The Synthesis of Selected B20 Materials

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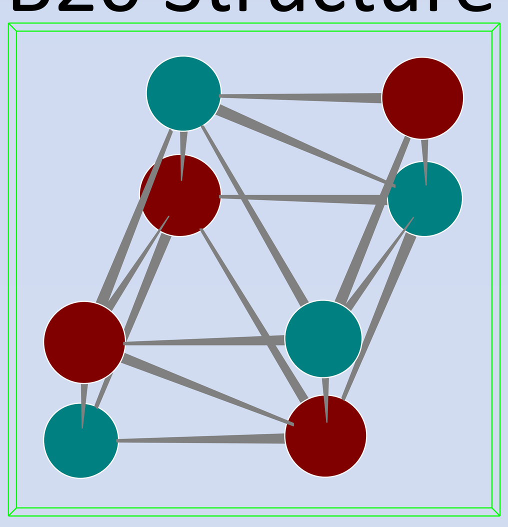
Identification of the B20 Cubic Structure

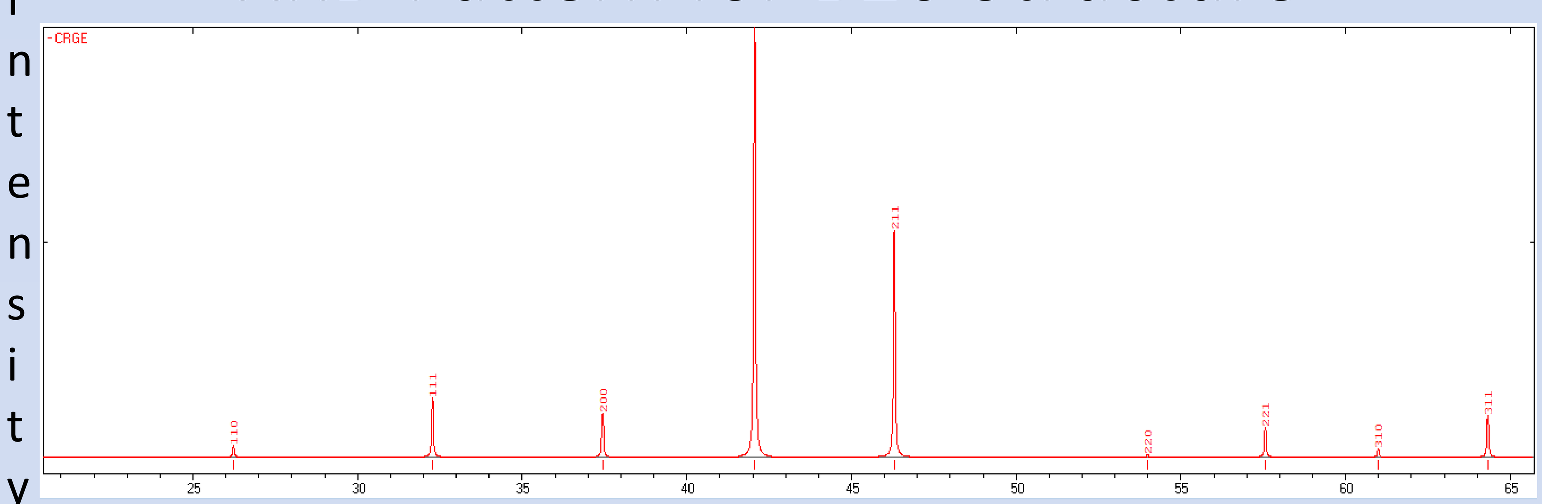
Crystal structures are often classified by their lattice planes. These planes are results of the repeating periodic structure of the lattice. A particular structure has a unique combination of planes at angles to one another. The overall structure can be determined from the diffraction of x-rays through these planes. The x-rays constructively interfere at particular angles governed by Bragg's Law. Powder x-ray diffraction (Powder XRD) is used to correct for skewed relative peak intensities from polycrystalline samples. Once an XRD pattern is taken, it can be compared to calculated or experimental examples of the suspected structure for confirmation.

