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

Using McStas Virtual Experiments

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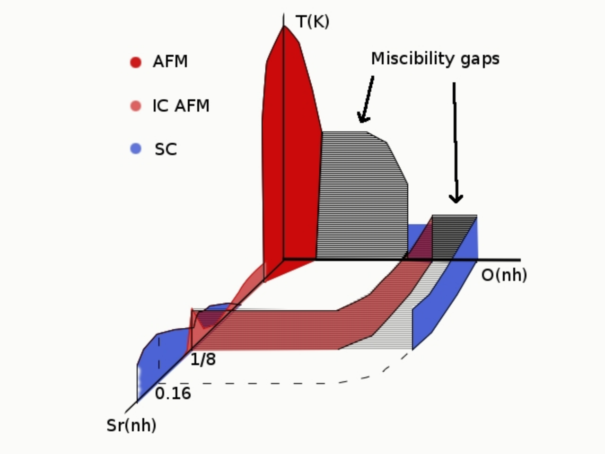
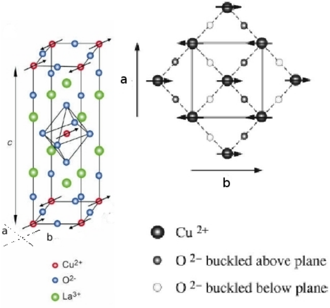
Phase diagramme of $La_{2-x}Sr_xCuO_{4+y}$

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

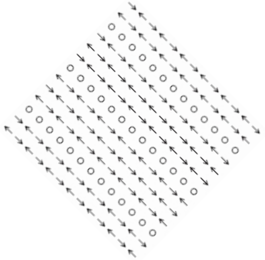


H.E. Mohottala *et al*, Nature Materials **5** 377 (2006)

Undoped AFM:

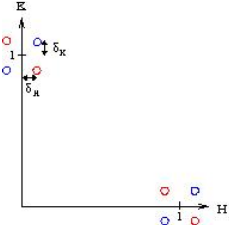


LNSCO IC AFM:

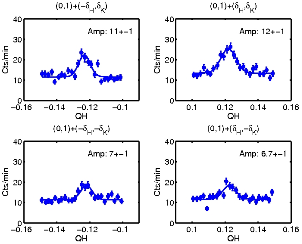


N.B. Christensen et al. PRL **98** (2007)
J.M. Tranquada et al (1995-)

LSCO+O:



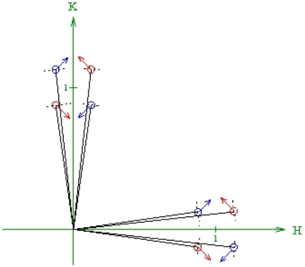
x	δ_H[rlu]	δ_K[rlu]
0	0.130(3)	0.125(3)
0.04	0.124(3)	0.124(3)
0.065	0.122(3)	0.122(3)
0.09	0.115(3)	0.123(3)

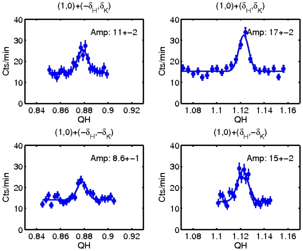


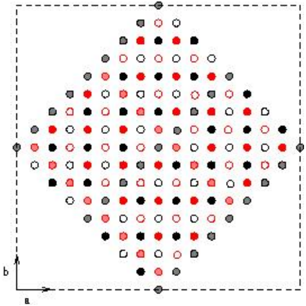
$x = 0.065$ ($x = 0.04$)

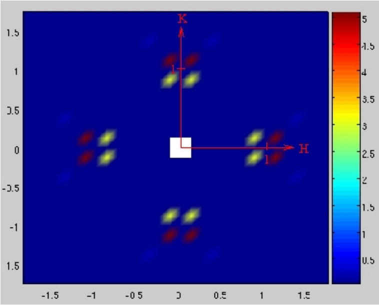
5% diff in proj of moment

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







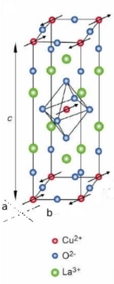


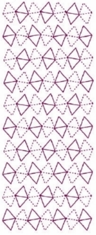
$$
\begin{aligned}
\frac{d\sigma_M}{d\Omega}(\mathbf{Q}) &= N\frac{2\pi}{V_0}\sum_{\tau}|pf(\mathbf{Q})w^{-W}|^2|F_{M\perp}(\mathbf{Q})|^2\delta(\mathbf{Q}-\tau) \\
F_{M\perp}(\mathbf{Q}) &= \mathbf{Q}\times(F_{M\perp}(\mathbf{Q})\times\mathbf{Q})) \\
F_M(\mathbf{Q}) &= \sum_d \mathbf{m}_d e^{i\mathbf{Q}\cdot\mathbf{r}_d}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

