Characterizing Weyl-mediated Magnetic Interactions in Non-centrosymmetric Rare-earth Materials

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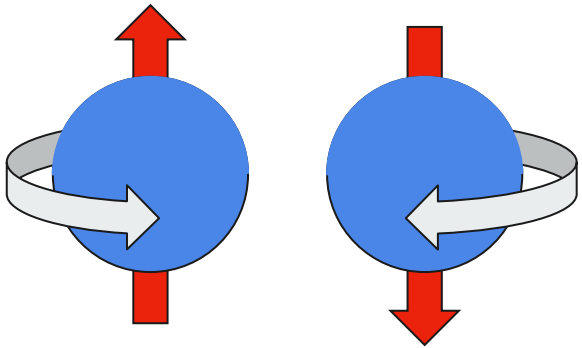
Goal

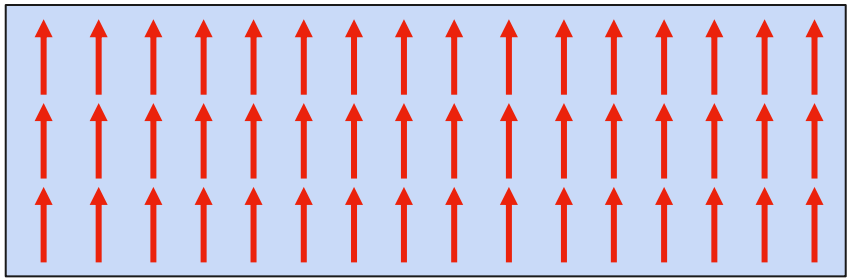
Explore novel behaviors induced by Weyl electrons in Weyl semimetals through modeling and probing magnetic structure.

Background Information

Spin and Magnetism

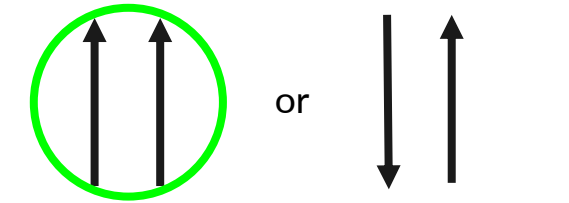
- Spin is an inherent property of elementary particles
  - Can be thought of as a **“tiny magnet”** for the purposes of this presentation
- Large regions of aligned spin are called **ferromagnetic domains** and result in a net magnetization





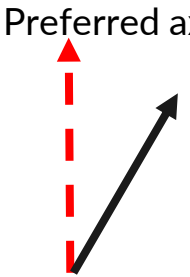
Magnetic Interactions

Exchange - Local interaction of neighboring atoms through overlapping wavefunctions

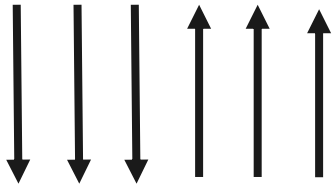


Ferromagnetic Antiferromagnetic

Anisotropy - Preferred axis of alignment

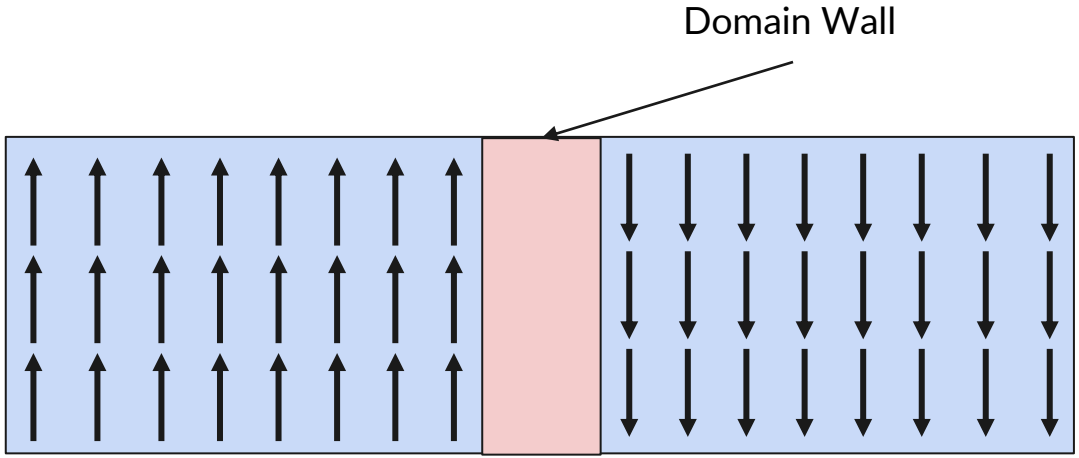


Dipole/Demagnetization - Long range effect due to the net magnetization



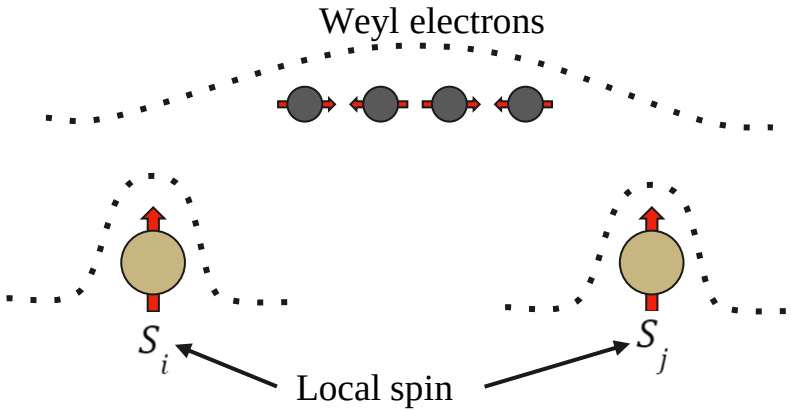
Multiple Domains and Domain Walls

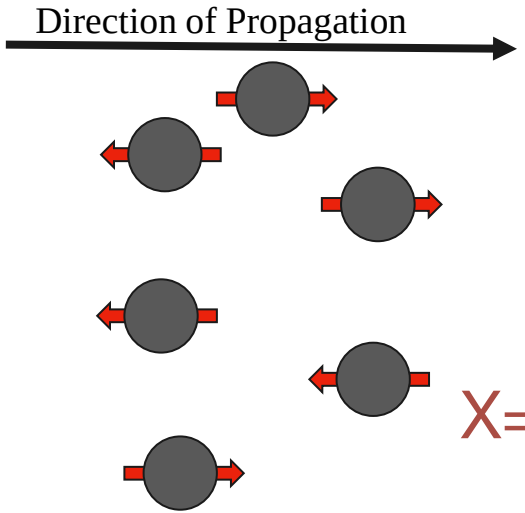
- A single crystal can have multiple domains of differing alignments.
  - Transition region is called a domain wall



