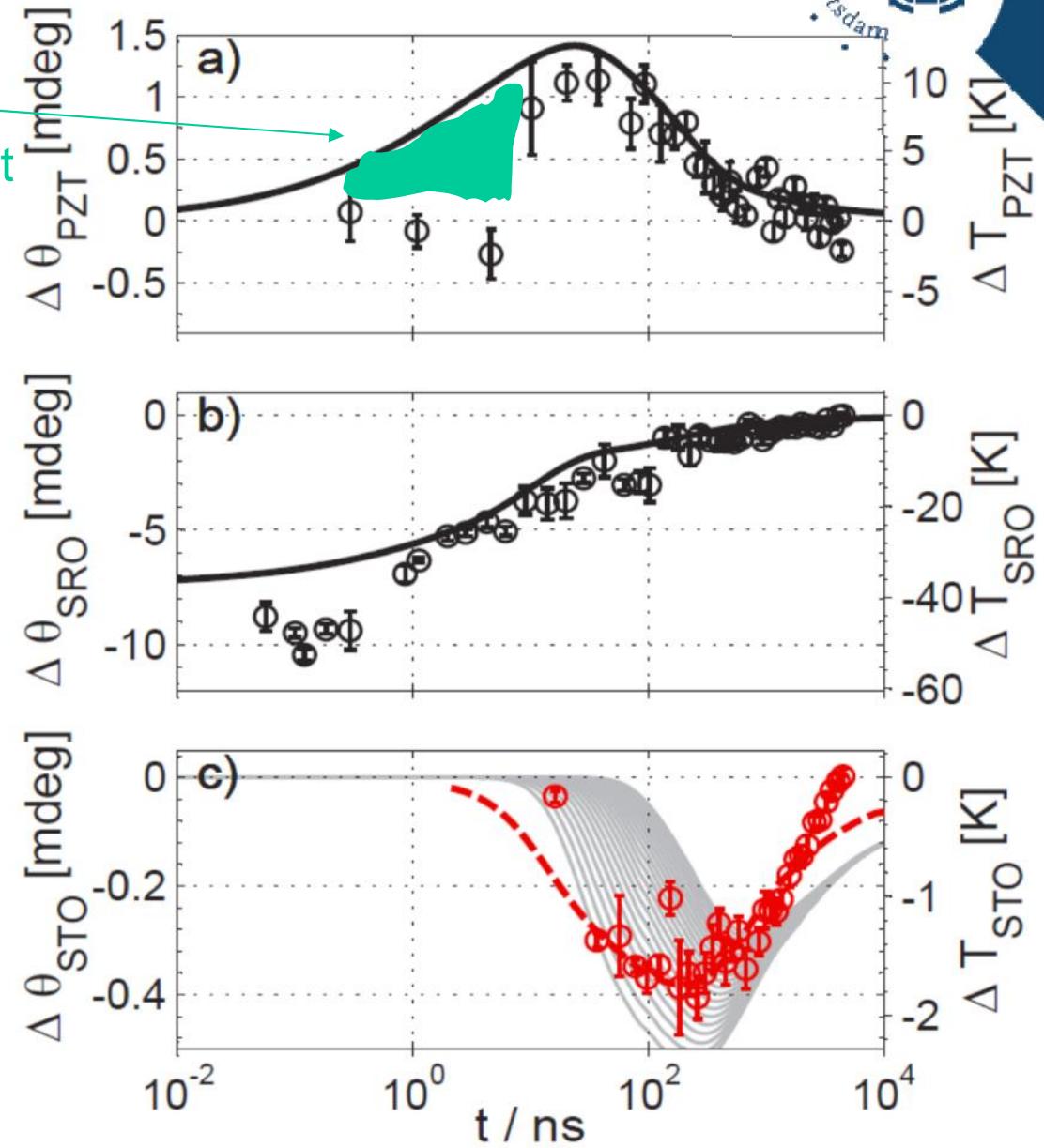
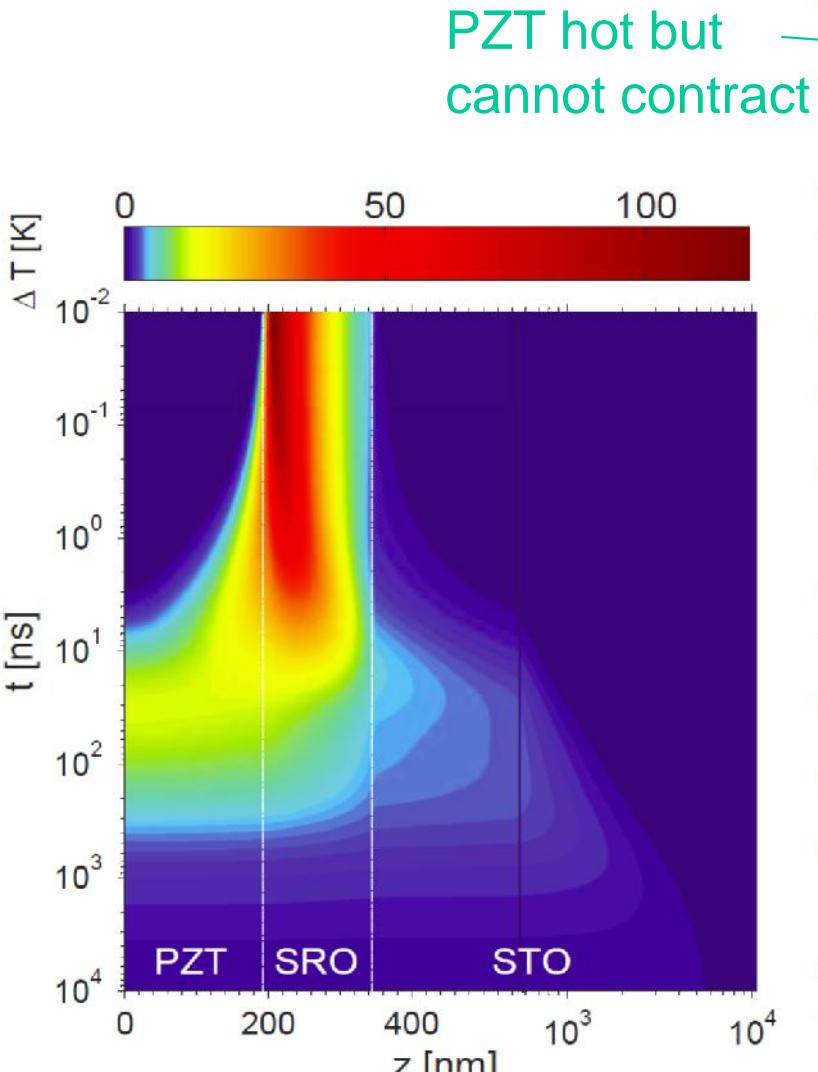
# Laser Heating of a Thin Ferroelectric Film



