Analysing Diffraction Data of $La_{2-x}Sr_xCuO_{4+y}$

Using McStas Virtual Experiments

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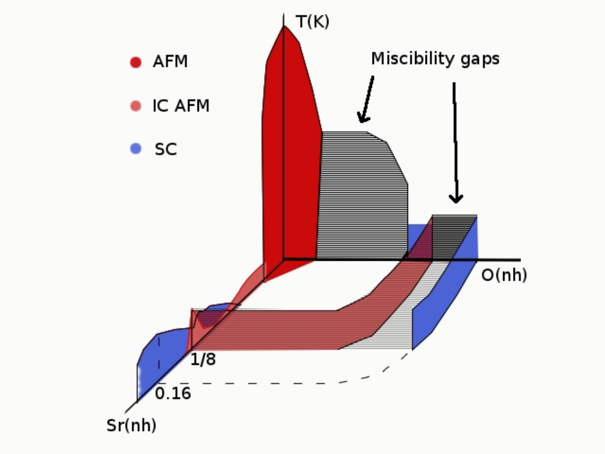
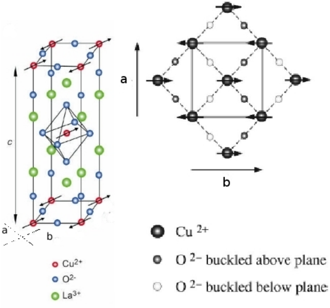
- Sr doping: T_M peaking at $n_h \sim 1/8$. T_c peaking at $n_h \sim 0.16$
- (High) O doping: $T_M = T_c = 40K$. Staging for $y > 0.06$
- Sr + O doping: $T_M = T_c = 40K$. Staging for $x < 0.06$

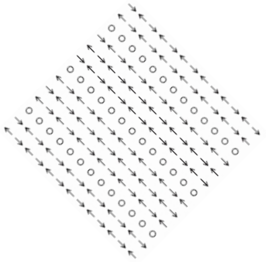


H.E. Mohottala *et al*, Nature Materials **5** 377

Undoped AFM:

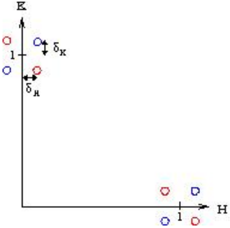


LNSCO IC AFM:

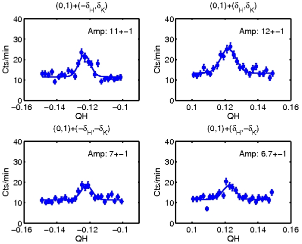


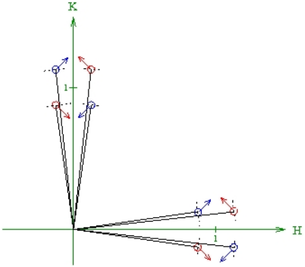
N.B. Christensen et al. PRL **98** (2007)
J.M. Tranquada et al (1995-)

LSCO+O:



x	δ_H[rlu]	δ_K[rlu]
0	0.130(3)	0.125(3)
0.04	0.124(3)	0.124(3)
0.065	0.122(3)	0.122(3)
0.09	0.115(3)	0.123(3)

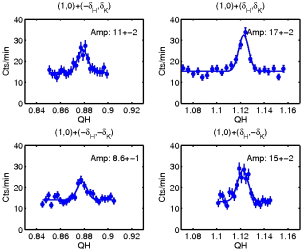


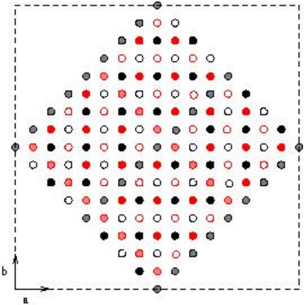


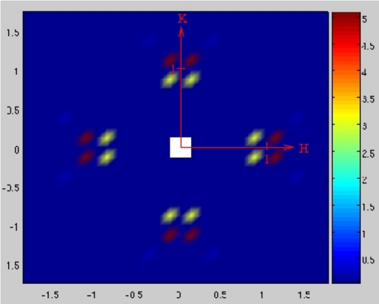
$x = 0.065$ ($x = 0.04$)