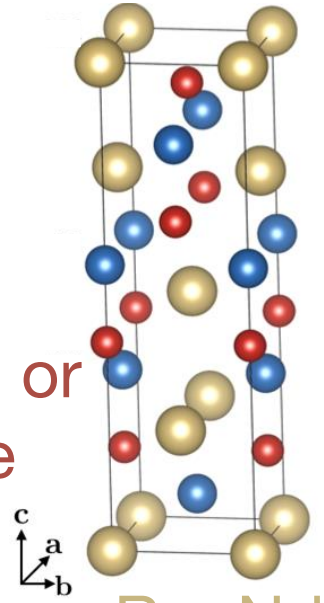
What is special about Weyl semimetals?

- Weyl electrons
  - “**Massless**” - highly mobile
  - **Chiral** - “handedness”
  - Mediates the Dzyaloshinskii-Moriya(DM) interaction that tends to **misalign** neighboring spins



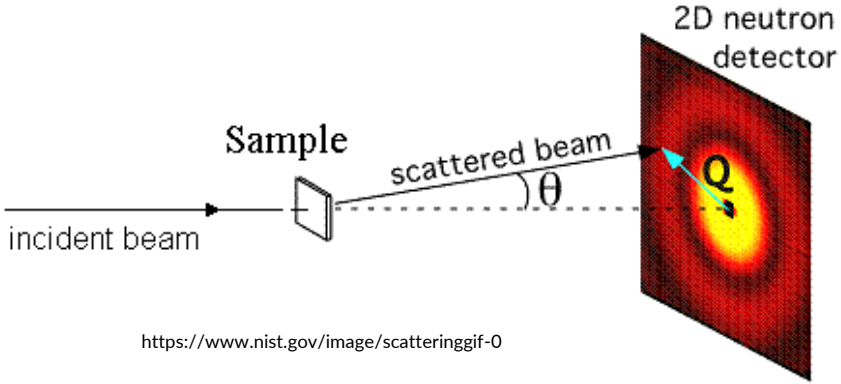


RAIX

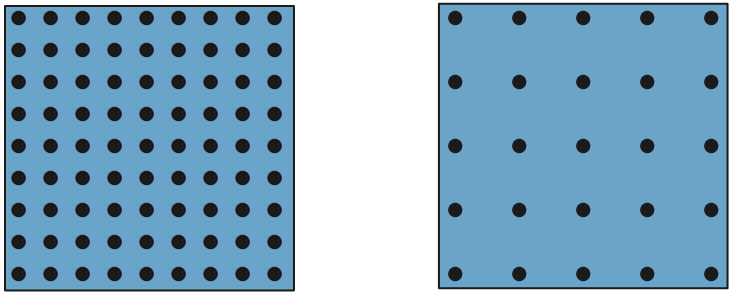


Neutron Scattering

- Why is it useful?
  - Measures **magnetic** and **structural** properties
  - Highly penetrating, so it is able to measure **bulk** properties
  - Sensitive on **nanometer** to **micron** length scales(for Small Angle Neutron Scattering(SANS))
    - **Ångstroms** for diffraction



