University of North Carolina at Asheville
Journal of Undergraduate Research
Asheville, North Carolina
May 2013

# Magnetic Properties of $BaFe_2As_2$

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## Abstract

Magnetism plays an important role in superconductivity. Specifically, there must be a complete absence of magnetic ordering for superconductivity to occur[1]. It is known that $BaFe_2As_2$ becomes superconducting only after being doped with nickel or cobalt[2]. Doping lowers the Curie temperature of $BaFe_2As_2$ such that it never becomes magnetically ordered. Introducing nickel or cobalt changes the electron density, which has a strong effect on magnetization. We can learn about the transition into superconductivity by studying the magnetic properties of $BaFe_2As_2$ using Mössbauer spectroscopy. A duel sextet model is used to fit Mössbauer spectra as an improvement over single sextet fittings[3].

## 1. Introduction:

$BaFe_2As_2$ is part of a family of recently discovered high temperature superconductors. Understanding the magnetic structure in $BaFe_2As_2$ is essential to understanding the transition into a superconducting state. When the parent compound is doped with ~5% cobalt or nickel we observe the transition into superconductivity around 20K[4]. The substitution of cobalt or nickel introduces additional electrons to the conduction band, which are thought to disrupt magnetic ordering and allow the onset of superconductivity. Using Mössbauer spectroscopy we study the iron sites of $BaFe_2As_2$ which are an indicator of the magnetism present in our sample.

Mössbauer spectroscopy is a sensitive tool, which we use to measure magnetic field strength on the iron nucleus, as well as determine the Debye temperature of the crystal lattice. Figure 1 shows the experimental setup by which a radioactive source interacts with our sample to produce an absorption spectrum.

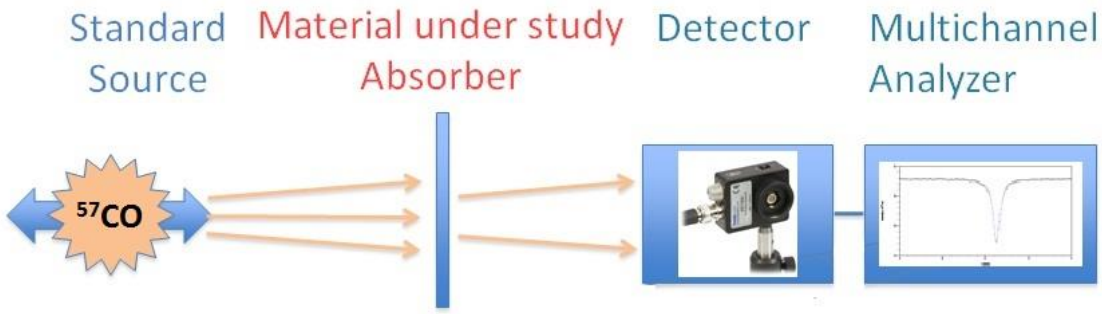


Figure 1: A source emits radiation which interacts with a sample to produce an absorption spectrum.

Radioactive $^{57}Co$ is used as the source which decays into an excited state of $^{57}Fe$. The excited iron nucleus has a $10^{-7}$s half-life and emits a 14.4KeV photon when it transitions to the ground state. Photons

may then interact with the sample via recoil free resonant absorption. Using a Doppler drive, which allows us to scan a range of frequencies, we obtain an absorption spectrum that gives a wealth of information about our sample including isomer shift and hyperfine splitting.

Isomer shift is the shift of spectral lines relative to the spectral lines of a standard absorber. Figure 2 shows an example of an isomer shift as seen in a Mössbauer spectrum. In our case, when we compare the

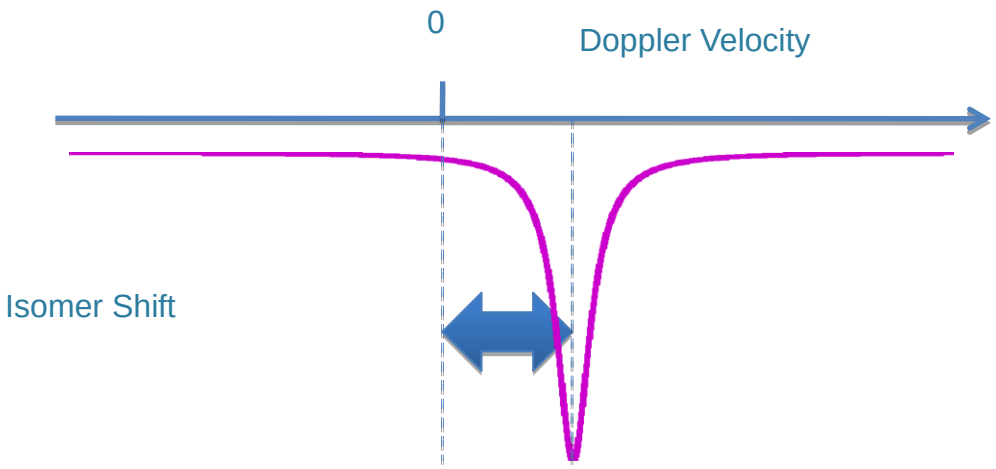


Figure 2: A spectral line is shifted to the right.