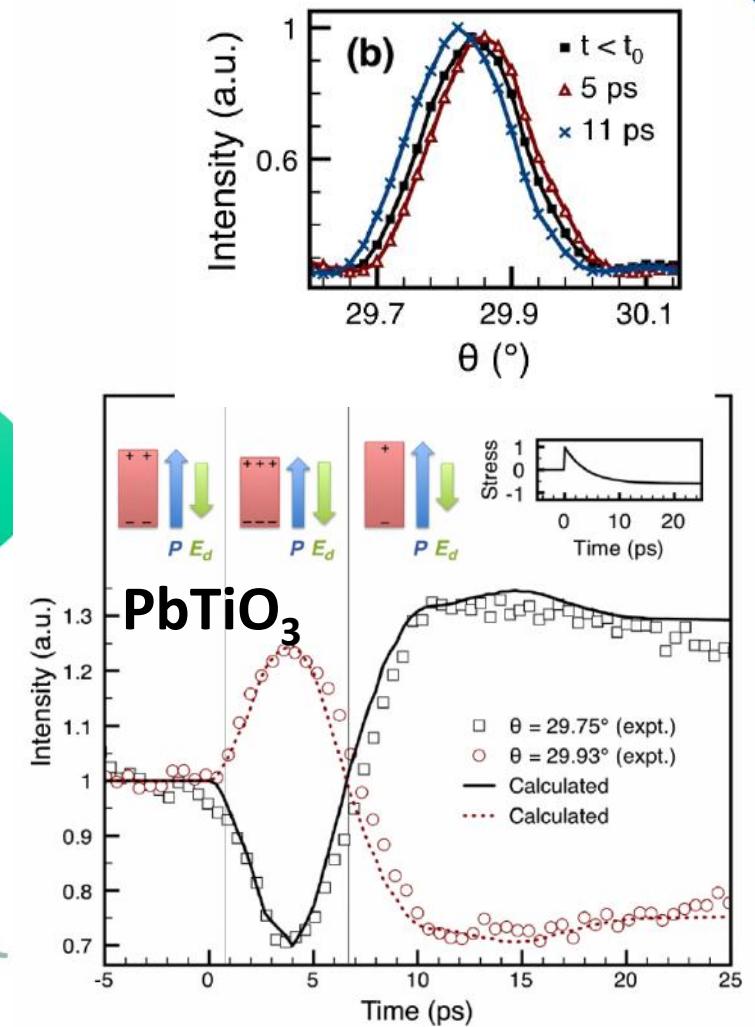
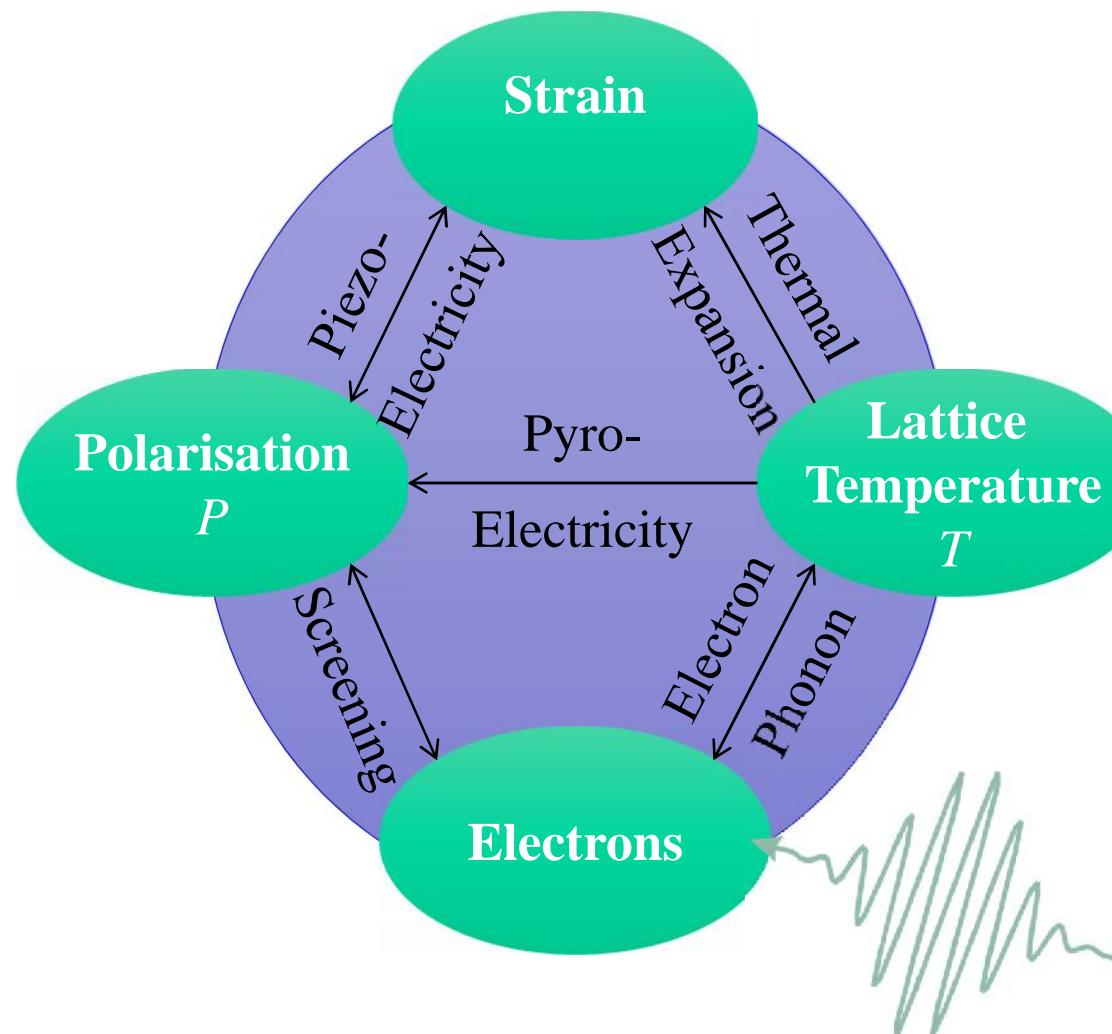
Does PZT contract when heated?