https://www.nist.gov/image/scatteringgif-0



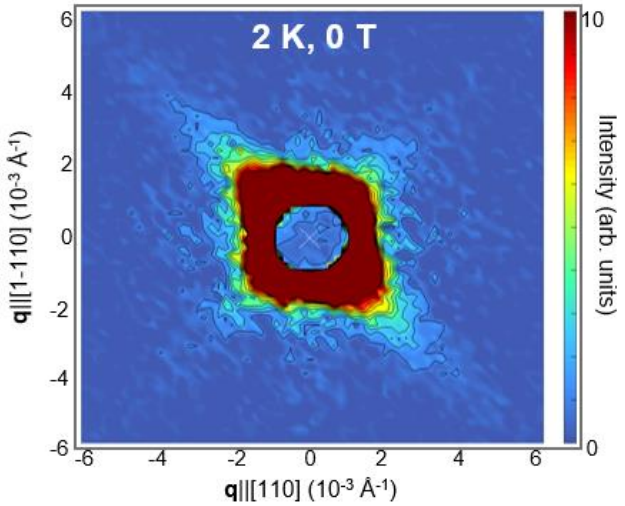
High-q

Low-q

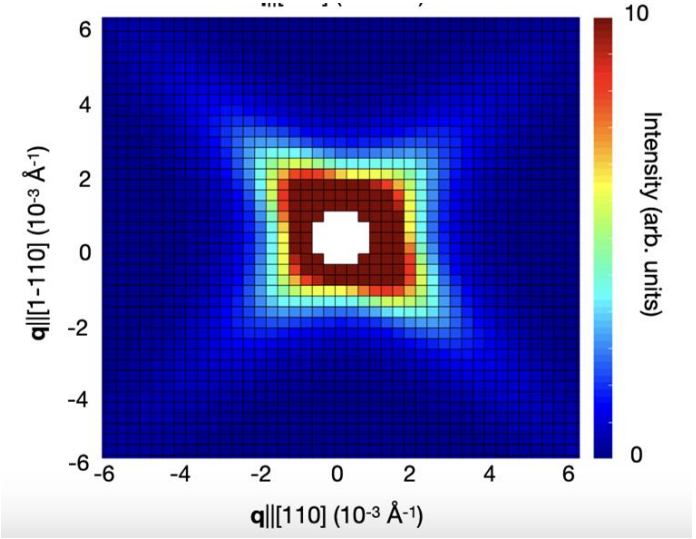
Modeling CeAlSi Striped Domains

Comparison to Neutron Scattering Data

Measured Scattering Data

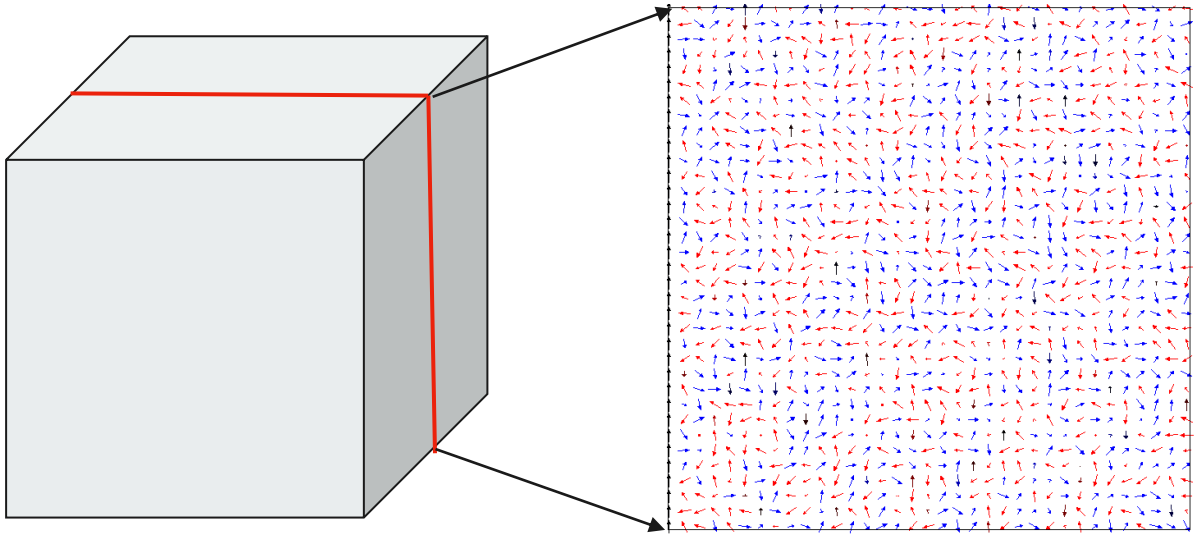


Simulated Scattering of Bilayer Striped Domains

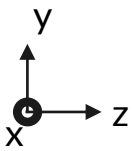


OOMMF Toolkit and Procedures

- Initiate from a random configuration of spins
- “Solves” the spin configuration by minimizing energy
- Should be thought of as a small part of a larger crystal



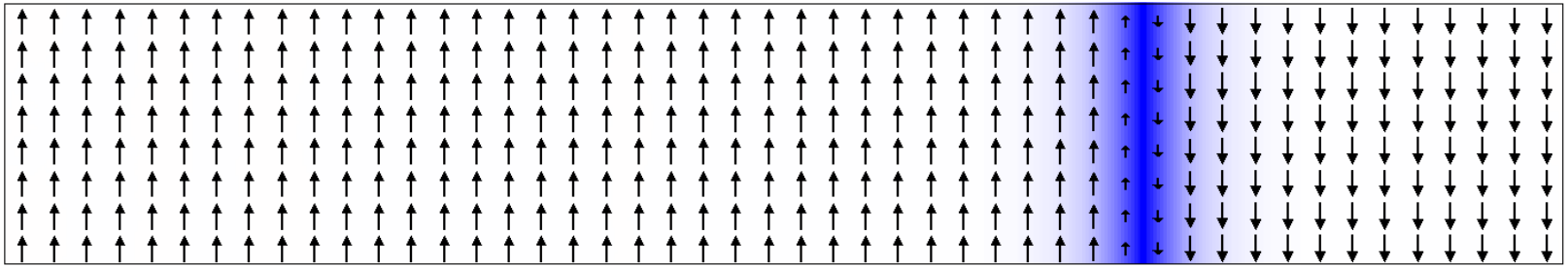
Modeling the DM Interaction



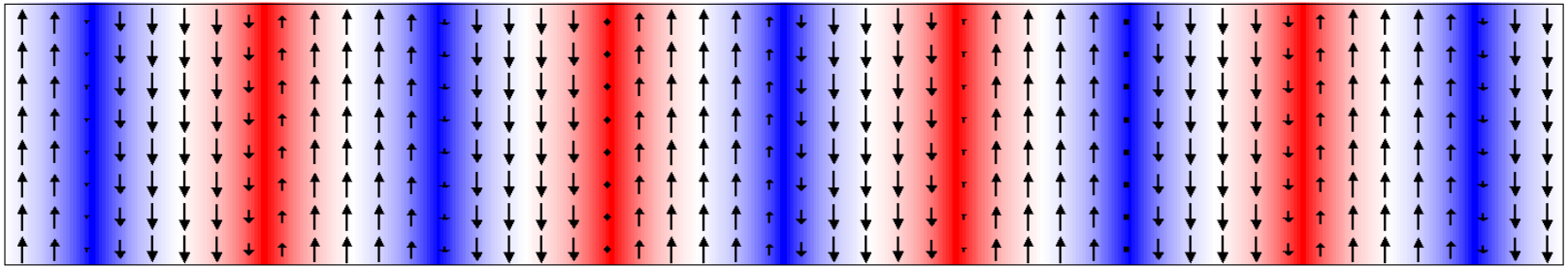
- Expectations
  - More domains, leading to stripes
  - Chiral domain wall transitions

Red - Out of Plane(+x)
Blue - Into Plane(-x)