5% diff in proj of moment

but $>$ 50% int diff high/low Q





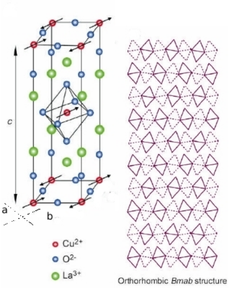


$$
\begin{aligned}
\frac{d\sigma_M}{d\Omega}(\mathbf{Q}) &= N\frac{2\pi}{V_0}\sum_{\tau}|pf(\mathbf{Q})w^{-W}|^2|F_{M\perp}(\mathbf{Q})|^2\delta(\mathbf{Q}-\tau) \\
F_{M\perp}(\mathbf{Q}) &= \mathbf{Q}\times(F_{M\perp}(\mathbf{Q})\times\mathbf{Q}) \\
F_M(\mathbf{Q}) &= \sum_d \mathbf{m}_d e^{i\mathbf{Q}\cdot\mathbf{r}_d}
\end{aligned}
$$

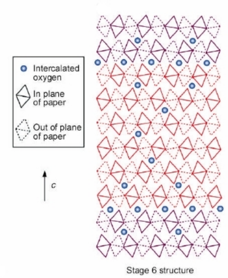
- The intensity difference in high/low Q peaks is qualitatively explained by a model with stripes in 3 layers.

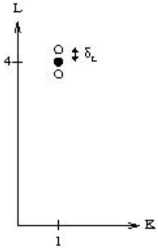
Model work by T.B.S. Jensen, Risø DTU

LCO:

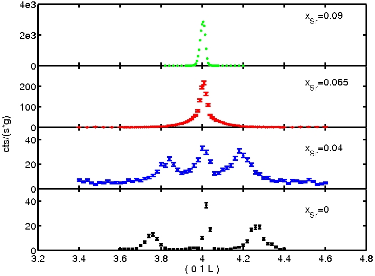


LSCO+O:





- Staging number = $1/\delta_L$



x	Staging number
0	3.8
0.04	5.5
0.065	disordered tilts
0.09	none

- The staging number increases with Sr content
- Decreasing O content with increasing staging number

- Intensity - cross-section
- Position - periodicity
- Width - domain size

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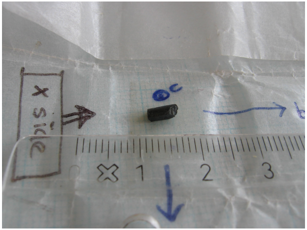
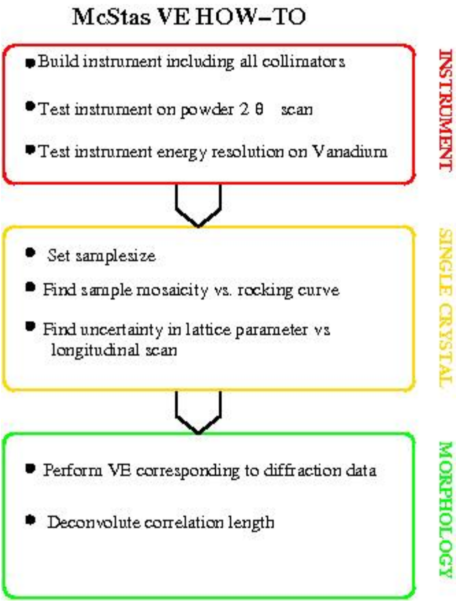
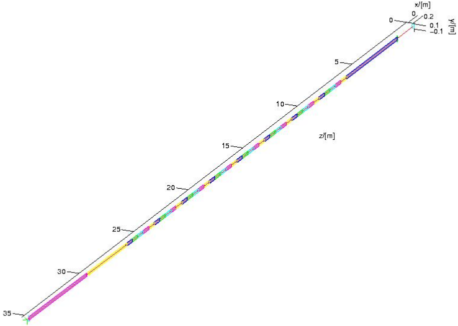
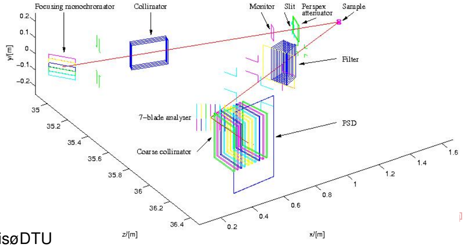
- Would be nice to have resolution limited linescans for comparison
- Virtual experiments on homogenous samples!