B20 Structure



Generated in PowderCell

XRD Pattern for B20 Structure



Intensity

2θ (degrees)

Bragg's Law

$$n\lambda = 2d\sin\theta$$

n is an integer

λ is the incident wavelength

d is the distance between crystal planes

θ is the angle between the incident ray and the plane

Chromium Germanide

Chromium Germanide, CrGe, is a material which naturally crystallizes in the B20 Cubic structure. This structure places alternating elements in a three dimensional grid so that each Cr has nearest neighbors of Ge and vice versa.

At temperatures below 62K the spins of the chromium atoms antialign with the spins of nearest neighbor chromium atoms. This is a potentially interesting phenomenon, because the chromium sublattice of the B20 structure is made up of triangles. These triangles build in a frustration in that any three points cannot perfectly antialign with one another.

Synthesis

Arc Melter

First method: Arc Melter

- -Measure Cr and Ge in 1:1 stoichiometric ratio
- -Combine in Arc Melter
- -Seal in evacuated quartz tube
- -Anneal at 880°C for 80 hrs

New method: Solid State Reaction

- -Measure Chromium and Germanium in 1:1 stoichiometric ratio
- -Grind and mix thoroughly with mortar and pestle
- -Press into a pellet under 3 metric tons for ~1 hr
- -Seal in evacuated quartz tube
- -Heat at 900°C for 80 hrs

Solid State Reaction Sample

Manganese Silicide

Manganese Silicide, MnSi, is also a material with the B20 Cubic structure. In this case at low temperatures the spins of the Manganese atoms arrange so that the magnetization progresses helically over a distance of about 18 nm.

Unlike the proposed measurements for CrGe, the future experiments for this MnSi sample require large single crystals. Because of this arc melting and solidstate reaction cannot be used.

Synthesis

The Flux Method

- -Measure Mn and Si in 1:1 stoichiometric ratio
- -Place in small crucible with much larger portion of Gallium
- -Stuff the top of the crucible with silicon wool
- -Seal in evacuated quartz tube
- -Heat above the melting point of the constituents
- -Slowly lower the temperature to a level below the melting points of the Mn and Si but above that of the flux
- -While hot, remove from the oven and centrifuge sample upside down

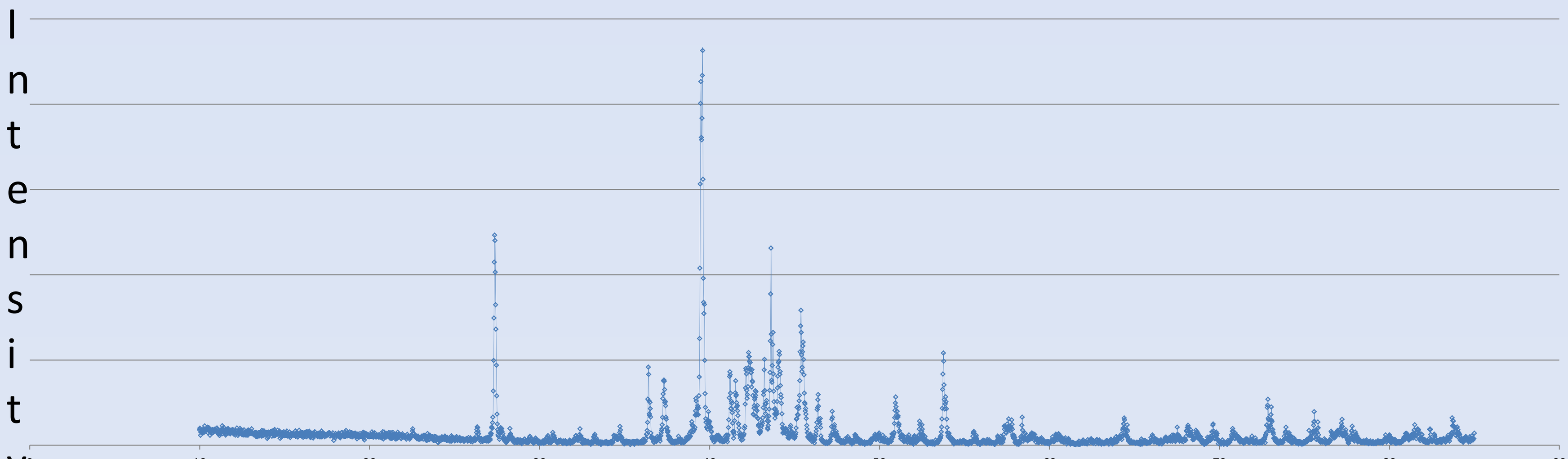
At the time of this poster's creation single crystal x-ray diffraction information was not yet available for the Manganese Silicide sample.