Without DM

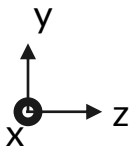


With DM

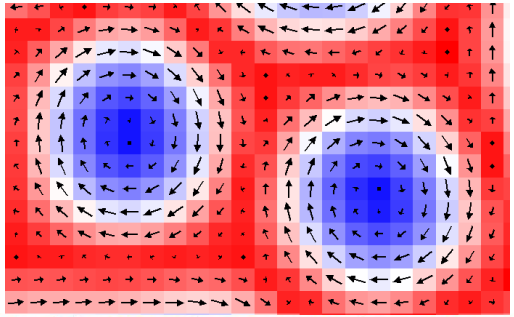


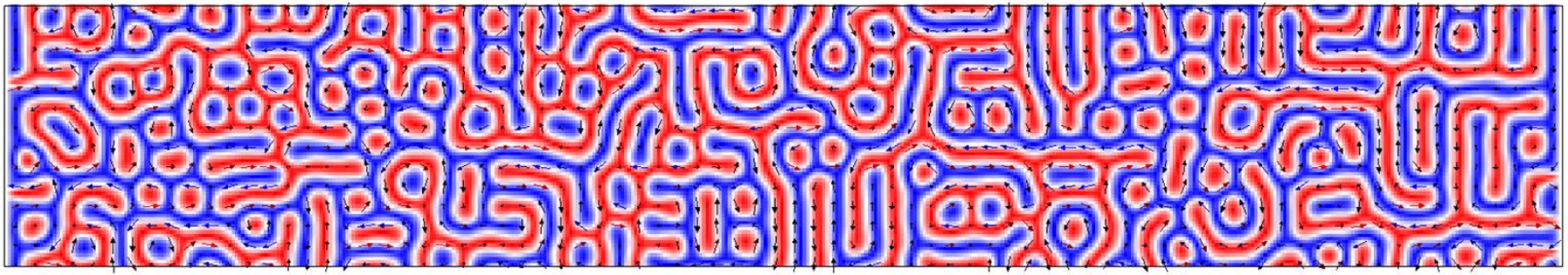
Further Increased DM Interaction

- Destroys striped order
- Promotes vortices of spin- “skyrmions”



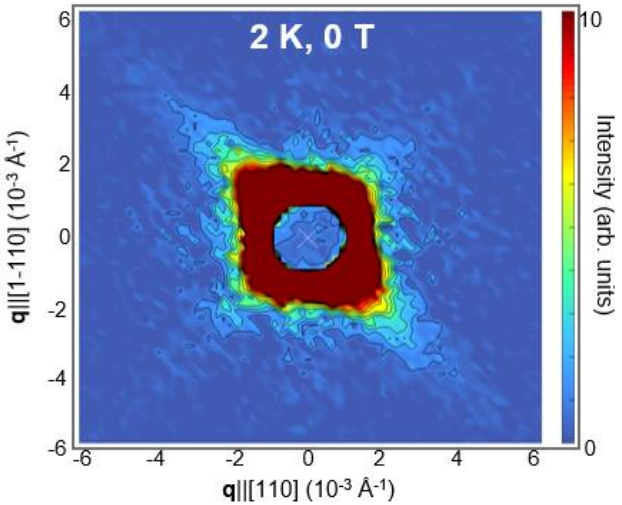
Red - Out of Plane(+x)
Blue - Into Plane(-x)

