# Static and Dynamic Disorder in Ba-doped Bismuth Sodium Titanate

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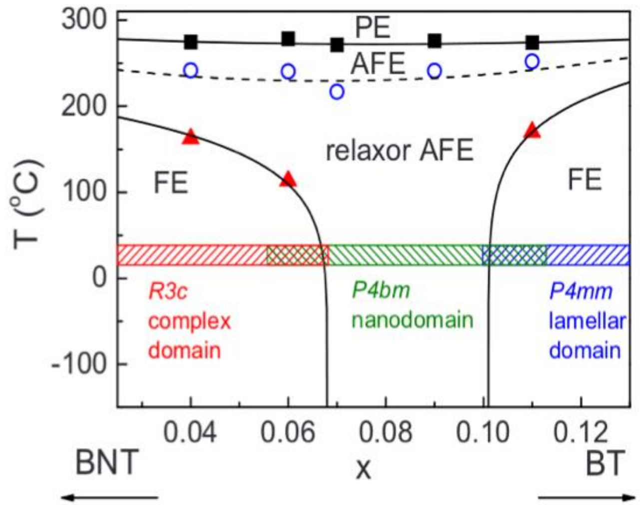
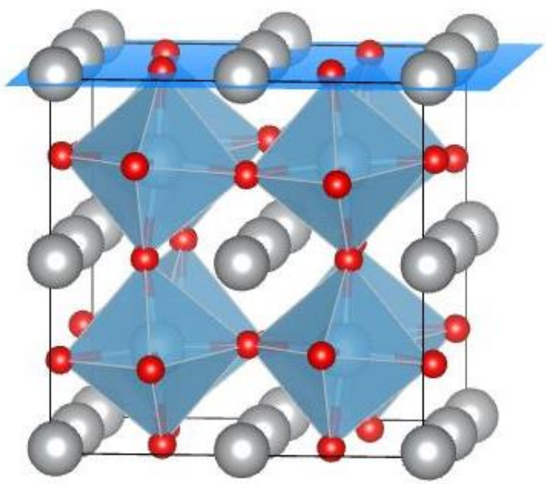
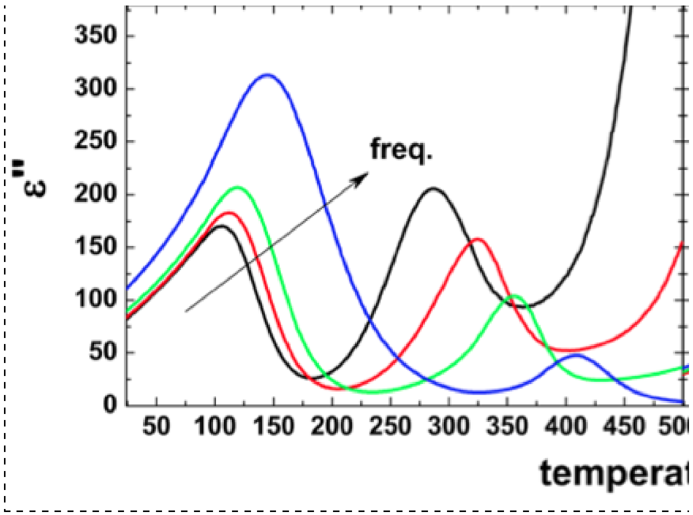
# Barium-doped Bismuth Sodium Titanate



- Octahedral tilt system changes at morphotropic phase boundary: high susceptibility

What are the „relaxors“? → disorder

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# Diffuse Scattering:
# Measures the Deviations from Ensemble Averages

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Regular arrangement of atoms and molecules leads to Bragg reflections (Fourier-components of order)

Deviations from this regular arrangement leads to diffuse scattering (Fourier-components of disorder)

$$F(\mathbf{h}) = \sum < f > \; e^{2\pi i \mathbf{h} < \mathbf{u} >} + \sum (f - < f >) \; e^{2\pi i \mathbf{h} < \mathbf{u} >} +$$

$$\sum < f > \; e^{2\pi i \mathbf{h}(\mathbf{u} - < \mathbf{u} >)} + \sum (f - < f >) \; e^{2\pi i \mathbf{h}(\mathbf{u} - < \mathbf{u} >)}$$