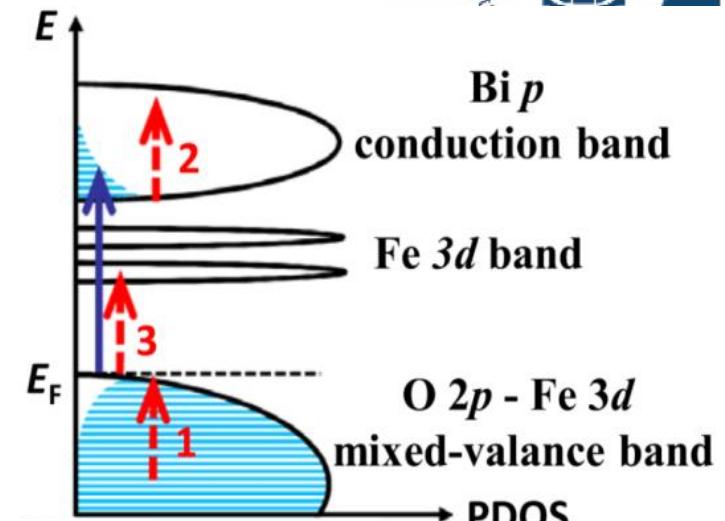
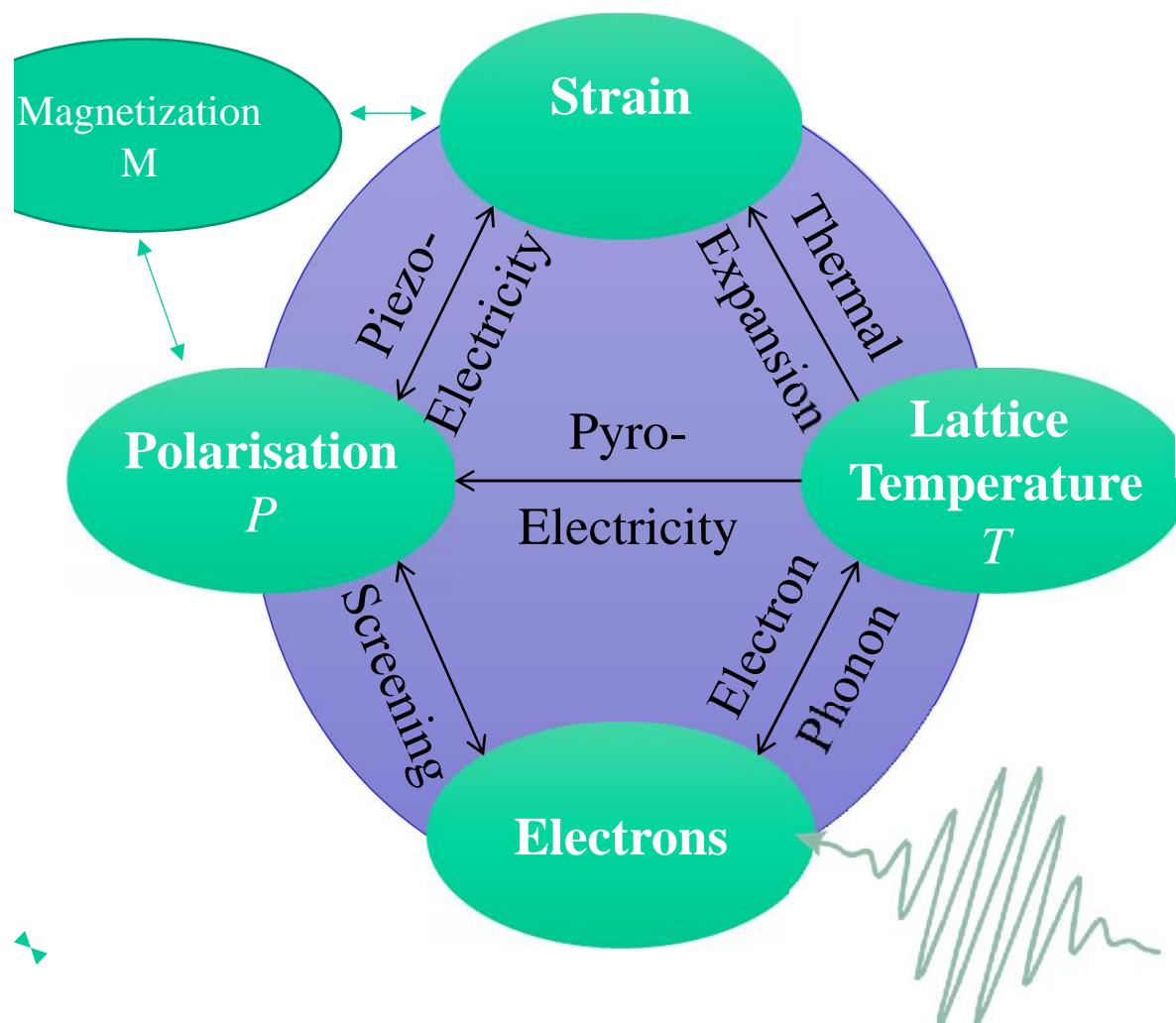
# PZT: c-Axis Expansion and Contraction



