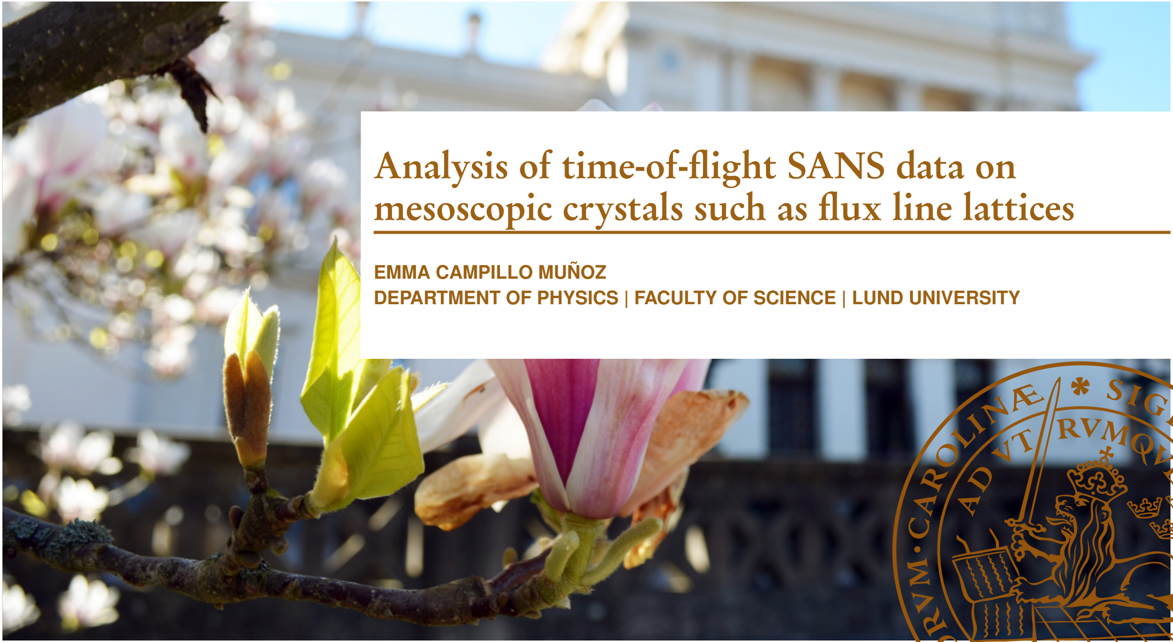

Analysis of time-of-flight SANS data on mesoscopic crystals such as flux line lattices

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Acknowledgements

Collaborators

- **Prof. Elizabeth Blackburn**
- **Prof. Edward M. Forgan**
- Dr. Maciej Bartkowiak
- Dr. Oleksandr Prokhnenko
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- Dr. Alistair Cameron, Dr. Randeep Riyat, Dr. Erik Jellyman
- Prof. Hazuki Kawano-Furukawa
- Dr. Jonathan S. White
- Dr. Robert Cubitt
- Dr. Alexander Holmes

Research institutions

Overview

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Small Angle Neutron Scattering (SANS)

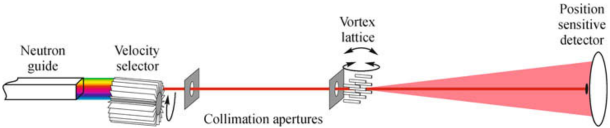
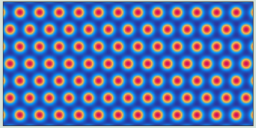


Figure: Schematic diagram of a typical SANS setup. M. R. Eskildsen, *et al.*, *Front. Phys.*, **6(4)**, 398—409 (2011).

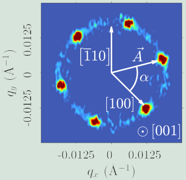
- Neutron magnetic moments interact with the VL.
- Resolve structures with $d \sim 100 - 300$nm.

