CONTROL your SPIN

Au$_2$Mn

Maria Pascale
University of Maryland
NIST Center for Neutron Research
Background on $\text{Au}_2\text{Mn}$

Body Centered Tetragonal
Background on Au$_2$Mn

- Ferromagnetic within each $x\ y$ plane
- Helicoidal (Helical) Structure

Background on $\text{Au}_2\text{Mn}$

- Ferromagnetic within each $x\ y$ plane
- Helicoidal (Helical) Structure


Wayne R. C., Smith F. A. Journal of Physics and Chemistry of Solids, 30(184) 1969
Motivation

- Spin Properties have only been tested down to 77 K and up to 8.83 kbar
- Single crystal has not been made
Au$_2$Mn Crystal Fabrication

Tetra Arc

Czochralski Process

Seed / Pulling rod

http://www.miracrys.com/CCinit.php?id=technologyam_4
Au$_2$Mn Single Crystal Fabrication

Au-Mn Phase Diagram (1990 Massalski T.B.)

© ASM International 2006. Diagram No. 900230

The graph depicts the phase diagram of the Au-Mn system, showing various phases and their phase transitions at different temperatures and atomic percentages of Mn. The diagram is used for the fabrication of Au$_2$Mn single crystals.
Au$_2$Mn Crystal Growth
MEASUREMENTS

X Ray Diffraction
Energy Dispersive Spectroscopy
Magnetic Susceptibility
Electrical Resistivity
Neutron Scattering
X-Ray Diffraction

Operates using Bragg’s Law

\[ n\lambda = 2d \sin \theta \]

Gives interatomic distances, which can be used to confirm or to deduce crystal structures

X-Ray Diffraction

Meas. data: I-Lin-Au2Mn-3

Intensity (cps)

2-theta (deg)

Pulled Sample: Primarily Au₃Mn

CAUTION! XRD Data may be unreliable due to sample preparation
Energy Dispersive Spectroscopy

Pulled Au-Mn Crystal  Proportions vary slightly depending on the location in the material

Possibly mix of different structural phases
Magnetic Susceptibility

Magnetic response of a sample to an applied field

\[ 4\pi \chi - T \text{ for } 100.5 \text{ mg Au-Mn Alloy} \]

\[ X_p = \frac{C}{T - \Theta} \]

\[ T_C = 130 \text{ K} \]

\[ S = 2 \text{ or } \frac{5}{2} \]

\[ y = m1 + 37.1/(m0 - m3) \]

<table>
<thead>
<tr>
<th>Value</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>m1</td>
<td>1.4453</td>
</tr>
<tr>
<td>m3</td>
<td>127.06</td>
</tr>
<tr>
<td>\chiq</td>
<td>0.0014495</td>
</tr>
<tr>
<td>R</td>
<td>0.99924</td>
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</tbody>
</table>
Au$_2$Mn Crystal Fabrication

Anneal at 730°C

Why?
- Concerned about existence of different phases
- Encourage steady state diffusion
- Obtain Au$_2$Mn
- Increase Grain Size
X-Ray Diffraction

Annealed Sample: Primarily $\text{Au}_3\text{Mn}$

Remember… Potentially unreliable!

Energy Dispersive Spectroscopy

Annealed Au-Mn Crystal

Proportions vary slightly depending on the location in the material

Looks like Au$_2$Mn!
Magnetic Susceptibility

Annealed Sample: $T_C = \text{above 320 K}$

Irreversibility implies magnetic ordering
Electrical Resistivity

- The intrinsic property of a material to prevent the flow of electricity
- Calculated using the $\rho = \frac{RA}{l} = \frac{VA}{I* l}$

**4 Point Test**

![Image of 4 Point Test](image)

$CeRhSi_3$
Electrical Resistivity

Physical Property Measurement System
Neutron Scattering

Disc Chopper Spectrometer

- Cold Neutron Instrument
- Time of Flight Spectrometer
- Closed Cycle Refrigerator: base temperature 2.6 K

1.56 g

NIST NCNR Web Page for DCS https://www.ncnr.nist.gov/instruments/dcs/
Neutron Diffraction

Disc Chopper Spectrometer

Powder Diffraction Rings
Neutron Spectroscopy

Disc Chopper Spectrometer

Magnetic Peaks

Structural Peak

Neutron Diffraction

Disc Chopper Spectrometer

Au$_5$Mn$_2$: Continuity and Contrast

<table>
<thead>
<tr>
<th></th>
<th>Au$_5$Mn$_2$</th>
<th>Au$_2$Mn</th>
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</thead>
<tbody>
<tr>
<td>T Order</td>
<td>354</td>
<td>365</td>
</tr>
<tr>
<td>At % Au</td>
<td>71</td>
<td>66</td>
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EDS

<table>
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<tr>
<th>Atom.</th>
<th>C Error</th>
<th>[at.-%]</th>
<th>[%]</th>
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</thead>
<tbody>
<tr>
<td>Au</td>
<td>63.84</td>
<td>3.9</td>
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</tr>
<tr>
<td>Mn</td>
<td>36.16</td>
<td>1.1</td>
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Conclusions and Outlook

- Structural phase homogeneity is a prevalent challenge
- Fabricate a new sample
- Upcoming Experiment – Pressure and temperature dependence of spin angle using BT4 triple axis
THANK YOU!

