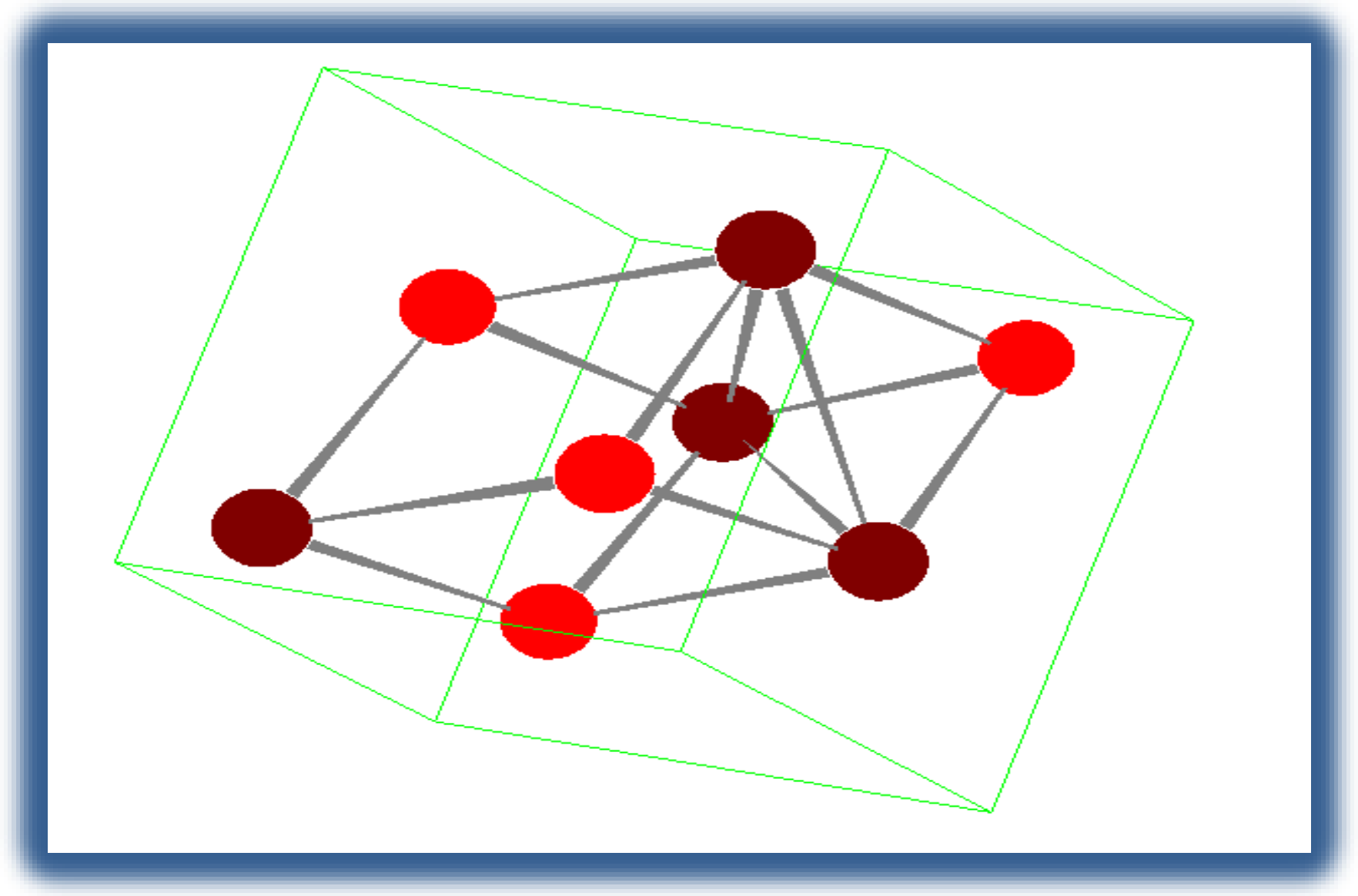
LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Optimizing FeSi Semiconductor by Means of Cobalt and Aluminum Doping

D. Lauriola[1], J.F.DiTusa[2]

[1]Rose Hulman Institute of Technology, Terre Haute, IN
[2]Louisiana State University, Baton Rouge, LA



Objective

To explore the effect of hole and electron co-doping of this semiconductor ($Fe_{1-x}Co_xSi_{1-y}Al_y$) on the magnetism and electrical transport..