Real space



r

Reciprocal space



$d = \lambda / 2 \sin \theta$ $\quad$ $q = 4\pi \sin \theta / \lambda$

Bragg diffraction in monochromatic SANS

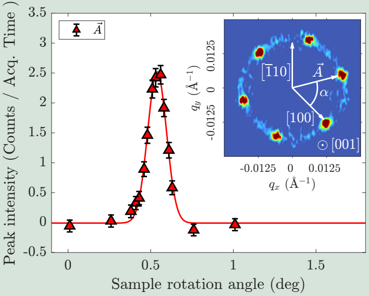


Figure: Rocking curve in ω at 130 mK and 1.5 T for the reflection labelled $\vec{A}$ in the inset for $CeCu_2Si_2$.

E. Campillo, *et al.*, *Phys. Rev. B*, **104**, 184508 (2021).

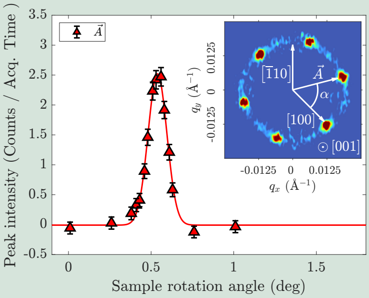
- Field as a Fourier series

$$B(\mathbf{r}) = \sum_{hk} \underbrace{|FF(\mathbf{q}_{hk})|}_{\text{Form Factor}} e^{i\mathbf{q}_{hk}\cdot\mathbf{r}}.$$

- Christen Formula

$$I(\mathbf{q}_{hk}) = 2\pi V \phi_n \left(\frac{\gamma}{4}\right)^2 \frac{\lambda_n^2}{\Phi_0^2 q_{hk}\cos(\zeta)} |FF(\mathbf{q}_{hk})|^2.$$

Bragg diffraction in monochromatic SANS



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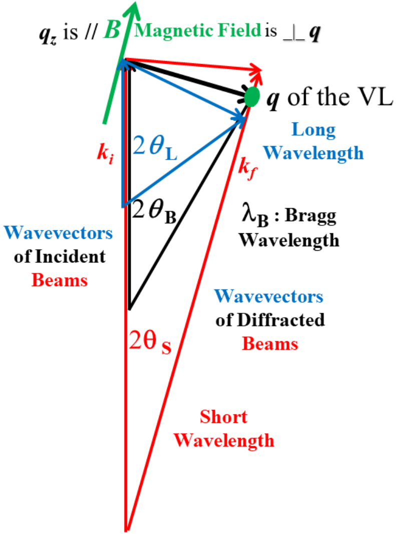
From $|FF(\mathbf{q}_{hk})|$

$$F_{\text{London}}(B) = \frac{B}{1 + q^2\lambda^2} \exp(-cq^2\xi^2)$$

Bragg diffraction in TOF SANS

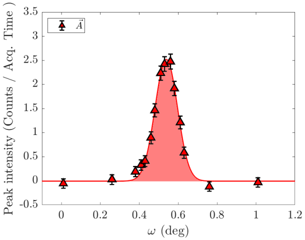
At one magnet angle α:

- Different wavelengths λ are scattered.
- Each α gives a range of q_z.
- Signal at Shorter and Longer λ = Signal at different ω.



E. Campillo, *et al.*, *J. Appl. Cryst.*, **55**, 1314-1323 (2022).

Vortex lattice form factor



Starting from the Christen formula

$$|F(\mathbf{q})|^2 = \frac{\Phi_0^2}{2\pi V\left(\frac{\gamma}{4}\right)^2} \times \frac{q\, I(\mathbf{q})}{\phi\lambda^2},$$

we define the integrated intensity under a rocking curve as:

$$\frac{qI(\mathbf{q})}{\phi\lambda^2} = \frac{1}{\phi\lambda^2}\int \sum_{q_x,q_y} I(q_x,q_y,\omega)\, q\, d\omega.$$

Vortex lattice form factor

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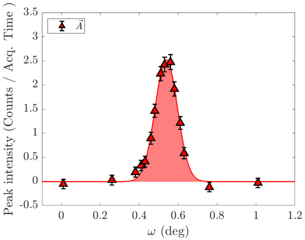

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In the TOF case:

- Illuminating beam: $\phi_j = \phi(\lambda_j)\Delta\lambda$.
- Scattered intensity: $I_j = I(q_x,q_y,q_z,\lambda_j)\Delta\lambda$.
- NOTE: $\Delta\lambda$ cancels in the ratio I_j/ϕ_j.