# Diffuse Scattering from BNT-BT: Bananas and Streaks (no Butterflies)

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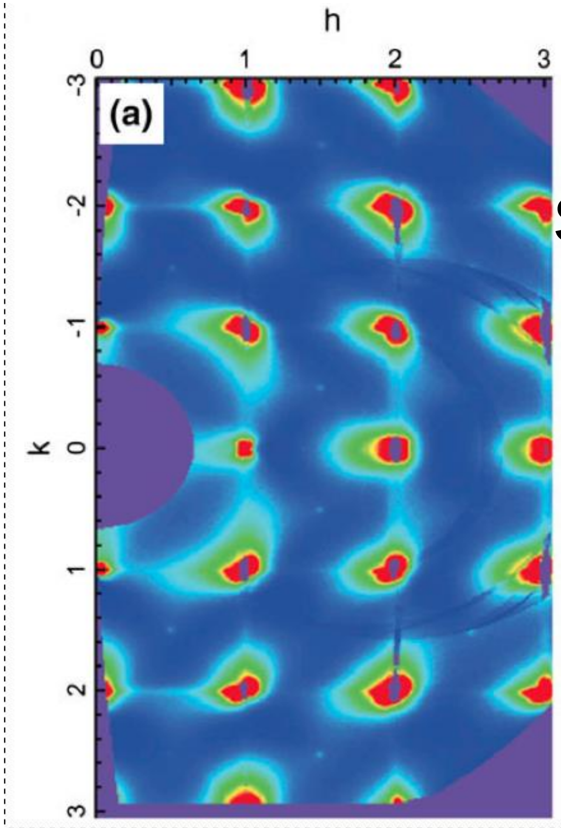
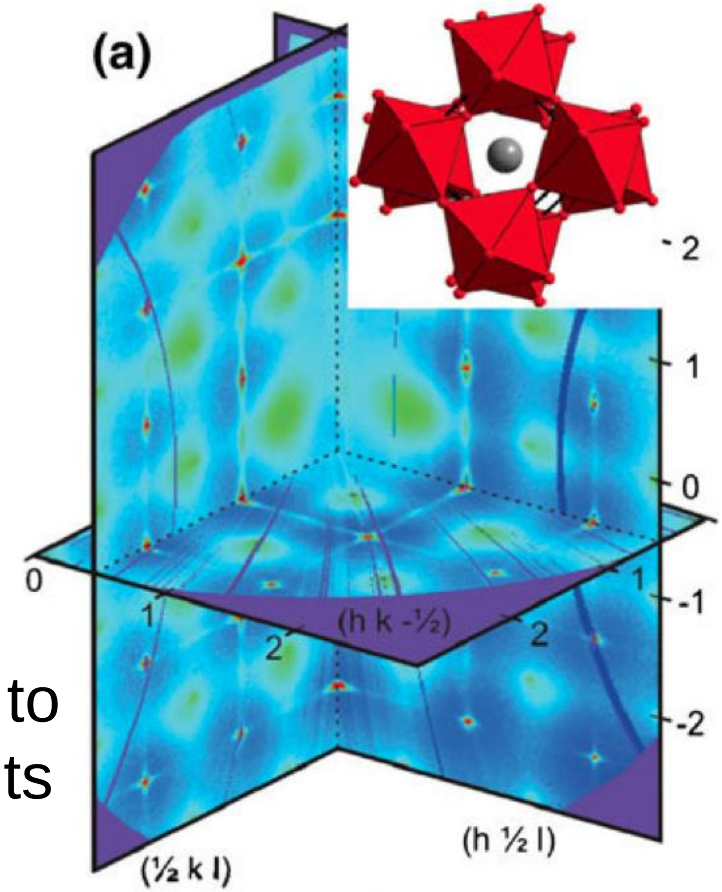



SRO scattering

Streaks due to stacking faults




(hk0) plane

3d-cut

*J. Daniels, W. Jo, W. Donner, JOM 2012*



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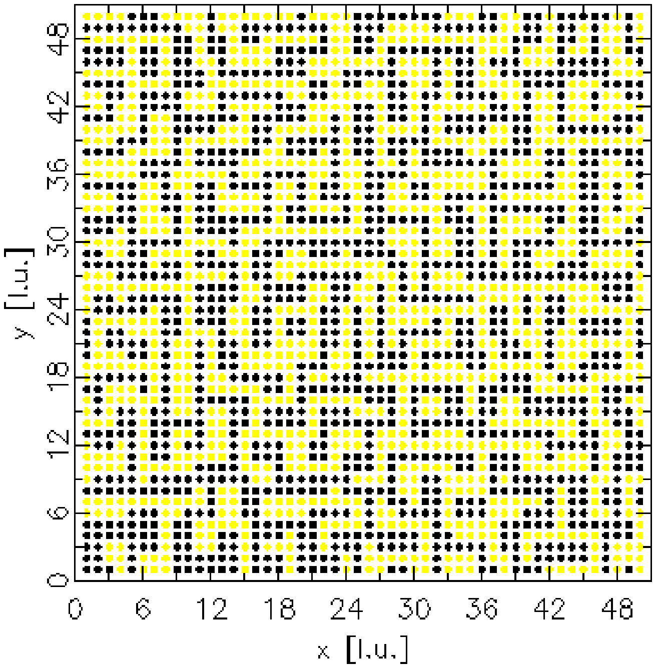
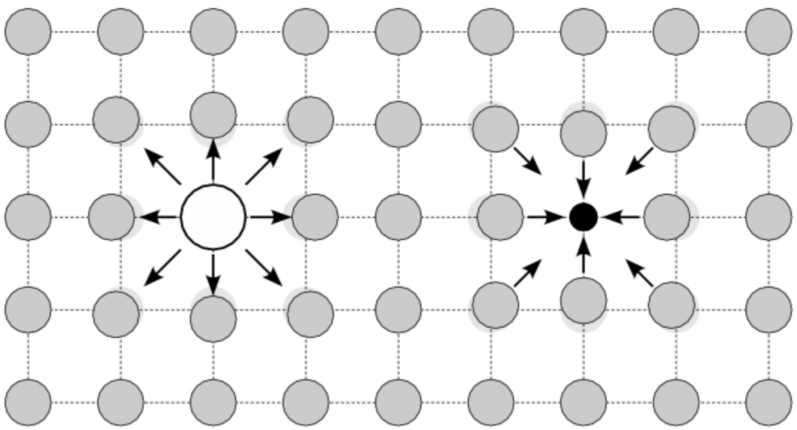
# SRO and Size-Effect

$$I_{diff}(\mathbf{q}) \propto N c_A c_B (f_B - f_A)^2 \left[ \sum_{mn} \alpha_m \cos(\mathbf{q}\mathbf{r}_{mn}) + \sum_{mn \neq 0} \beta_m \mathbf{q}\mathbf{r}_{mn} \sin(\mathbf{q}\mathbf{r}_{mn}) \right] .$$