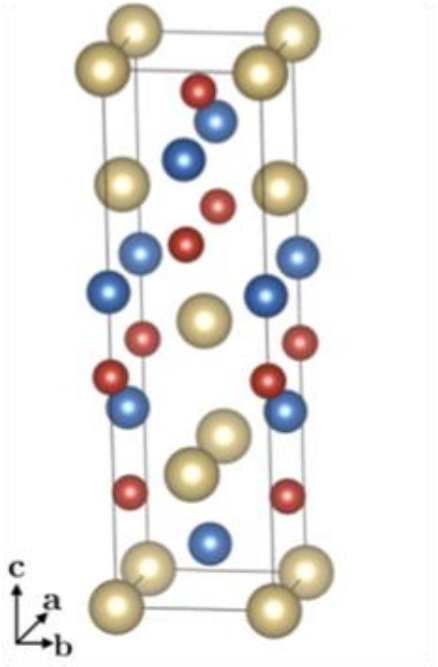




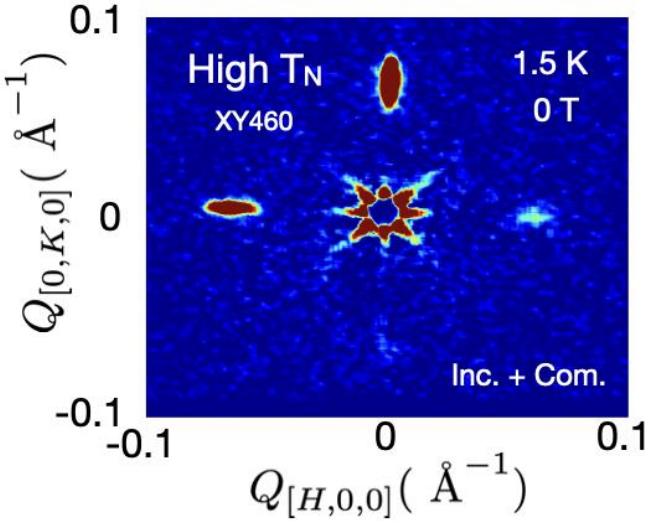
Compounds of Interest

CeAlSi

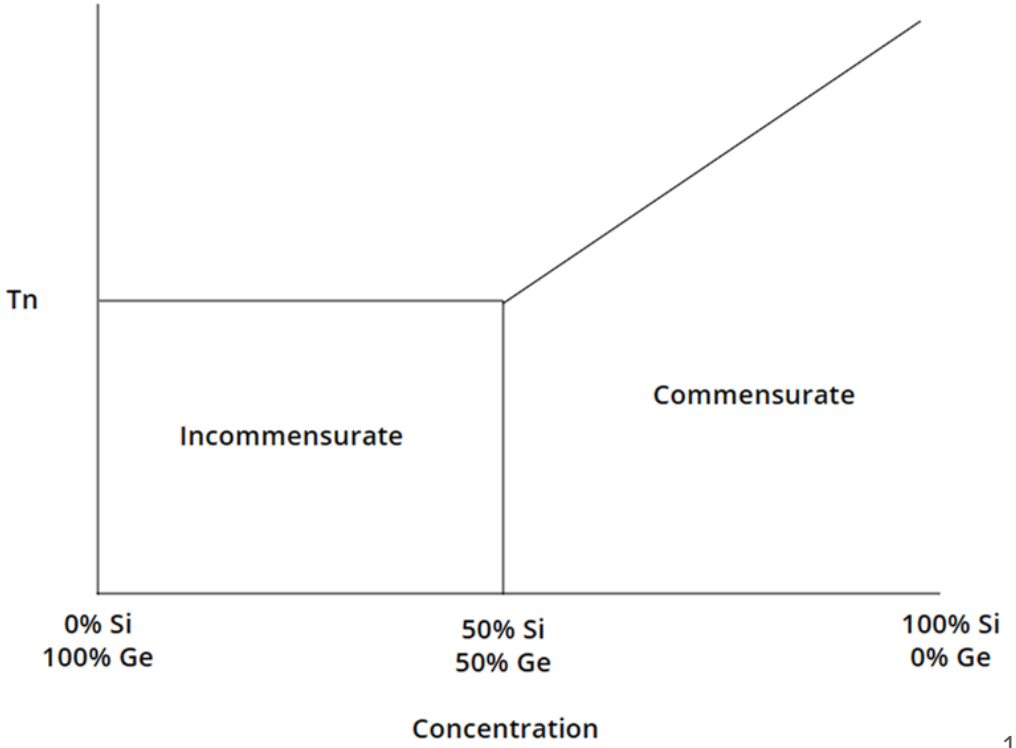




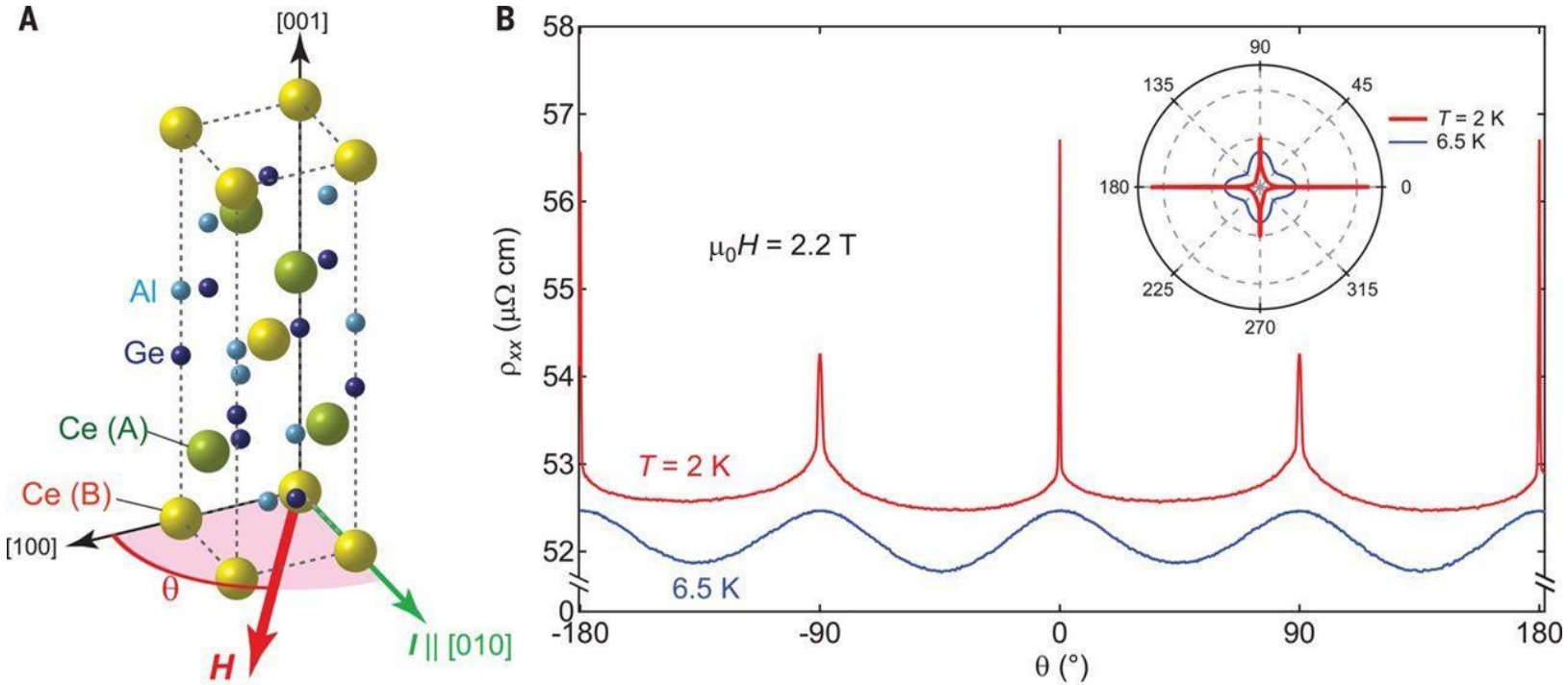
CeAlGe



Phase Change



Singular Angular Magnetoresistance(SAMR)



T. Suzuki *et al.* Singular angular magnetoresistance in a magnetic nodal semimetal. *Science* 365,377-381(2019).DOI:10.1126/science.aat0348

Conclusion and Future Direction

Results

- Successfully modeled DM interaction.
  - Showed striped domains match experimental results.
- Mapped out the magnetic phase diagram in more detail relative to its Ge/Si content.