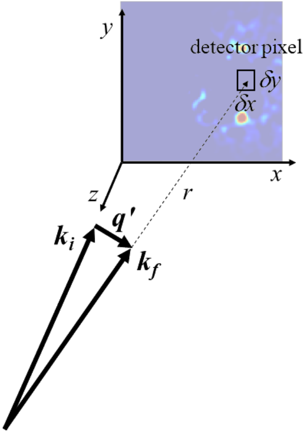
Geometry of the scattering

In the laboratory frame **q/** = $\mathbf{k}_f$ - $\mathbf{k}_i$, with magnitude k_j:

$$\mathbf{q}/ = \left(k_j\frac{x}{r},\ k_j\frac{y}{r},\ \frac{k_j}{2}\left[\left(\frac{x}{r}\right)^2 + \left(\frac{y}{r}\right)^2\right]\right).$$

In the sample frame, for small sample/magnet rotations:

$$\mathbf{q} = \left(k_j\frac{x}{r},\ k_j\frac{y}{r},\ q/_z - k_j\frac{x}{r}\sin\alpha\right).$$



E. Campillo, *et al.*, *J. Appl. Cryst.*, **55**, 1314-1323 (2022).

TOF form factor

Differentiating, the relationship between pixel-space and **q**-space:

$$\frac{dq_x}{dx} = \frac{dq_y}{dy} = \frac{k_j}{r},$$

and for detector area $\Delta x \Delta y$ and the **q**-pixel $\Delta q_x \Delta q_y$:

$$\Delta x \Delta y = \Delta q_x \Delta q_y \times \frac{r^2}{k_j^2}.$$

TOF version of the formula for the form factor:

$$|F(\mathbf{q})|^2 = \frac{\Phi_0^2}{2\pi V\left(\frac{\gamma}{4}\right)^2} \times \frac{1}{\lambda^2} \times \underbrace{\frac{\Delta q_x \Delta q_y r^2}{k_j^2 \delta x \delta y}}_{N \text{ detector pixels}} \times \int \sum_j \frac{I_j(\Delta q_x, \Delta q_y, q_z)}{\phi_j} dq_z.$$

TOF form factor

Differentiating, the relationship between pixel-space and **q**-space:

$$\frac{dq_x}{dx} = \frac{dq_y}{dy} = \frac{k_j}{r},$$

and for detector pixel $\Delta x \Delta y$, the **q**-pixel is $\Delta q_x \Delta q_y$:

$$\Delta x \Delta y = \Delta q_x \Delta q_y \times \frac{r^2}{k_j^2}.$$

TOF version of the formula for the form factor

$$|F(\mathbf{q})|^2 = \frac{\Phi_0^2}{2\pi V\left(\frac{\gamma}{4}\right)^2} \times \frac{\Delta q_x \Delta q_y}{4\pi^2} \times \frac{r^2}{\delta x \delta y} \times \int \sum_j \frac{I_j(\Delta q_x, \Delta q_y, q_z)}{\phi_j} dq_z.$$

Experiment chronology

Three different experiments were performed at HFM/EXED:

- January 2016:

  High-field dependence measurements on YBCO.

λ = 2.55 Å to 8.15 Å.

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Experiment chronology

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Experiment chronology

Three different experiments were performed at HFM/EXED:

- January 2016:

  High-field dependence measurements on YBCO.

  λ = 2.55 Å to 8.15 Å.