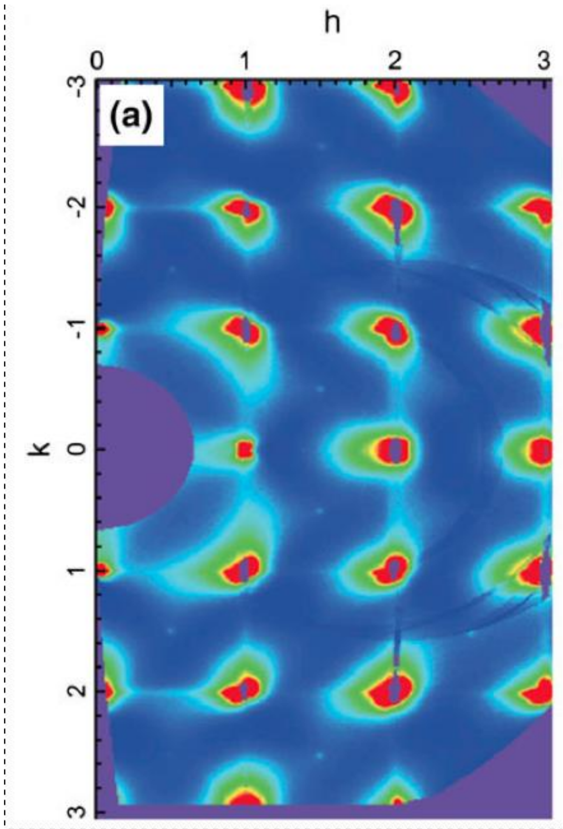



Correlation of Bi/Na atoms positive in <100> direction, negative in <110> direction