Future Direction

- Fit the model parameters to experimental data to understand the length scales of the interactions.
- Conduct more thorough measurements of CeAlGe to better understand its behavior

Acknowledgments

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NIST CENTER FOR NEUTRON RESEARCH

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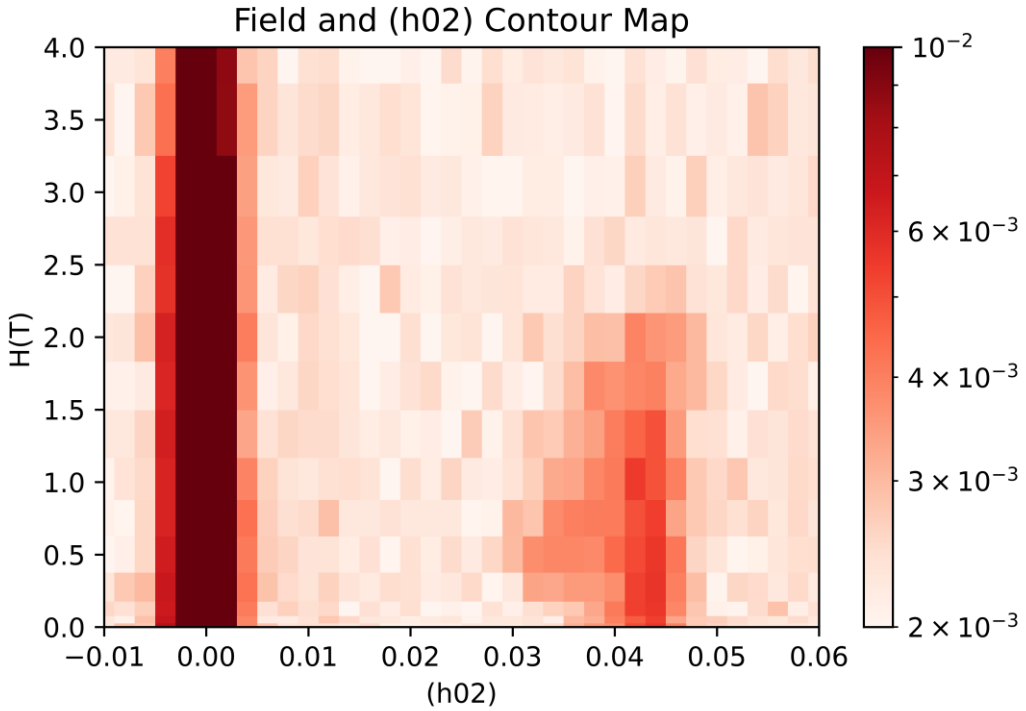
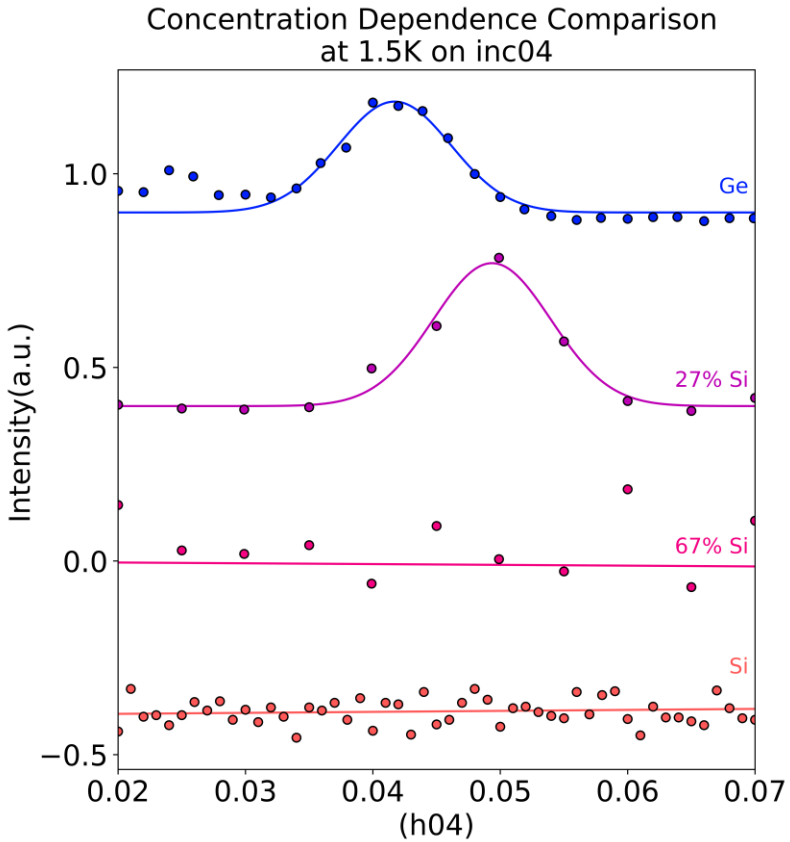
OOMMF User's Guide, Version 1.0
M.J. Donahue and D.G. Porter
Interagency Report **NISTIR 6376**,
National Institute of Standards and Technology, Gaithersburg, MD (Sept 1999)

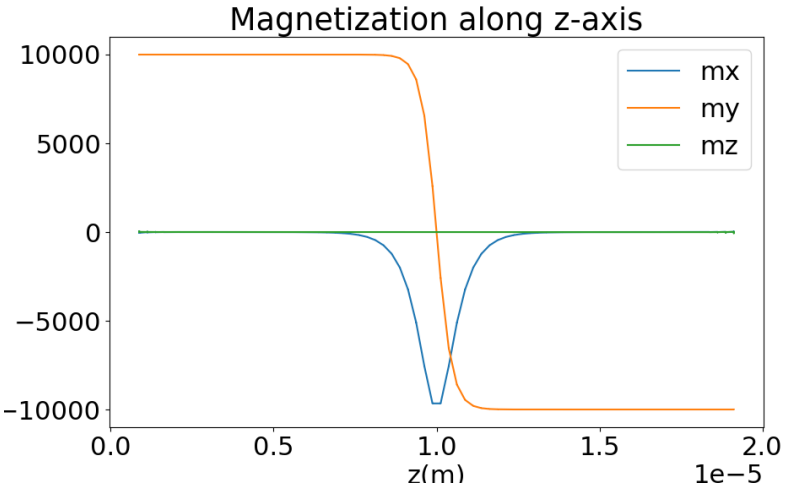
Questions?