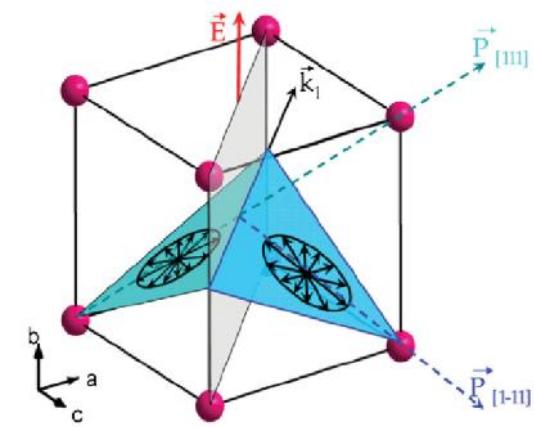
# Depolarization Fields and Shift Currents in $\text{PbTiO}_3$



# Depolarization Fields and Shift Currents in $\text{BiFeO}_3$



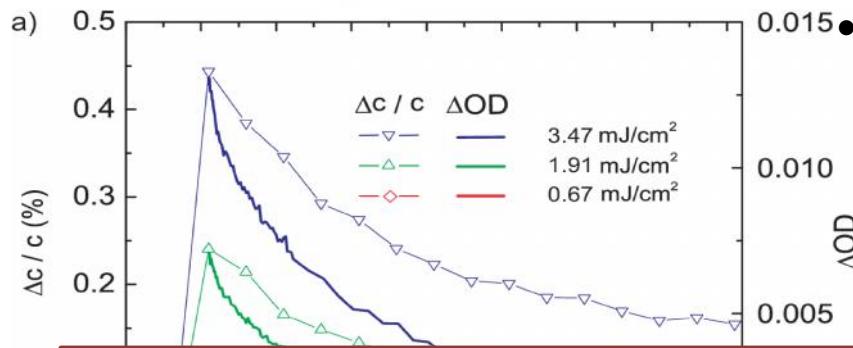
Magnetoelectric Effect



# Depolarization Fields and Shift Currents in BiFeO<sub>3</sub>



@APS  $\tau_{x-ray} \approx 100\text{ps}$

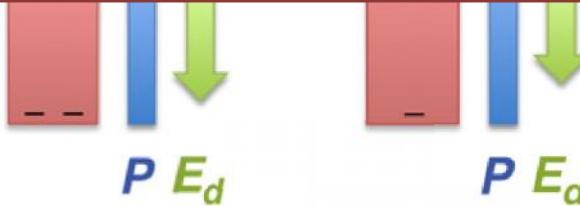
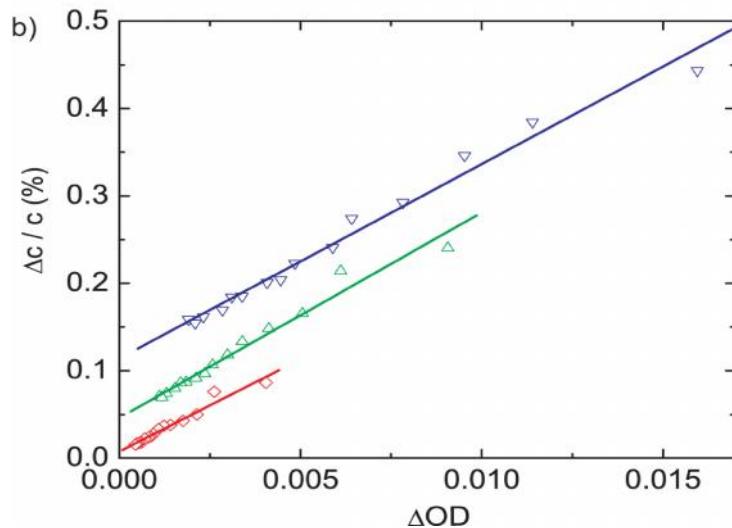