- 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

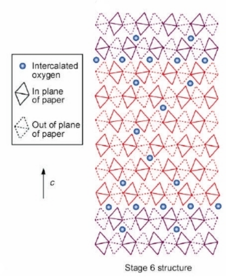
LCO:



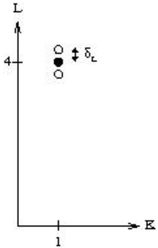


Orthorhombic *Bmab* structure

LSCO+O:

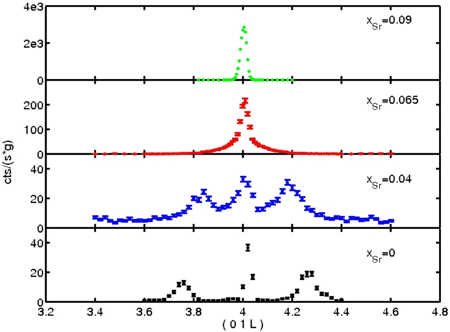


Stage 6 structure



- Staging number = $1/\delta_L$

B.O. Wells *et al.*, Zeitschrift f. Physik B **100** (1996)



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

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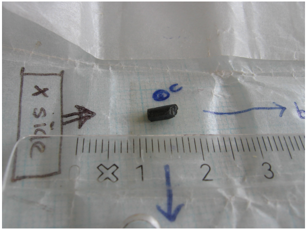
- Would be nice to have resolution limited linescans for comparison
- Virtual experiments on homogenous samples!



McStas VE HOW–TO

INSTRUMENT

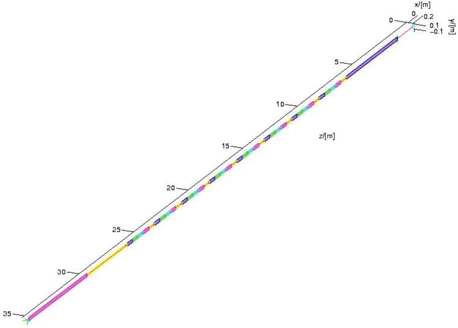
- Build instrument including all collimators
- Test instrument on powder 2 θ scan
- Test instrument energy resolution on Vanadium

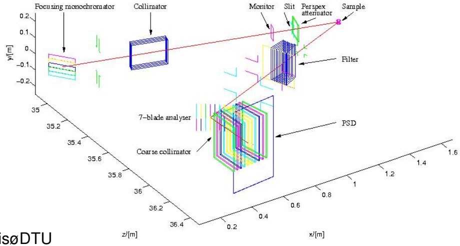
SINGLE CRYSTAL

- Set samplesize
- Find sample mosaicity vs. rocking curve
- Find uncertainty in lattice parameter vs longitudinal scan

MORPHOLOGY

- Perform VE corresponding to diffraction data
- Deconvolute correlation length



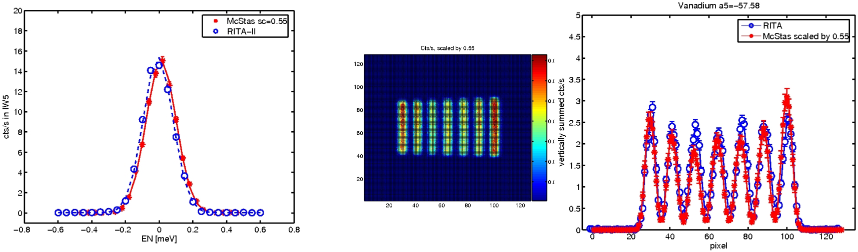


Effective instrumental resolution and thereby the linewidth of a particular scan depends on

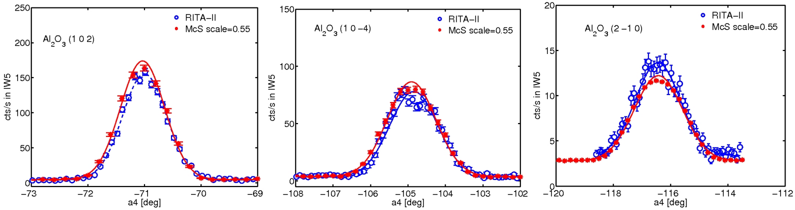
- Divergence of the beam before the monochromator: Size of source, geometry and m-values of guide elements
- Mosaicity of the monochromator - listed by producer as 37'
- Mosaicity of the analyser
- Geometrical factors: Sizes of components and distances between them
- Divergence of collimators
- Point-spread 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)