Introduction

Semiconductor doping is essential for microelectronics and solid state physics. The FeSi semiconductor is particularly good for doping as it has interesting magnetic and electrical properties. Al substitution for Si donating holes, while Co substitutes for Fe donating electrons. Measuring the magnetic moment of this new compound will give further insight on how this semiconductor reacts to doping and its possible future applications in spintronics technology. Previously there had been research on single doping of the FeSi semiconductor but combining hole and electron doping may give the possibility to separately control magnetic and electronic properties of the semiconductor.

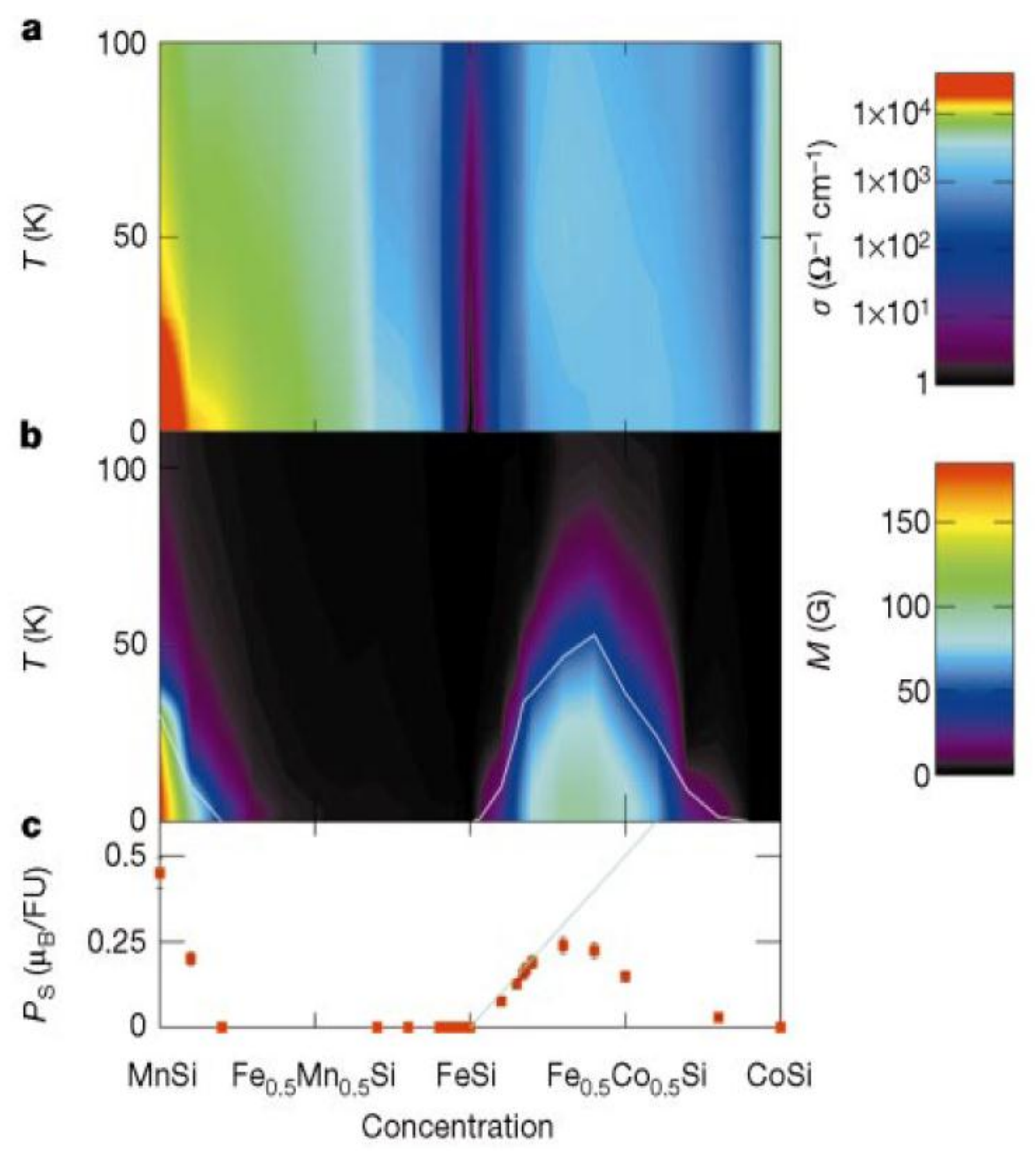
Properties of $Fe_{1-x}Co_xSi$

FeSi

- **60 meV band gap insulator**
- **Cubic B20 noncentrosymmetric crystal structure**
- **Vanishing low temperature susceptibility**