- **depolarization field screening (DFS)**

- photogenerated free charge carriers
- macroscopic transport to interfaces
- strain generation via inverse piezoelectric effect



What happens in the first 100ps?



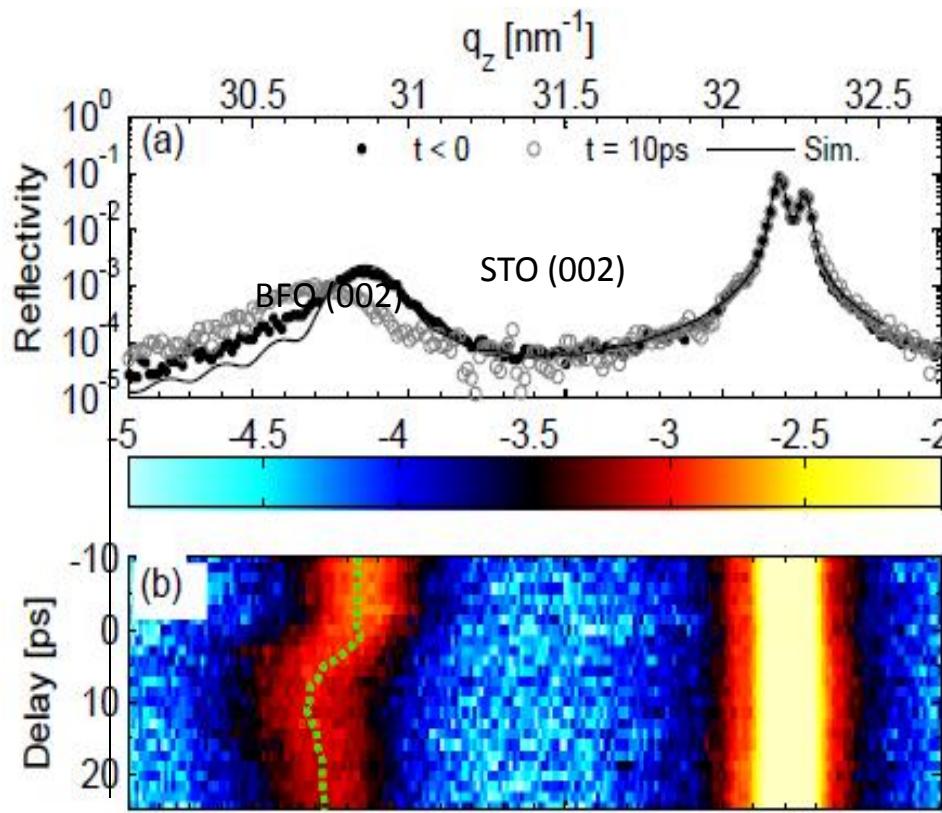
$$\tau_c = \frac{d}{v_d} = \frac{d}{\mu E} > 5\text{ps}$$

carrier mobility:  $\mu = 0.1 - 3.0 \text{ cm}^2/\text{Vs}$   
internal electric field:  $E \approx 200 \text{ kV/cm}$