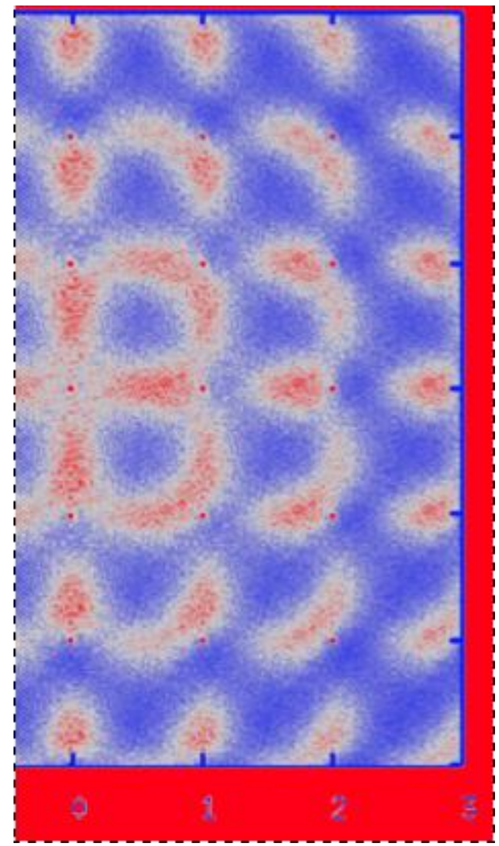


Asymmetry of diffuse scattering due to size effect

# SRO and Size-Effect (Bananas)

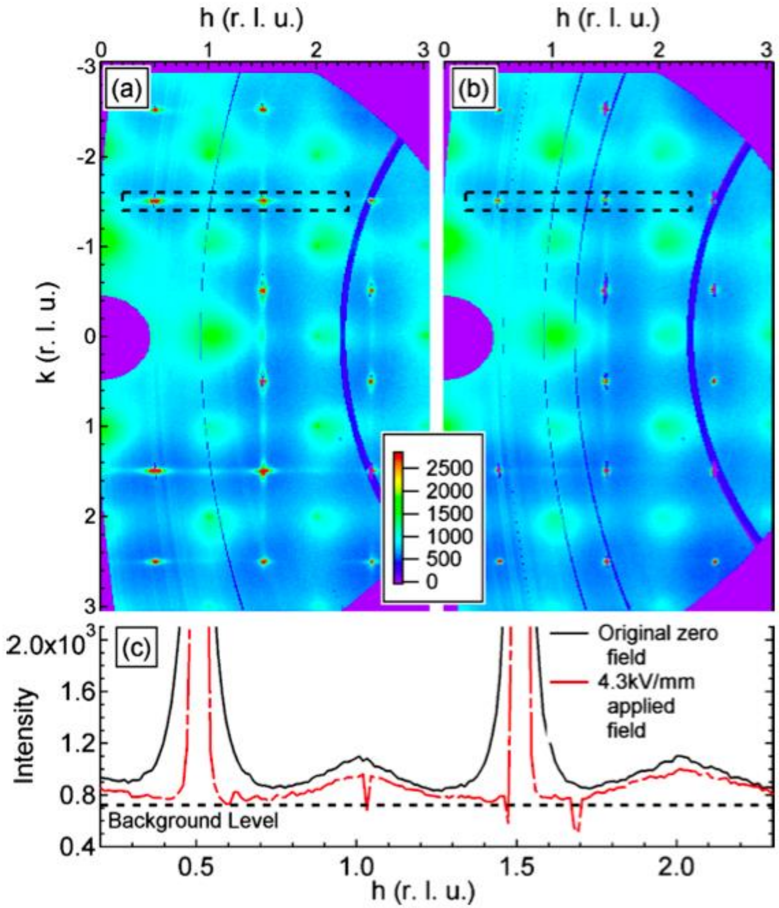



Correlation of Bi/Na atoms positive in <100> direction, negative in <110> direction



Asymmetry of diffuse scattering due to size effect

# Field-dependence of Half-order Intensity (Streaks)




Measurement at ID15 (ESRF)
by J. Daniels, W. Jo

One tilt system grows on the cost of the other: 20nm initial size

How do these (electrically active) stacking faults look like?

# The Double Fault Structure
# (Single Faults Produce Inverted Domains)

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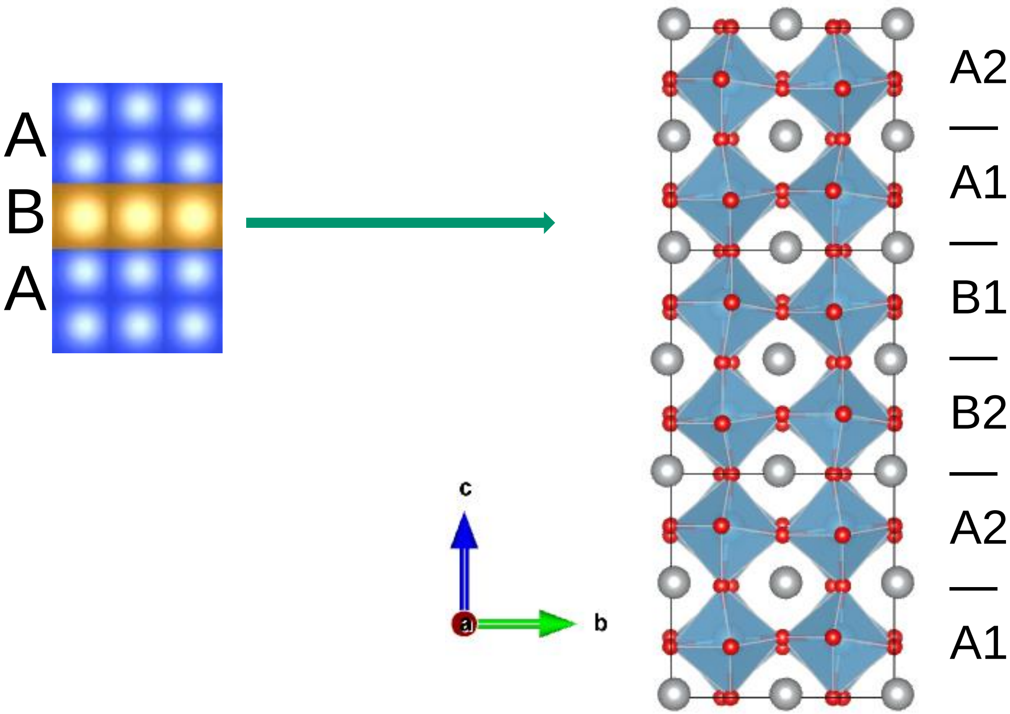
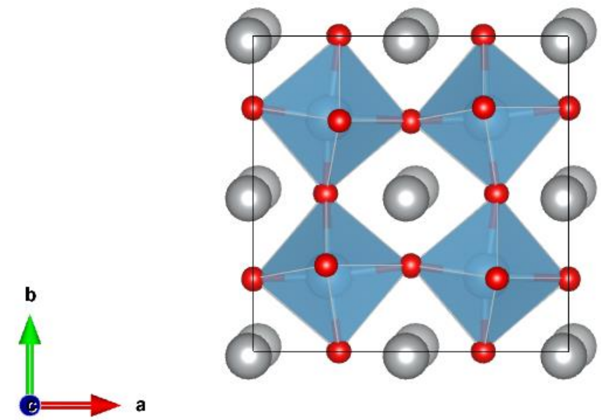



The A2-B2 part from top:




R3c | Pbnm
$a^-a^-a^-$ | $a^-a^-a^+$



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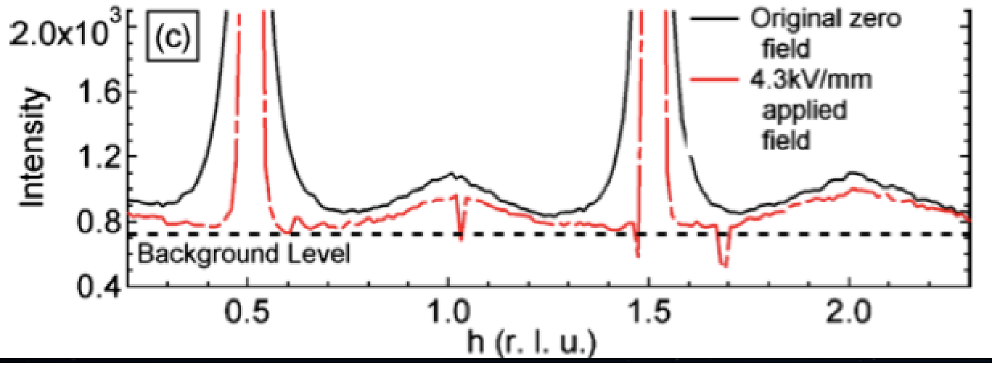
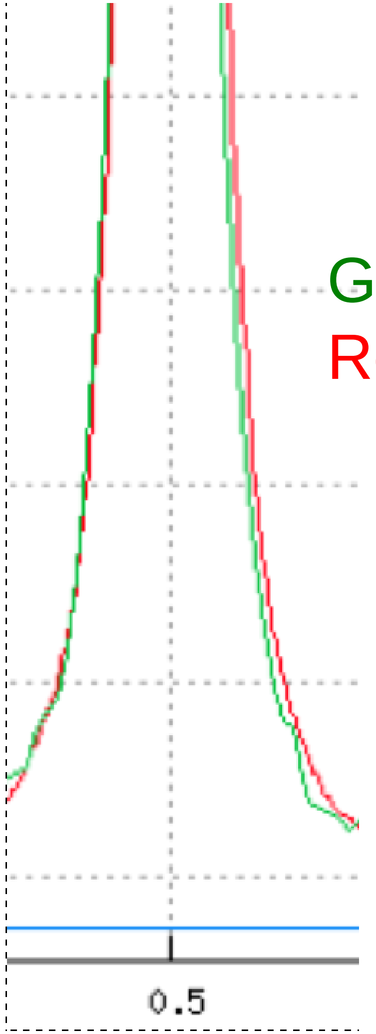
# Line Scan Through Half-order Streak (and simulation with DISCUS)



