Crystallographic and Magnetic Structure of CaFe$_2$As$_2$

By Methods of X-Ray and Neutron Diffraction
Contents

- What We Measure - Reciprocal Space
- How We Measure It
  - Powder Diffraction
  - Single Crystal Diffraction with Single/Area Detectors
- What We Learn From It
  - Orthorhombic Structural Distortion
  - Stripe-type Magnetic Order
What We Measure – Reciprocal Space

- Reciprocal space is the Fourier Transformation of Real Space.

- (HHL) plane of $(\text{Ca}_{1-x}\text{Sr}_x)\text{Co}_2\text{As}_2$, Same Space Group as $\text{CaFe}_2\text{As}_2$
Reciprocal Space

Note the Log Scale
Weak Features are Exaggerated
Reciprocal Space

- **Mosaic** - Perpendicular to $Q$ (Transverse), Same d-spacing

- **Lattice Parameters** - Parallel to $Q$ (Longitudinal)

- Quasi-elastic/Inelastic contribution, e.g. phonons, if no analyzer.

- Polycrystalline rings

- What we measure is always the Convolution of signal with Instrument Resolution.
How We Measure it – Transverse and Longitudinal Scans
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**Powder Diffraction – Identity Check**

![Graph of powder diffraction spectrum with arrows indicating peaks and labels for phase and lattice parameters.]

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**FIG. 2.** (Color online) Powder x-ray diffraction spectrum of ground single-crystal CaFe$_2$As$_2$. Note that Si powder was added as a standard and Sn is present from residual flux on surface of samples used.

- Correct Phase?
- Longitudinal, Refine Lattice Parameters
- Need to know Crystal Structure in advance (Space Group, Atomic Positions)
Rocking Scan (Transverse/S1/Theta/Omega Scan) – Quality Check

FIG. 1. (Color online) Rocking curve through the (1 1 10) reflection of the CaFe$_2$As$_2$ single crystal used for the x-ray diffraction study. Inset: picture of a CaFe$_2$As$_2$ single crystal on millimeter grid paper. The crystallographic c axis is perpendicular to the plate of the crystal. The small droplets on the surface are residual Sn flux.
CaFe$_2$As$_2$: Tetragonal to Orthorhombic Distortion with Stripe-type Magnetic Order

Jing Han Soh, Inelastic neutron scattering studies of magnetic fluctuations in the tetragonal and collapsed tetragonal phases of CaFe2As2
Tetragonal to Orthorhombic Distortion with Stripe-type Magnetic Order

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Single Crystal Neutron Diffraction

![Graphs showing diffraction patterns](image)

**FIG. 1.** (Color online) (a) $Q$ scans through the positions of the tetragonal $(1 -1 -2)$ nuclear peak (referenced to the tetragonal unit cell) and the magnetic peak positions at 180 K. No intensity is observed at the positions of the magnetic reflections. (b) Below the tetragonal-to-orthorhombic transition, two twin domains are observed in longitudinal scans through the $(2 0 -2)$ (indexed to the orthorhombic cell) nuclear peak position. The magnetic peak $(1 0 -1)$ is associated with only one of these domains. (c) Two-dimensional plots showing the $Q$ and $\omega$ (sample rotation in the scattering plane) dependences of peaks in (b).
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**Magnetic Propagation Vector -> Magnetic Structure -> Moment Direction**

\[ \frac{d\sigma}{d\Omega} = N(yr_0)^2 \sum_{\tau} \delta(Q - \tau)[\vec{Q} \times \vec{M} \times \vec{Q}]^2 \]

Sensitivity to Transverse Components ONLY

Comparison between the measured and calculated structure factors for the proposed magnetic structure of CaFe$_2$As$_2$ from the FULLPROF refinement.
Orthorhombic Structural Distortion

- 2D area detector gives an (almost) longitudinal scan
- Rocking the sample covers 3 dimensional reciprocal space. Integrated Intensity gives volume fraction
Twinning – One of the Real-World Complications

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Order Parameters

- Structural Phase Transition is First Order, Order Parameter defined as $\frac{a - b}{a + b}$
- Magnetic Phase looks Second Order, but First Order is Normalized properly

Fig. 3. (Color online) (a) Temperature dependence of the orthorhombic splitting (red curves) and magnetic integrated intensity (blue symbols) normalized to the orthorhombic volume fraction upon warming (filled circles) and cooling (open circles) through the transition. Below 170 K, both the orthorhombic distortion and the magnetic peak intensity are saturated. The dashed lines are guides to the eye. (b) The raw integrated intensities of the magnetic $(-101)_M$ reflection (blue symbols) and the orthorhombic (400) nuclear peak.
THANK YOU
Q&A

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