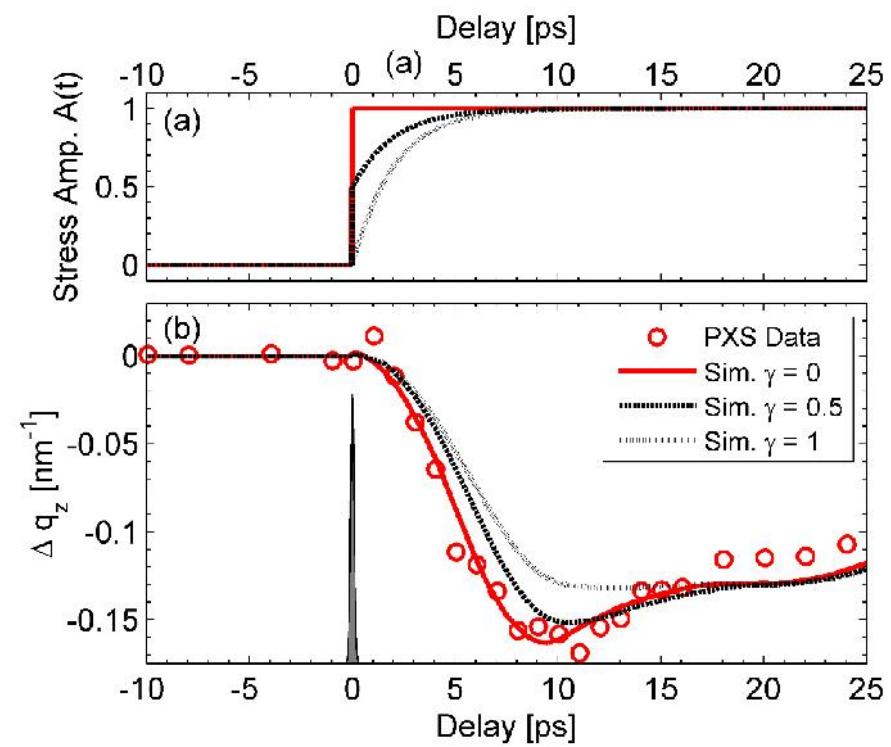
# Above-Band-Gap Excitation of BFO



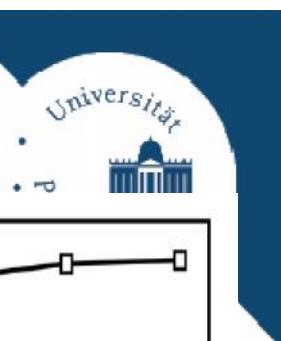
Shift of BFO Bragg peak



Stress is dominantly instantaneous  
No long range carrier motion!



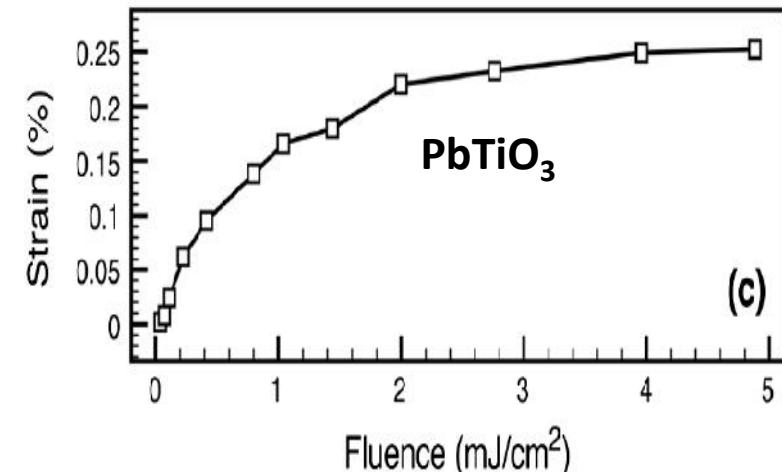
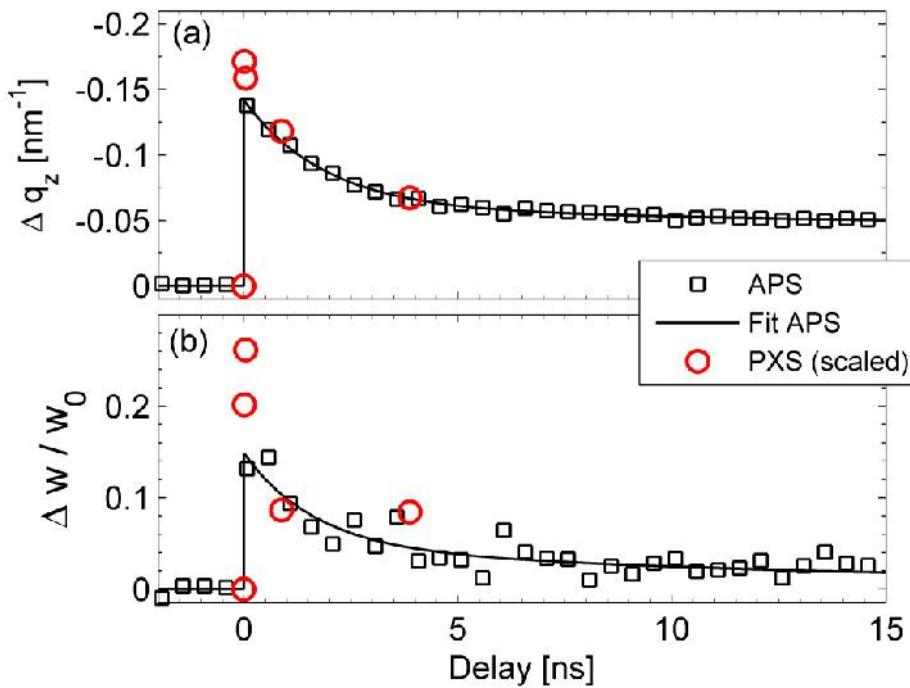
# Arguments against Depolarization Field Screening