$Fe_{1-x}Co_xSi$

- **Co substitutes for Fe and increases the conductivity**
- **Co doping increases the magnetization**
- **Half metal at lower Co doping percentages.**



Schlesinger, et al. PRL. V71. n11. 1993.
Manyala, et al. Nature. V404 2000

Methods and Crystal Structure

Arc-melting

The sample was created by *arc-melting* together the different elements in an evacuated argon chamber. The sample reached a temperature of about 2500 K.

Annealing

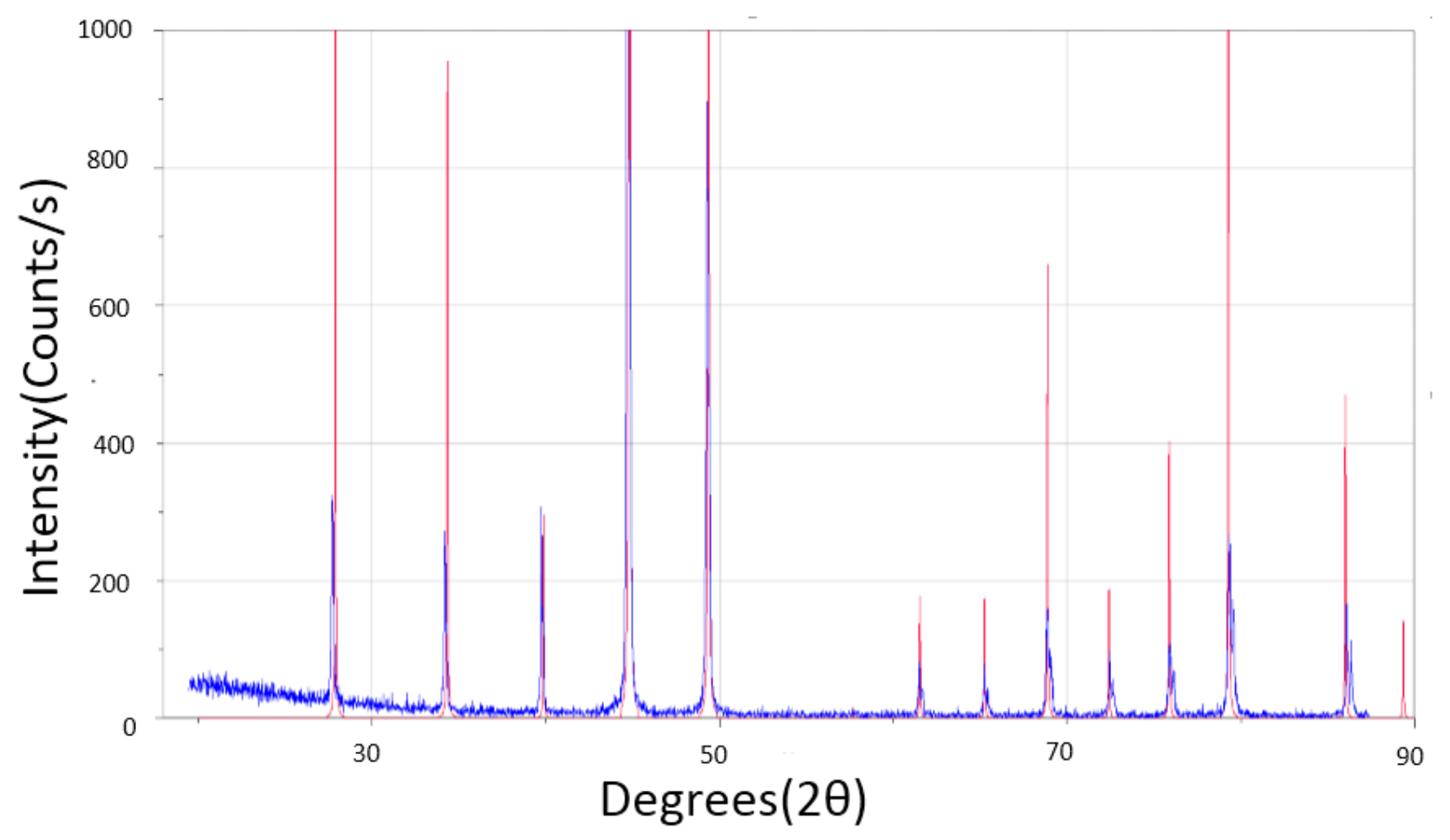
The sample was put into an evacuated quartz tube and heated in a box furnace. It remained at 1000 C for a minimum of 24 hours. This ensured that the sample was well mixed and uniform in phase. Then the sample was quenched in cold water in order to maintain the correct crystalline structure.