- Change of the detector.

- July 2017:
  - Temperature dependence measurements on YBCO.
  - Field and temperature dependence on BKFA.

- December 2019:

  High-field dependence measurements on 15% Ca-doped YBCO.

  λ = 5.0 Å to 8.15 Å.

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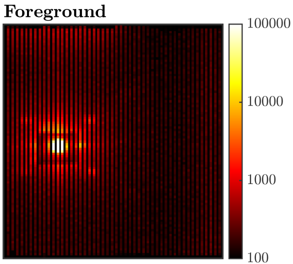
Data treatment



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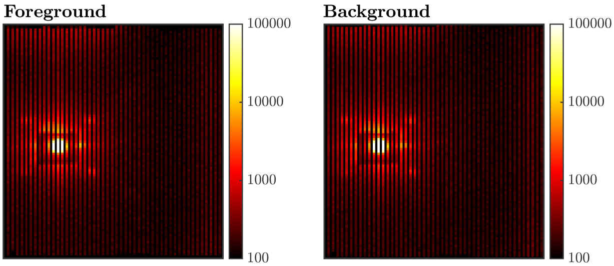

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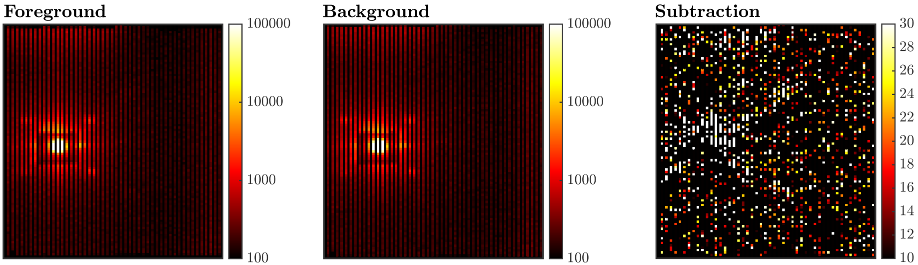


E. Campillo, *et al.*, *J. Appl. Cryst.*, **55**, 1314-1323 (2022).

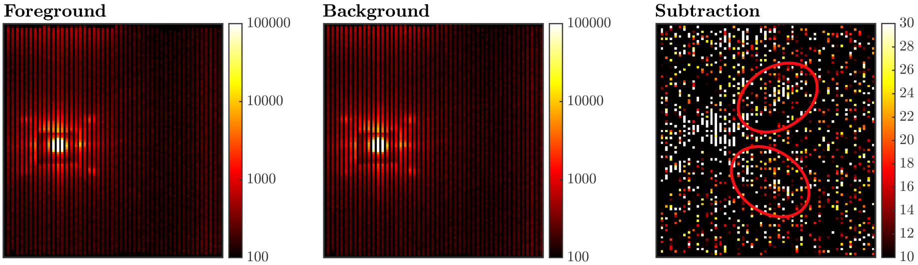
Data treatment

Monochromatic VS TOF

TOF form factor expression

Experiments and data treatment

Results



Procedure:

- Load FG and BG files.
- Rebin from time bins to $\Delta\lambda$ bins.
- Divide FG and BG files by efficiency.
- Rebin from detector pixels to **q**-space.
- Normalise FG and BG by beam I.
- Subtract BG from FG.

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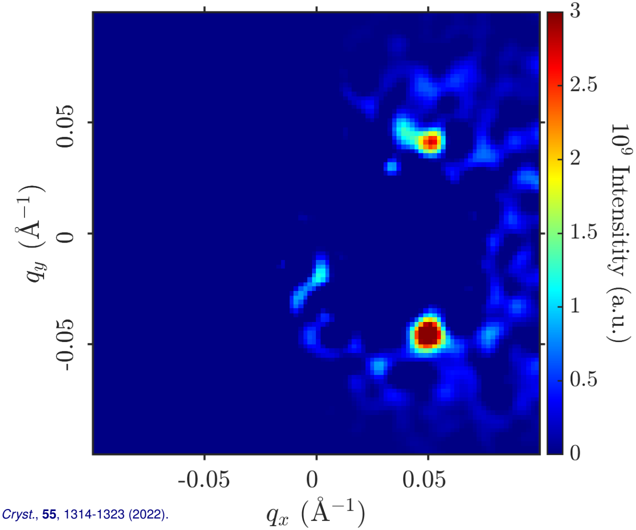
Data treatment