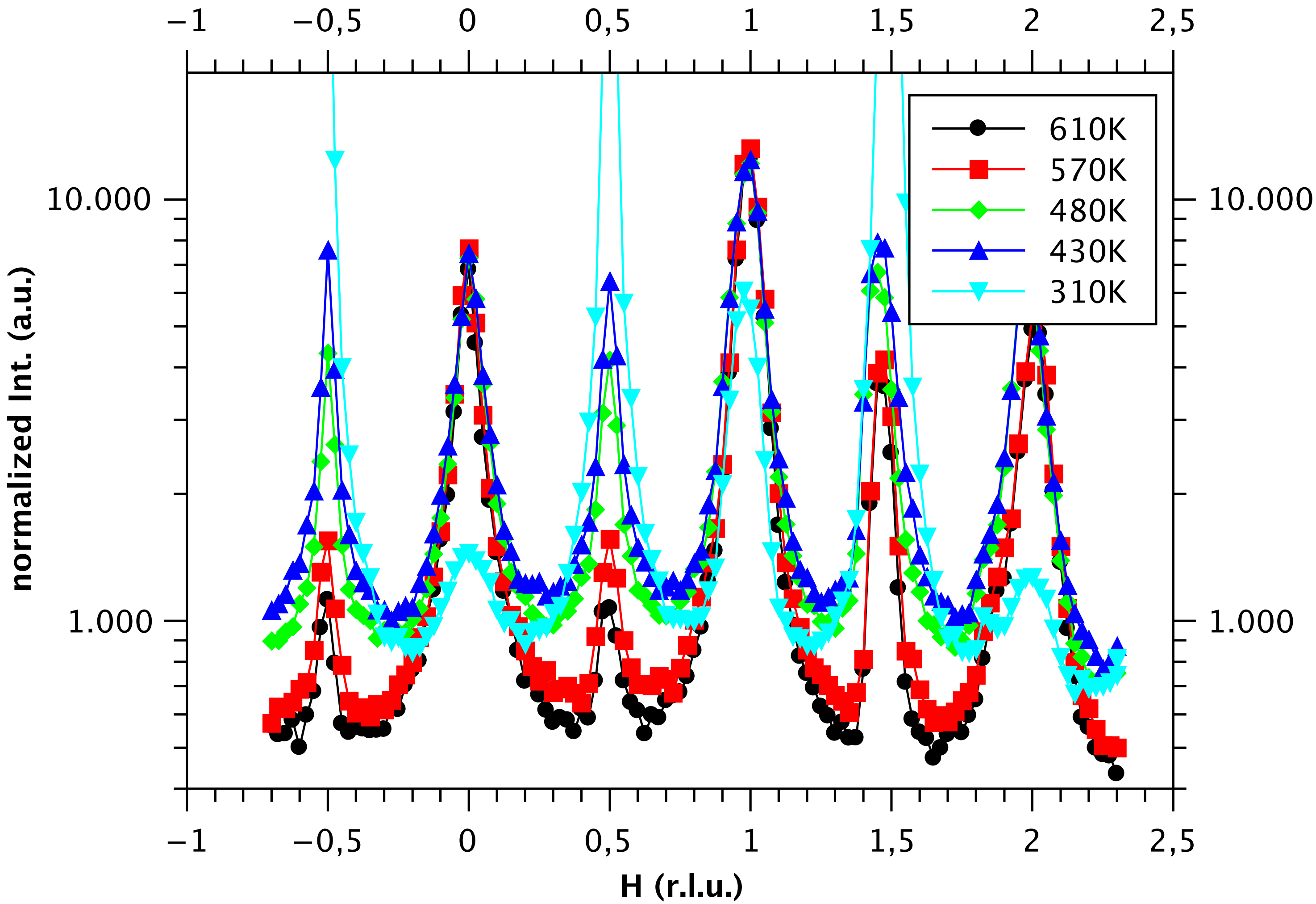




Green: data

Red: simulation

Stacking fault probability: 2%

# Temperature Dependence of Half-order Streaks (EIGER, PSI)



# Compare Stacking Fault Density and Permittivity

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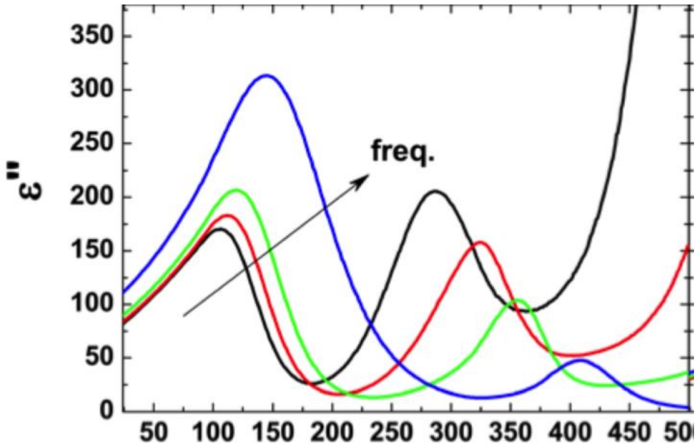
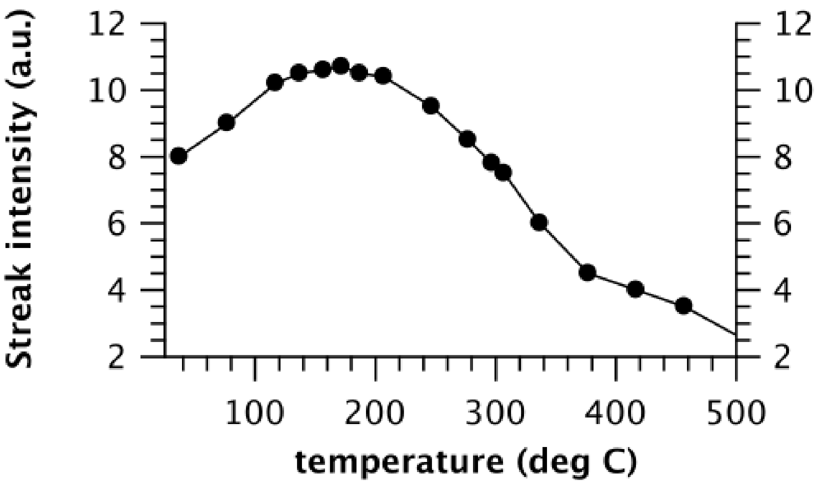



ε´´ is the damping of the permittivity