x side
c
1
2
3


McStas VE HOW–TO
Build instrument including all collimators
Test instrument on powder 2 θ scan
Test instrument energy resolution on Vanadium
INSTRUMENT
Set samplesize
Find sample mosaicity vs. rocking curve
Find uncertainty in lattice parameter vs longitudinal scan
SINGLE CRYSTAL
Perform VE corresponding to diffraction data
Deconvolute correlation length
MORPHOLOGY



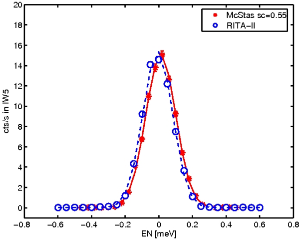


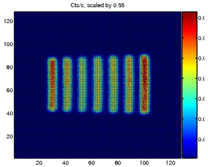
Effective instrumental resolution and thereby the linewidth of a particular scan depends on

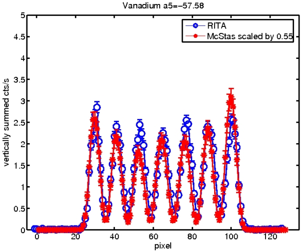
- Divergence of the beam before the monochromator: Size of source, geometry and m-values of guide elements
- Mosaicity of the monochromator - listed by producer as 37'
- Mosaicity of the analyser
- Geometrical factors: Sizes of components and distances between them
- Divergence of collimators
- Point-spread function of the position sensitive detector (PSD)
- Absolute energy of the incoming and scattered beam
- Sample parameters
  - shape/size (all samples including incoherent scatterer, powder, single-crystal)
  - particle size in sample (powder)
  - mosaicity and uncertainty in lattice parameters (single-crystal)

The samples in the virtual experiments are homogeneous and by deconvoluting the effective resolution the linewidth broadening due to finite size effect is found.

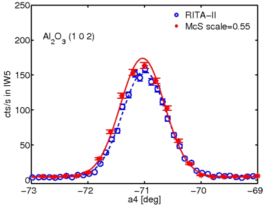
Vanadium sample

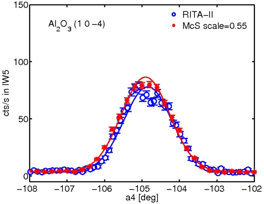


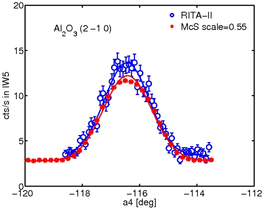


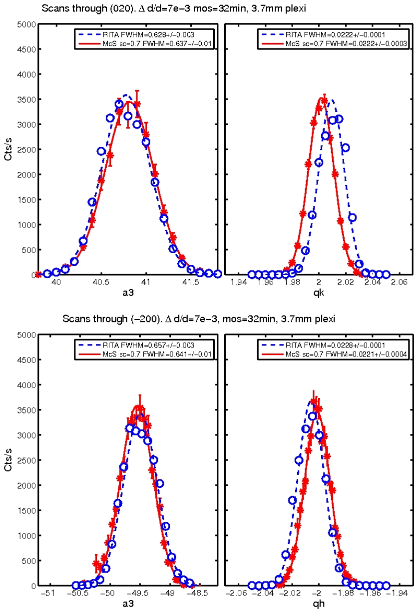


PowderN sample





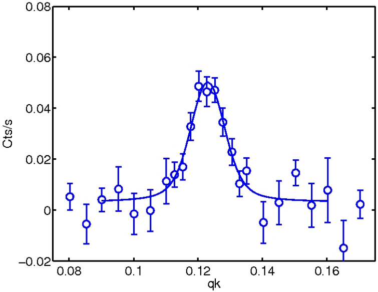




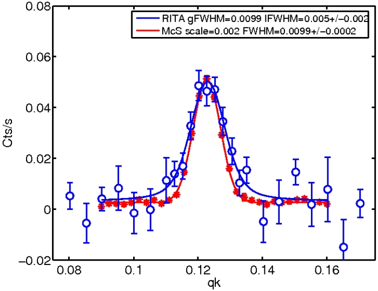
- McStas ○ RITA-II

Fundamental reflections (020) and (-200) used to set mosaicity and $\frac{\Delta d}{d}$