Clusters of needle shaped single crystals of MnSi

Results

XRD Pattern for Arc Melted Sample

Intensity



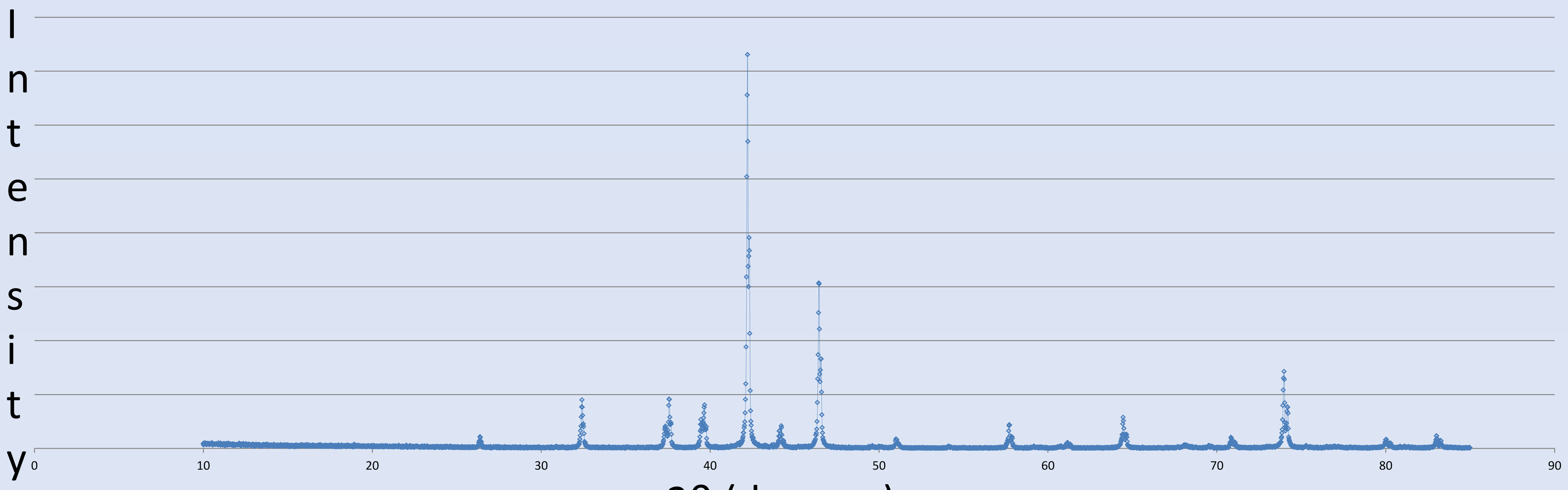
2θ (degrees)

Analysis:

Very messy. Many peaks exist in unrecognized positions. Many phases are present.

XRD Pattern for Solid State Reacted Sample

Intensity



2θ (degrees)

Analysis:

Sharp peaks. Two unknown peaks. Very close match.

Future Work

Once the sample has been confirmed as CrGe the resistivity and magnetic susceptibility will be studied at various temperatures with the help of liquid Helium. We are especially interested in measuring the Hall effect.

References

Introduction to X-ray Diffraction. Materials Research Laboratory, UC Santa Barbara. <http://www.mrl.ucsb.edu/mrl/centralfacilities/xray/xray-basics/index.html#x1>

Yasukochi, Ko, et al. "Antiferromagnetism of CrGe." Journal of the Physical Society of Japan 21 p557 (1966).

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

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