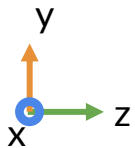

Field and (h02) Contour Map
H(T)
(h02)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
0.06
10^{-2}
6×10^{-3}
4×10^{-3}
3×10^{-3}
2×10^{-3}

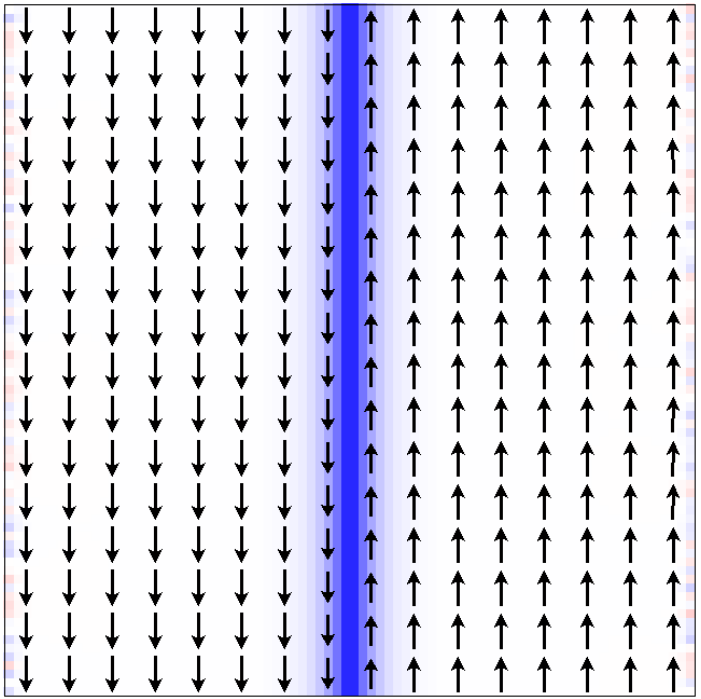

Concentration Dependence Comparison
at 1.5K on inc04
Intensity(a.u.)
1.0
0.5
0.0
−0.5
Ge
27% Si
67% Si
Si
0.02
0.03
0.04
0.05
0.06
0.07
(h04)

Verification of the OOMMF Simulation

- Includes only the exchange, anisotropy and dipole interactions which are well understood.
  - Expect domain wall to process along the in/out-of-plane direction.







Exchange

$$E = J\left[S_i \bullet S_j\right]$$

DM

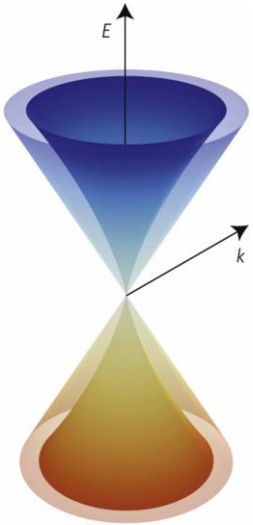
$$E = D \bullet S_i \times S_j$$

$$|A \times B| = |A||B|sin(\theta)$$

$$|A \bullet B| = |A||B|cos(\theta)$$

Break inversion symmetry

$$\vec{r} \neq -\vec{r}$$

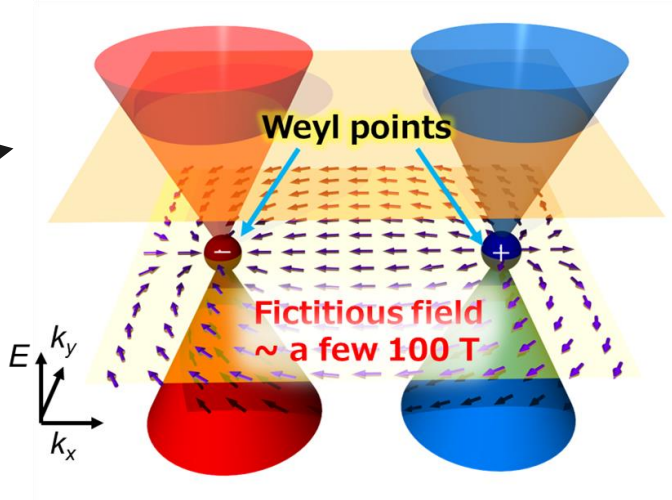


Elias, Nature Physics 7, 701-704 (2011)

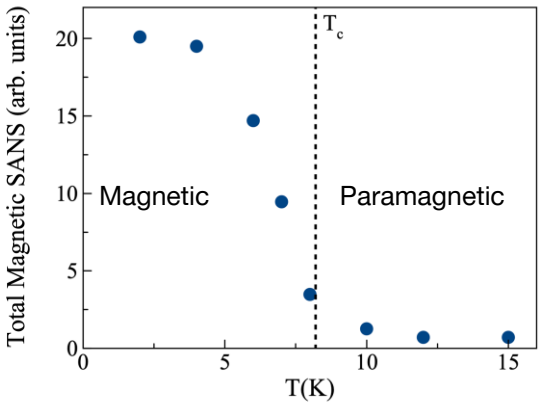
and/or

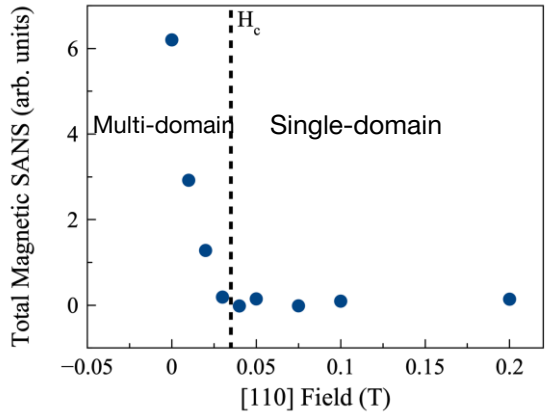
$$t \neq -t$$

Break time-reversal symmetry(magnetism)