max. at high frequencies

*Wook Jo et al.: JAP 2011*




intensity of streaks
→ probability of stacking faults
→ density of relaxors

*neutron data from EIGER @ PSI*



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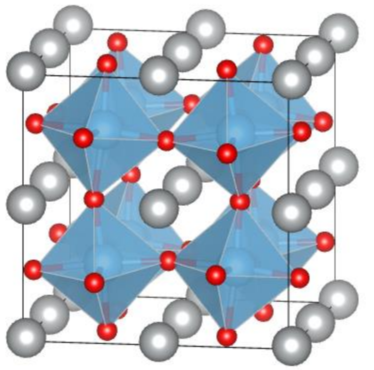
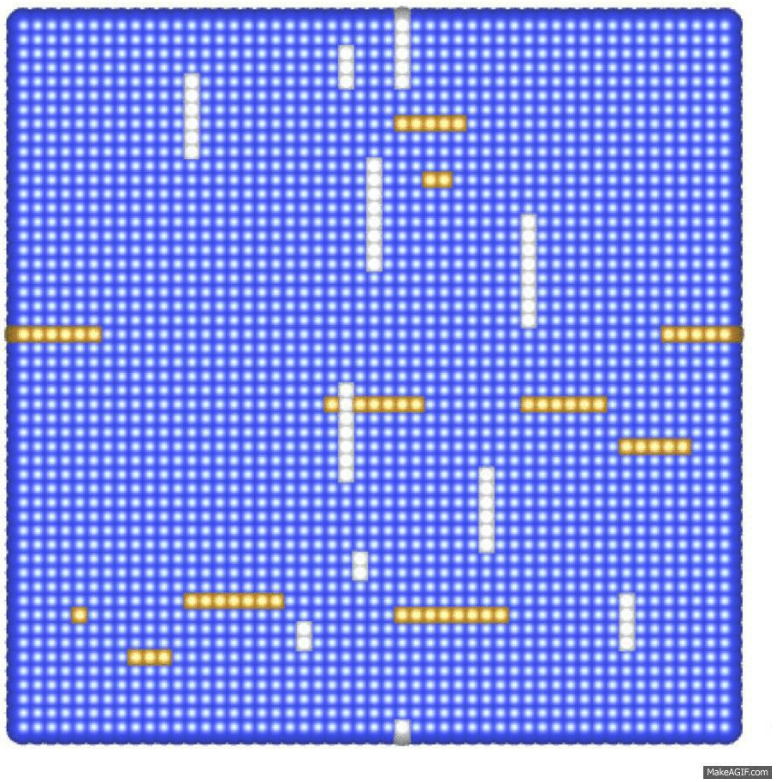
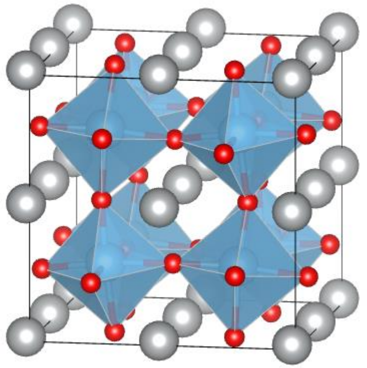
# Actual Model in Real Space (and Time):