X-Ray Diffraction

The annealed sample was then cut and part of it was ground to powder. The x-ray diffraction (XRD) was used to determine if the sample was single phased. Bragg's law (2d sinθ=nλ) was then used to determine the lattice constant

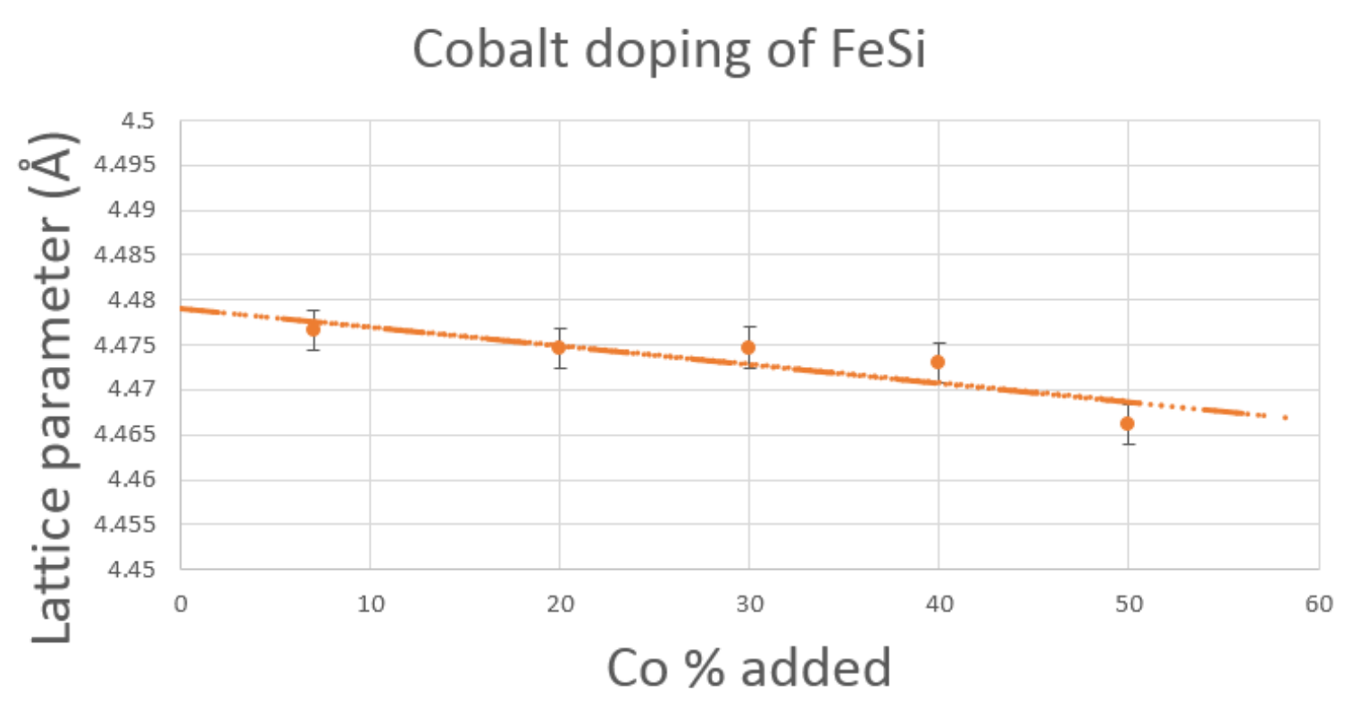
X-Ray Diffraction pattern:

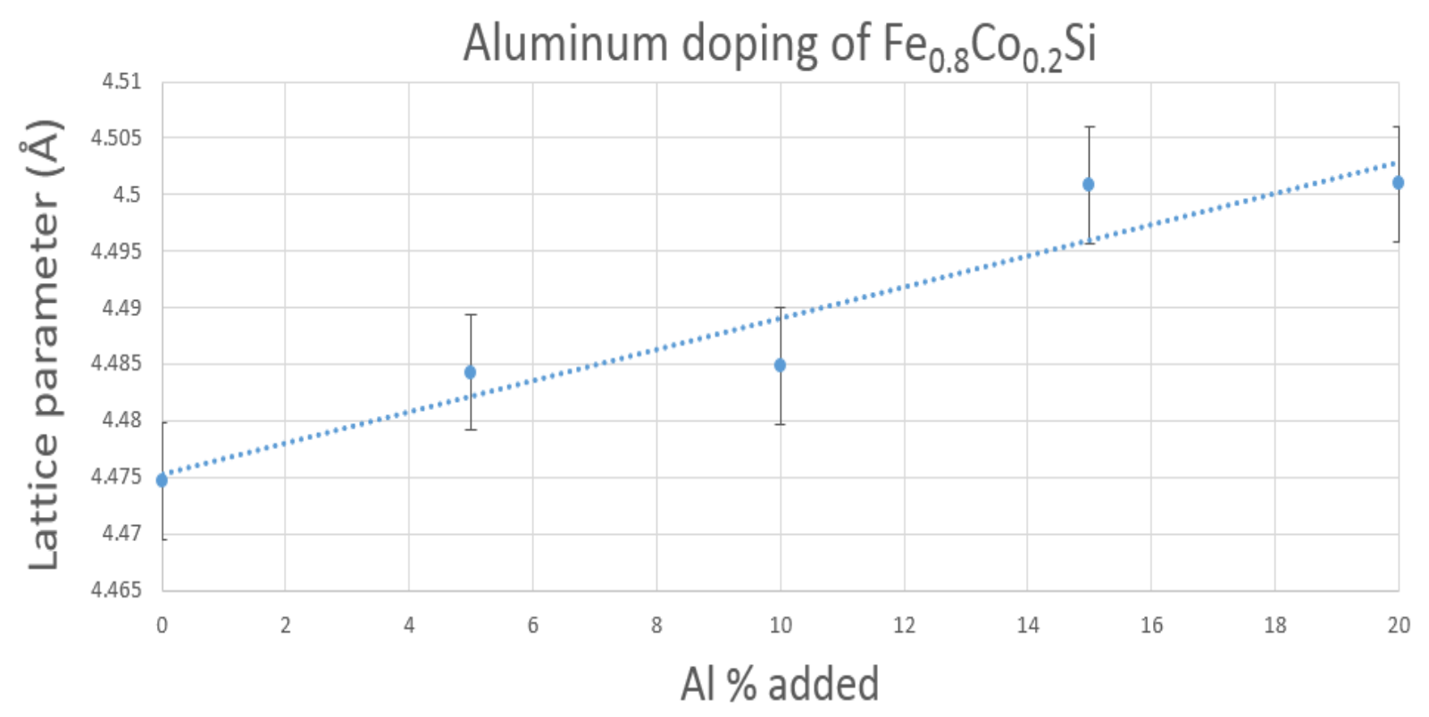
Comparison between theoretical (red) and experimental results(blue)