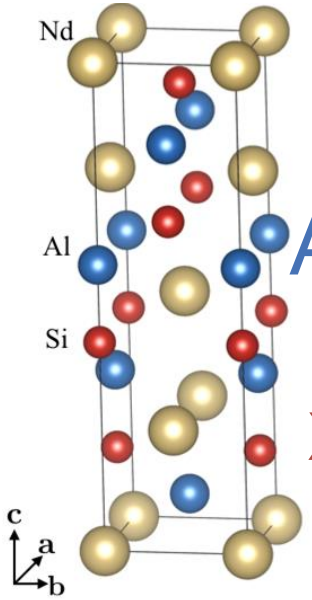
S. Nakatsuji and N. Kiyohara, Nature 527.7577 (2015)


Total Magnetic SANS (arb. units)
T(K)
T_c
Magnetic
Paramagnetic
0
5
10
15
20


Total Magnetic SANS (arb. units)
[110] Field (T)
H_c
Multi-domain
Single-domain
−0.05
0
0.05
0.1
0.15
0.2
0
2
4
6

2 K

RAlX

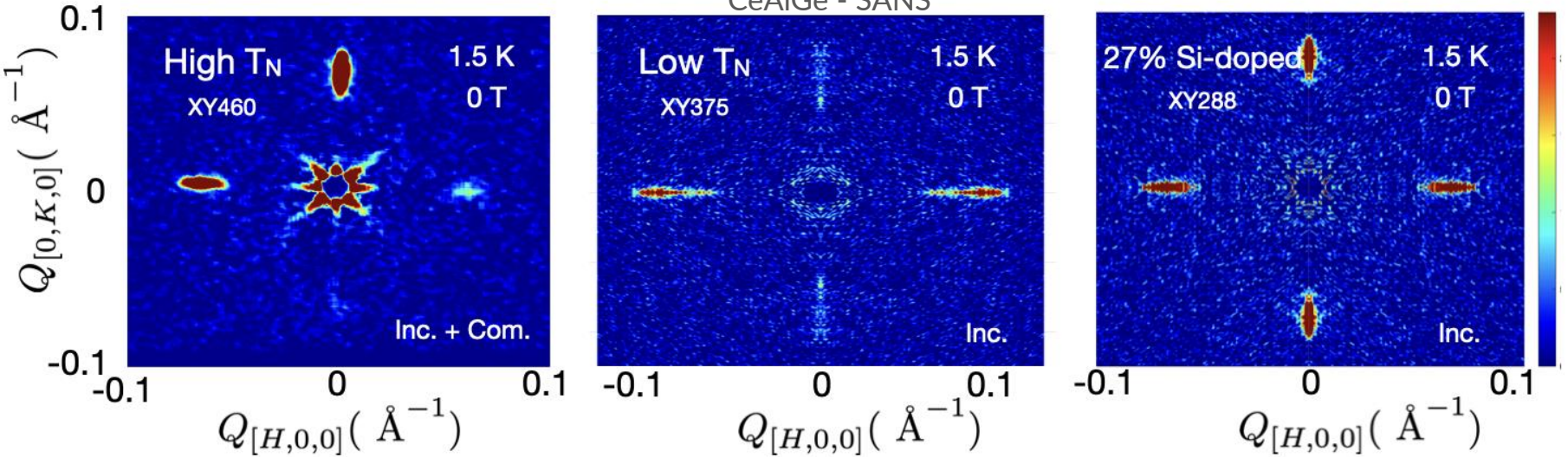


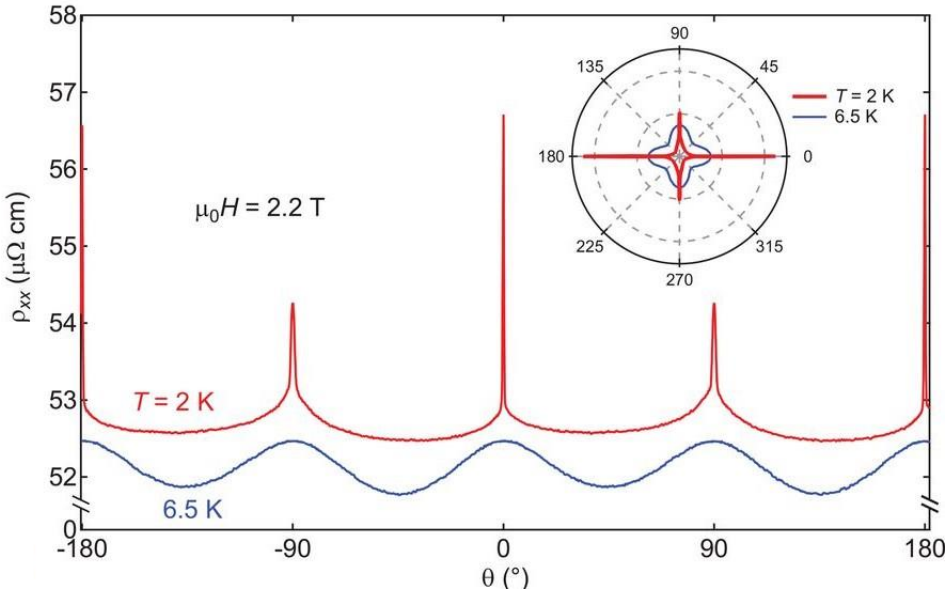
Al

X=Si or Ge

R = Nd, Sm, or Ce

CeAlGe - SANS


High T_N
XY460
1.5 K
0 T
Inc. + Com.
Low T_N
XY375
1.5 K
0 T
Inc.
27% Si-doped
XY288
1.5 K
0 T
Inc.
0.1
0
-0.1
$Q_{[0,K,0]}$(Å^{-1})
$Q_{[H,0,0]}$(Å^{-1})



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