Blue: “matrix” A1-A2

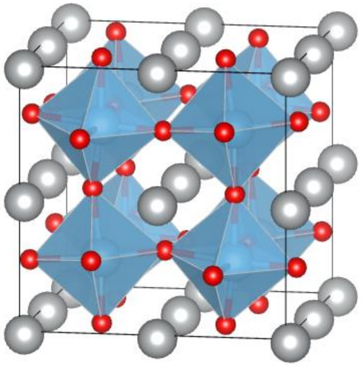




Yellow: vertical (double) fault B2-B1

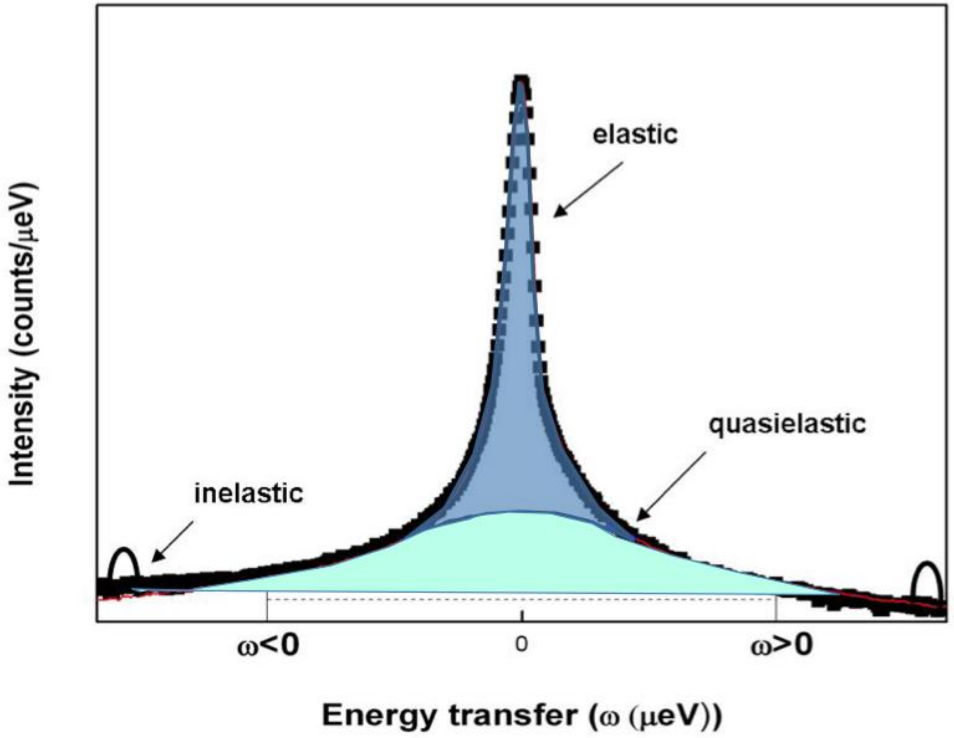


White: horizontal (double) fault B2-B1V

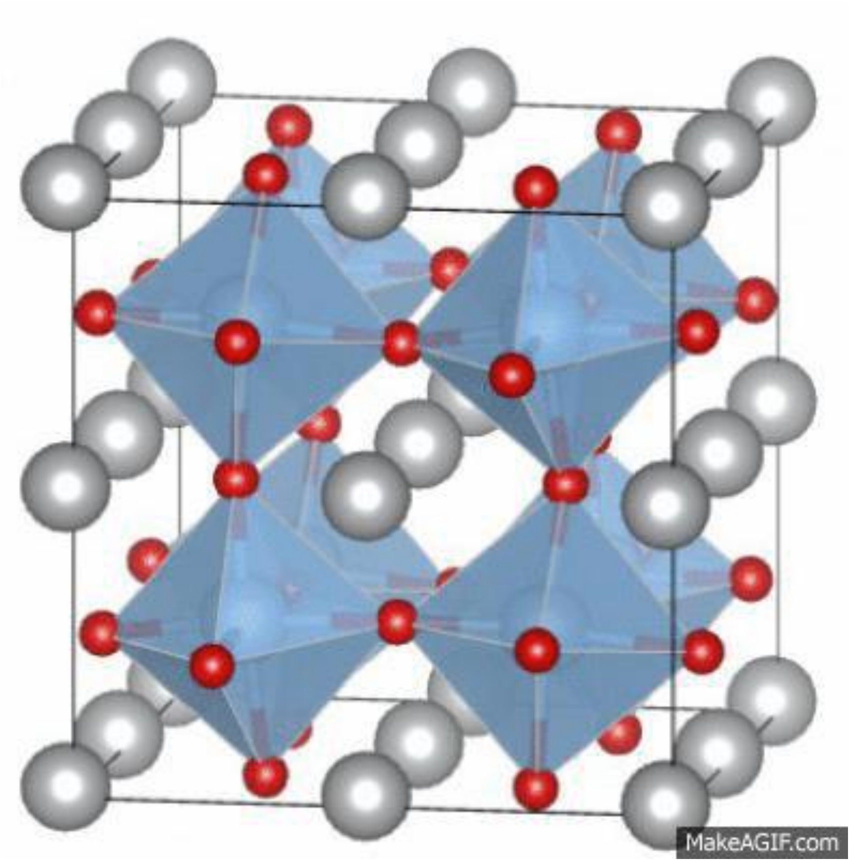


# Coherent Quasi-elastic Scattering: Measurement of Space and Time-correlations

$$I_{inc}(\mathbf{Q},t)=\frac{1}{N}\sum_i\left\langle \exp\{i\mathbf{Q}\bullet\mathbf{R}_i(t)\}\exp\{-i\mathbf{Q}\bullet\mathbf{R}_i(0)\}\right\rangle$$



# Coherent quasi-elastic scattering: Rotational diffusion between two states




Fluctuation-dissipation Theorem:

$$\chi_{\mathrm{QE}}(\mathbf{Q},\omega) = \frac{\chi(0)}{1+q^2\xi^2}\left(1 - \mathrm{i}\frac{\omega}{\Gamma_q}\right)^{-1}$$

# Coherent quasi-elastic scattering: Doping of Ba increase fluctuation frequency

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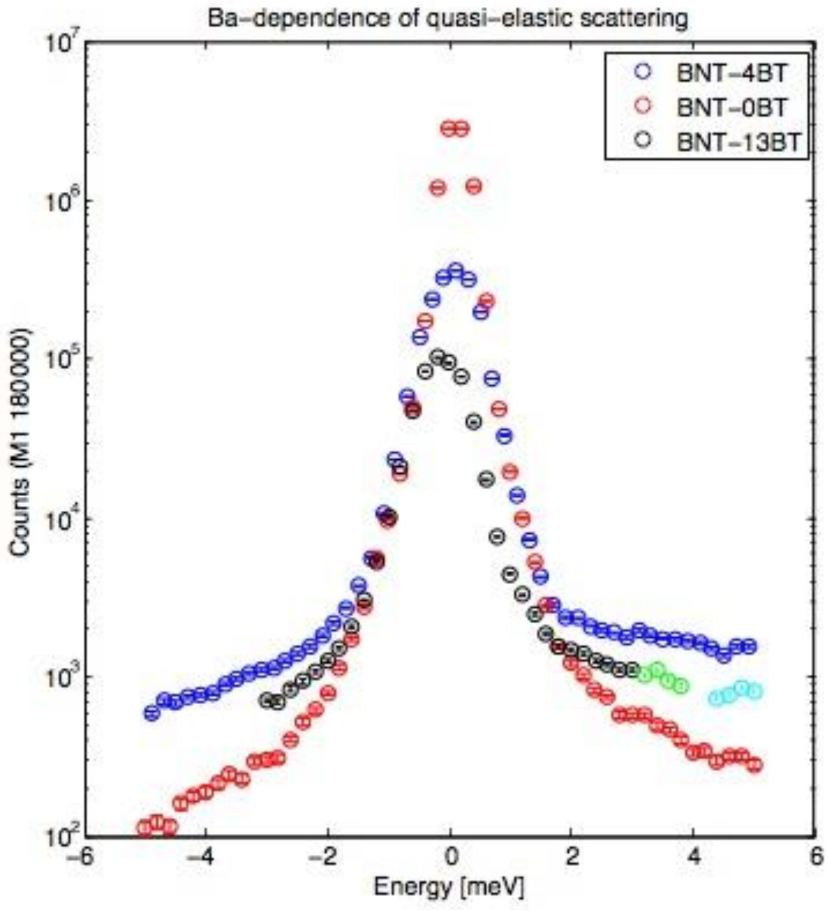


Beamtime IN8 (ILL)

**VISIT POSTER B3 !!**

# Conclusion and Outlook

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- Found the microscopic reason for relaxor behavior
- Working on reason for structural instabilities (soft phonon)
- Evaluating EXAFS data for local environment of Bi (SRO)
- Continue work on time dependence (QENS)



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