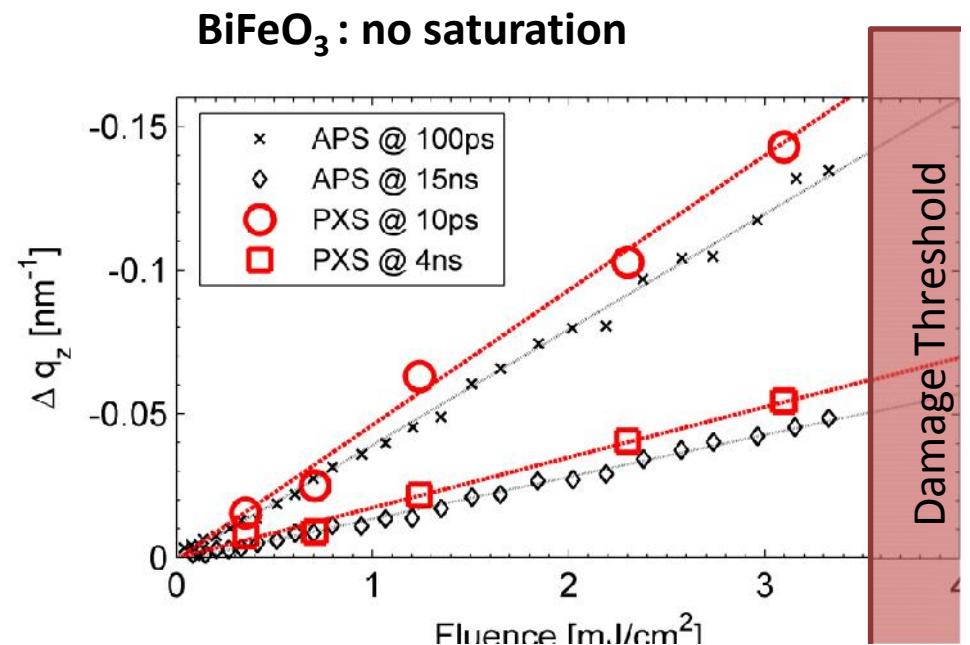
Shift and width have same decay time  
Inhomogeneous stress remains in BFO!

Fluence dependence without saturation.

$$\text{shift} = 2.29\text{ns} \quad \text{width} = 2.31\text{ns}$$



D. Daranciang et al, Phys. Rev. Lett. **108**, 087601 (2012)



**PostDocs and PhD students  
University of Potsdam  
+ HZB:**

Daniel Schick

Dr. Peter Gaal

Dr. Wolfram Leitenberger

Dr. Roman Shayduk

Dr. Hengameh Navirian

Yevgeni Goldshteyn



**Collaboration PZT**

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**Ionela Vrejoiu**

**Collaboration BFO**

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**Haidan Wen  
Yuelin Li**



Cornell University

**Carolina Adamo  
Darrell G. Schlorom**



**WISCONSIN**  
UNIVERSITY OF WISCONSIN-MADISON

**Pice Chen  
Paul G. Evans**

# Summary



- UXRD data from synchrotrons and plasma source
- Heat transport ~10 ps on ~20nm length scale
- Inhomogeneous transient strain (SRO)
- Domains trigger in-plane dynamics in PZT  
Damping different for expansion and compr.
- Heat transport in SRO/PZT + in-plane sound  
PZT cannot contract faster than 10 ns
- Above band gap excitation of BFO  
No charge carrier motion – inhomogeneous!  
Depolarization field screening not dominant
- Stress instantaneous – only orbital changes