Mentor: Nicholas Butch

Acknowledgements: I-Lin Liu, Kefeng Wang
Susceptibility

- The tendency of the magnetic moments (spins) within a material to become aligned with an applied magnetic field

- Higher susceptibility = easier to redirect the spins

![Diagram showing magnetic moments before and after applying a field](image)

Prior to applied Field

Field Applied

100.5 mg
27.1 mg

prior to applied field
X-Ray Diffraction

- X-Rays interact with electrons to reveal
  - Atomic structure and Lattice Parameters
  - Phases and Orientations
  - Thermal Expansion

- Advantages
  - Can use small samples
  - Little effect on sample

- Disadvantage
  - Difficult to distinguish atoms of similar atomic number
  - Hydrogen is virtually invisible
Susceptibility

$4\pi X - T$ for 27.1 mg Au-Mn Alloy

<table>
<thead>
<tr>
<th>Normalized Long Moment (emu/Oe/mol)</th>
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</thead>
<tbody>
<tr>
<td><strong>Value</strong></td>
</tr>
<tr>
<td>m1</td>
</tr>
<tr>
<td>m3</td>
</tr>
<tr>
<td>Chisq</td>
</tr>
<tr>
<td>R</td>
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$y = m1 + 120.125(m0 - m3)$
## Susceptibility

<table>
<thead>
<tr>
<th>Transition (K)</th>
<th>Grown: Top - 100.5 mg</th>
<th>Grown: Middle - 27.1 mg</th>
<th>Annealed</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZFC $T_c$ 1</td>
<td>-70.56 AFM</td>
<td>110.87 FM</td>
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</tr>
<tr>
<td>ZFC $T_c$ 2</td>
<td>34.81 FM</td>
<td>229.92 FM</td>
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<tr>
<td>FC $T_c$ 1</td>
<td>-115.31 AFM</td>
<td>81.30 FM</td>
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<tr>
<td>FC $T_c$ 2</td>
<td>195.58 FM</td>
<td>227.11 FM</td>
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Energy Dispersive Spectroscopy

Annealed Sample
Susceptibility

Annealed Sample: $T_C = \text{above 320 K}$
Energy Dispersive Spectroscopy

How does EDS work?

1. Electron beam excites the sample.

2. X-rays are emitted from the sample.

3. Output energies and their quantities are recorded.

4. Reports elements which are present and their proportional quantities.

Note: The difference between electron levels is atom specific.
Energy Dispersive Spectroscopy

**Pulled Au-Mn Crystal**

- Properties and Proportions vary depending on the location in the material

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Surface – Likely mix of Au$_3$Mn and AuMn

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![Graph with spectra and a table showing the elemental analysis of Au and Mn.

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>Au</td>
<td>M-series</td>
<td>80.44</td>
<td>84.94</td>
<td>61.14</td>
<td>3.2</td>
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<tr>
<td>Mn</td>
<td>K-series</td>
<td>14.26</td>
<td>15.06</td>
<td>38.86</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Total: 94.70 100.00 100.00
Reference

Gold-Manganese Binary Diagram (1990 Massalski T.B.)

Publication year: 1990
Diagram type: binary phase diagram
Concentration range: full composition; 0-100 at.% Mn
Temperature: -100 - 1400 °C
Nature of investigation: experimental
Authors: Massalski T.B., Okamoto H.
Title: Au-Mn (Gold-Manganese)
APDIC diagram: No

Callister D. William, Rethwisch G. David.


Yellow Submarine
https://garinglenn.wordpress.com/2013/10/18/magic-wand-and-quick-select-tools/

Electron Diffraction Spectroscopy

**Outer Core – Likely Au₃Mn and AuMn**

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<tbody>
<tr>
<td>Au 79 M-series</td>
<td>77.71</td>
<td>85.15</td>
<td>61.52</td>
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<tr>
<td>Mn 25 K-series</td>
<td>13.55</td>
<td>14.85</td>
<td>38.48</td>
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<tr>
<td><strong>Total:</strong></td>
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<td><strong>100.00</strong></td>
<td><strong>100.00</strong></td>
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</table>

**Inner Core – Primarily Au₂Mn**

<table>
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<th></th>
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<td>Au 79 M-series</td>
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<td>87.09</td>
<td>65.29</td>
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<tr>
<td>Mn 25 K-series</td>
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<td>12.91</td>
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<tr>
<td><strong>Total:</strong></td>
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<td><strong>100.00</strong></td>
<td><strong>100.00</strong></td>
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