Results

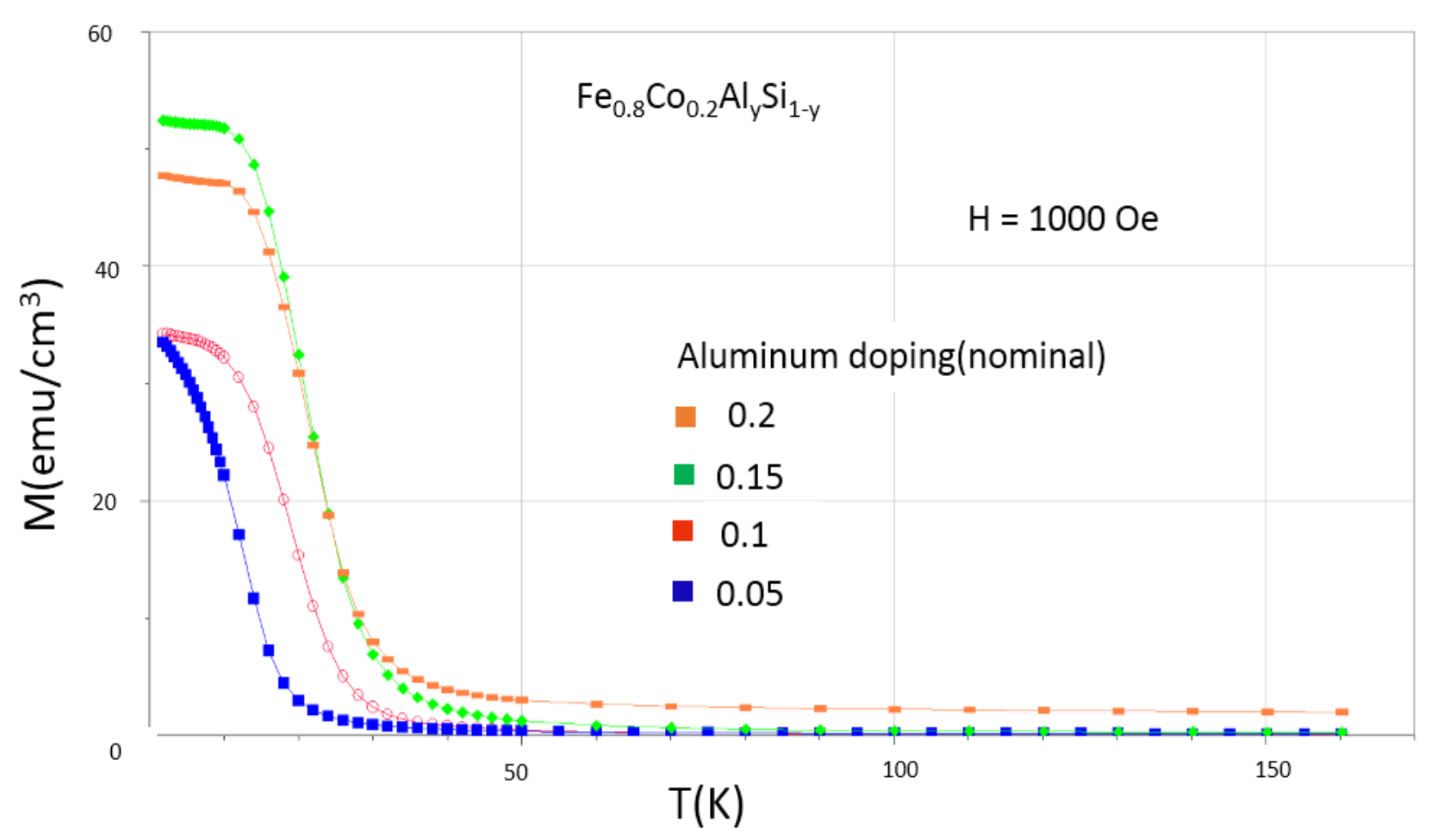
Change of lattice constant as samples are doped