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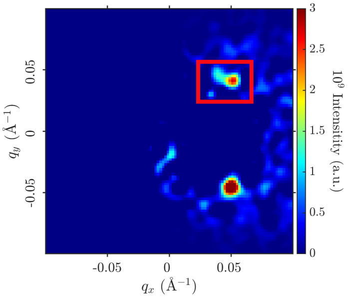
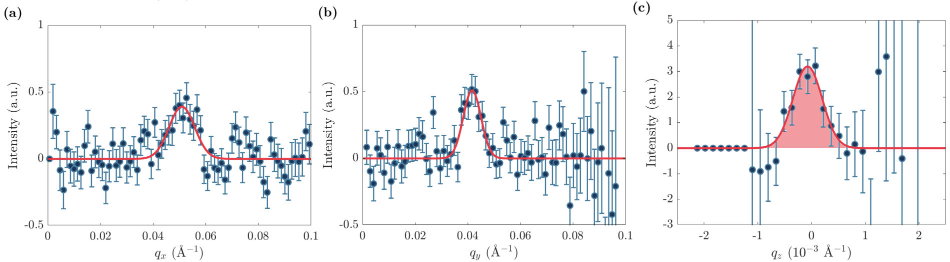


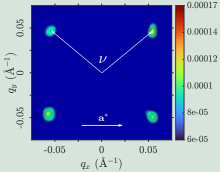
General considerations

- Choosing a range of λ.
- α determines the **q**-area covered: two or three angles needed.
- q_z width relevant: uninvestigated sample requires several angles.



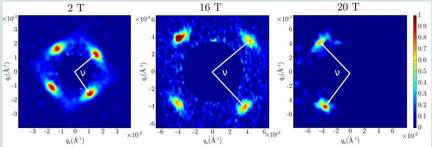
Form factor on YBCO and Ca-YBCO

$YBa_2Cu_3O_7$

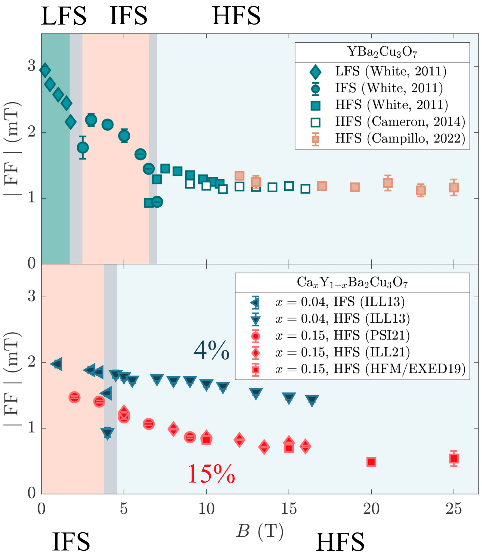


E. Campillo, *et al.*, *Phys. Rev. B*, **105**, 184508 (2022).

$Ca_{0.15}Y_{0.85}Ba_2Cu_3O_7$



A. S. Cameron & E. Campillo, *et al.*, *arXiv:2208.06706*.



A. S. Cameron & E. Campillo, *et al.*, *arXiv:2208.06706*.

Final remarks

- We developed a TOF Christen formula.
- We established an analysis procedure (developed in Mantid).
- We formulated general considerations for TOF experiments.
- We analysed unexplored data measured on YBCO and Ca-doped YBCO up to 25 T.
- Important contribution for future research at ESS.
- TOF can be used to study VL of superconductors.

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