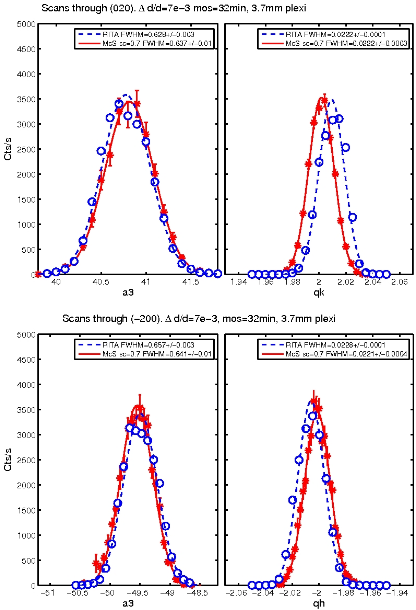
The samples in the virtual experiments are homogeneous and by deconvoluting the effective resolution the linewidth broadening due to finite size effect is found.

Vanadium sample



PowderN sample



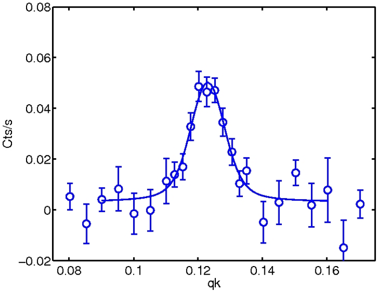


- McStas ○ RITA-II

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

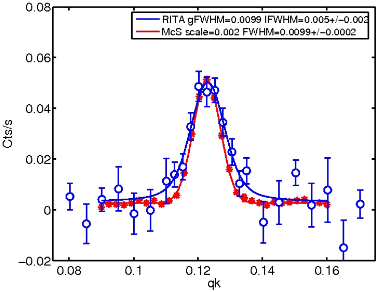
Simulated (resolution) width agrees within 5% of measured

x=0.09



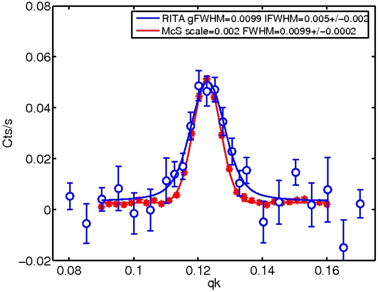
- The IC AFM peak is narrow and close to resolution limited...

x=0.09



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

x=0.09



IC AFM broadened:

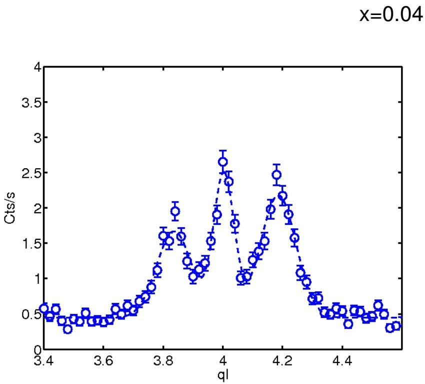
Fit to Voigt
lw=0.006(2) $Å^{-1} \Rightarrow$ Corr. = 340$\pm$130 Å

Fit to Gaussian

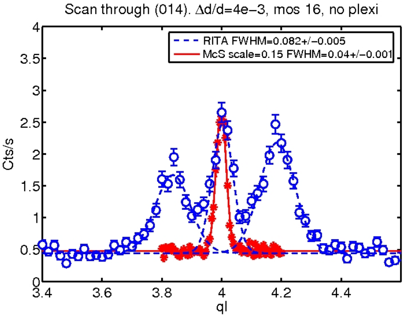
$w = \sqrt{w_m^2 - w_r^2}$

w=0.010$Å^{-1} \Rightarrow \frac{2\pi}{w} \sim$ 610$\pm$140Å

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


x=0.04
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

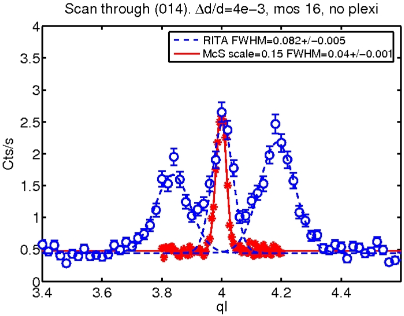
x=0.04



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

x=0.04



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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, J. ì Hjøllum and Bente Lebech
- PSI: Niels B. Christensen, Christof Niedermayer

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THANK YOU FOR LISTENING!