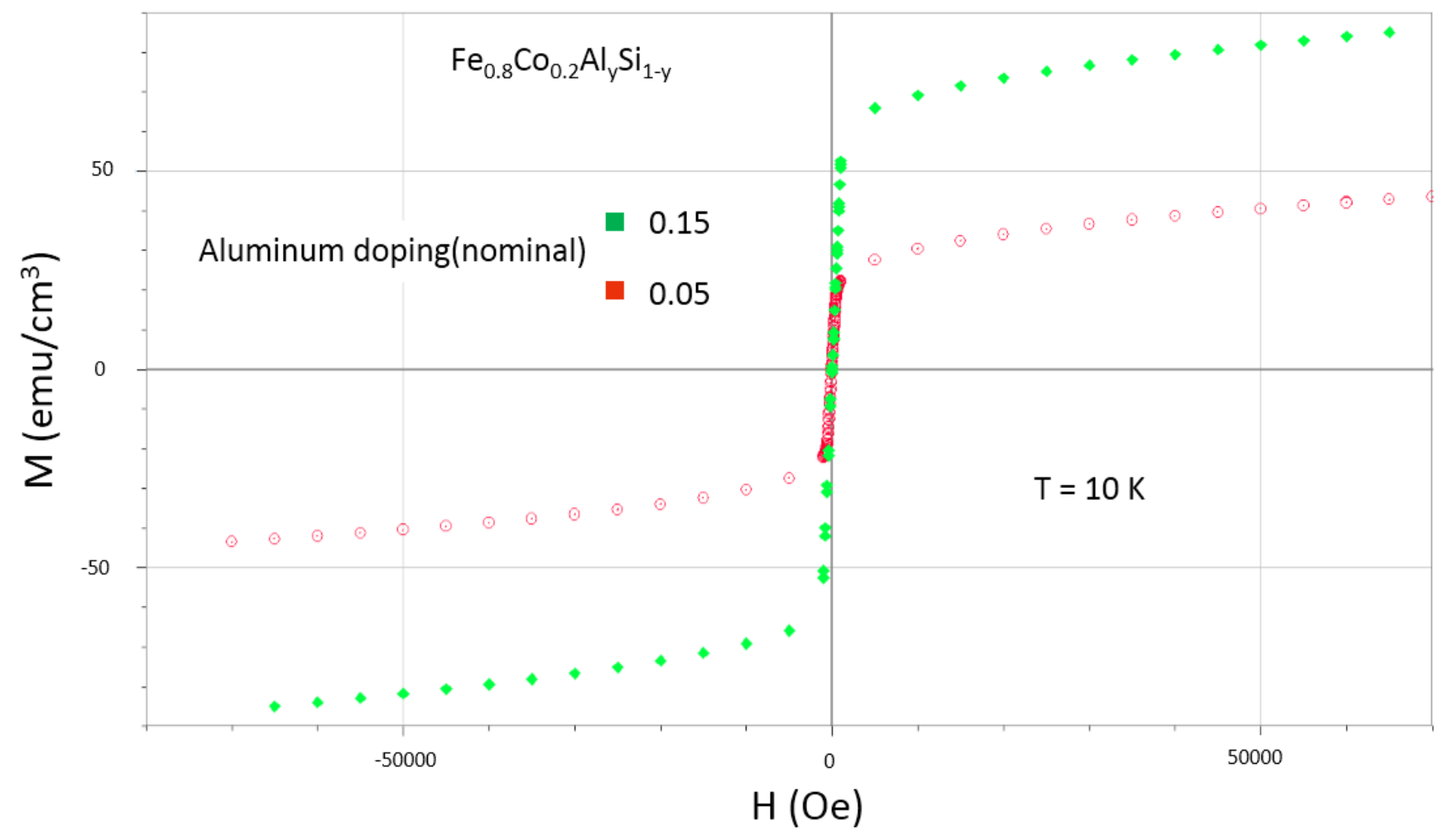


Magnetization Measurements

The Superconducting Quantum Interference Device (SQUID) was used to measure the magnetization of the sample. This measurement was done after the XRD revealed that the sample was single-phased.



- **Temperature sweep: 1.8 to 160 K**
- **Field sweep: -70000 to 70000 Oe**
- **Increased magnetization as Al and Co was added**



Conclusion

- **Lattice constant decreases linearly with Co, increases linearly with Al doping**
- **Magnetization increased with Co *and* Al doping**
- **Magnetization saturates at low temperatures with higher Al doping**

Ongoing Work

- **More measurements of magnetization with different doping percentages**
- **Measurements of magnetoresistance and the Hall effect to determine electron scattering mechanisms, carrier concentration and carrier type.**

ROSE-HULMAN INSTITUTE OF TECHNOLOGY

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Personal information

Daniel Lauriola
dk.lauriola@gmail.com
Rose Hulman Institute of Technology
260-413-4080