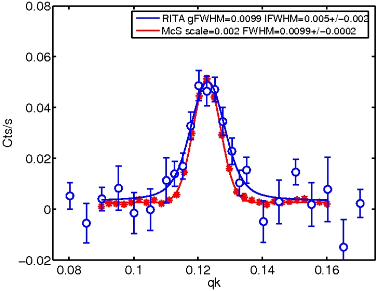
Simulated (resolution) width agrees within 5% of measured



- The IC AFM peak is narrow and close to resolution limited...



- The IC AFM peak is narrow and close to resolution limited... but effects larger than 10% are observable by McStas VE

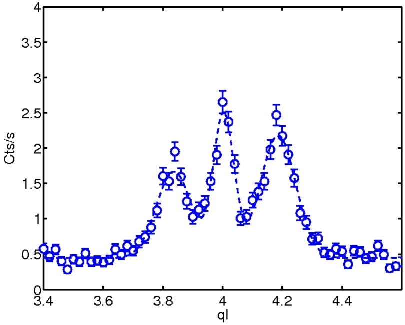


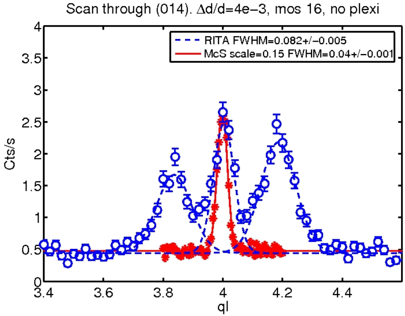
IC AFM broadened:

Fit to Voigt
lw=0.006(2) Å^{-1} ⇒ Corr. = 340±130 Å

Fit to Gaussian
$$w = \sqrt{w_m^2 - w_r^2}$$
w=0.010Å^{-1} $\Rightarrow \frac{2\pi}{w} \sim$ 610±140Å

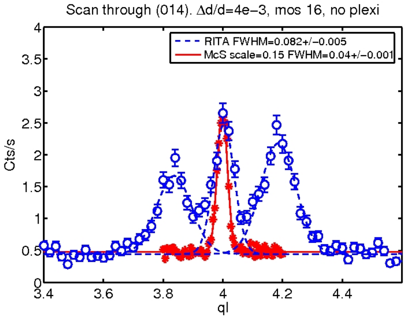
- The IC AFM peak is narrow and close to resolution limited... but effects larger than 10% are observable by McStas VE


Cts/s
ql
0
0.5
1
1.5
2
2.5
3
3.5
4
3.4
3.6
3.8
4
4.2
4.4



Bmab broadened: w=0.034 $Å^{-1}$
Domain size $\frac{2\pi}{w} \sim 185 \pm 30$ Å

Staging broadened: w=0.064 $Å^{-1}$
Domain size $\frac{2\pi}{w} \sim 100 \pm 8$ Å



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Domain size $\frac{2\pi}{w} \sim 100 \pm 8$ Å

- Mcstas VE is a useful tool when there is no instrumentally resolved peak in the vicinity

I would like to thank my coworkers:

- UConn: Barret O. Wells, Hashini E. Mohottala, Samuel B. Emery
- McStas: Peter K. Willendrup, Erik Knudsen, Kim Lefmann, Emmanuel Farhi
- Risø DTU: Niels H Andersen, Thomas B.S. Jensen, Asger B. Abrahamsen and Bente Lebech
- PSI: Niels B. Christensen, Christof Niedermayer

PLEASE VISIT OUR POSTER I1.2 IN THE POSTER SESSION TUESDAY AFTERNOON!

THANK YOU FOR LISTENING!