spectral lines of $BaFe_2As_2$ to those of pure iron (ferrite) we notice that the absorption lines have been shifted by an energy corresponding to a Doppler velocity of ~0.5mm/s. This shift is caused by the fact that an iron nucleus sitting in a ferrite lattice is surrounded by a different chemical environment than an iron nucleus in our $BaFe_2As_2$ lattice. More specifically, the sample will have a different electron density at the nucleus than the source. As a result an iron nucleus in the sample will resonate at a different energy than an iron nucleus in the source. Figure 3 shows an example of an absorber requiring more energy to resonate than is emitted by the source. The Doppler motion of the source makes up for this difference.

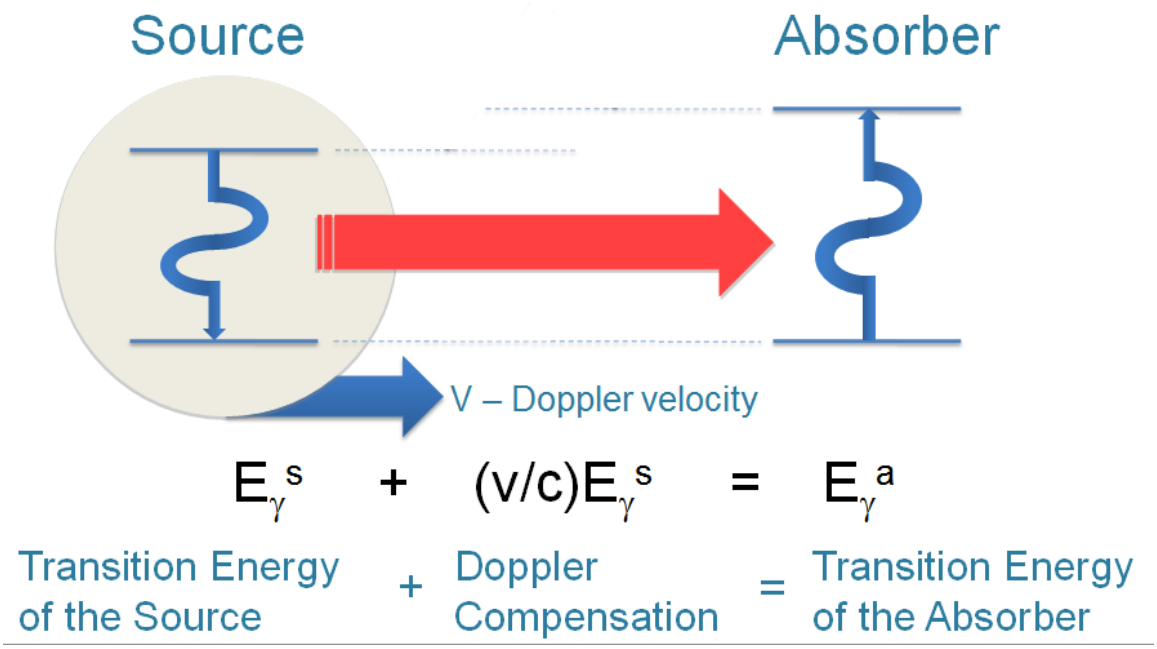


Figure 3: Isomer shift is measured by the Doppler velocity required for resonance.

It should be noted that there is a temperature dependence to the isomer shift caused by the Second Order Doppler shift (SOD). That is, *Isomer shift = chemical shift + SOD.* Temperature dependence of the isomer shift tells us about the Debye temperature and is given by equation 1 where *k* is Boltzmann's constant, $\Theta_D$

$$SOD = -\frac{3}{2}\frac{k\Theta_D}{Mc}\left[\frac{3}{8}+3\left(\frac{T}{\Theta_D}\right)^4\int_0^{\Theta_D/T}\frac{x^3dx}{e^x-1}\right] \quad (1)$$

is the Debye temperature, *M* is the mass of the nucleus, *c* is the speed of light and *T* is temperature[1].

Hyperfine splitting is the splitting of the energy levels of the nucleus and is caused by an applied magnetic field on the nucleus. Figure 4 shows the first excited state of $^{57}$Fe splitting into four energy levels, and the ground state splitting into two. As a result there are eight possible transitions instead of one. Two of

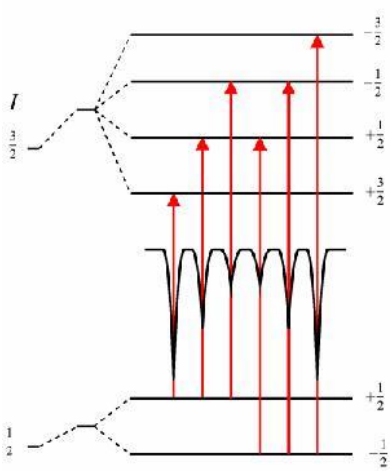

Figure 4: Splitting of the energy levels of the excited and ground state. Red arrows represent allowed transitions and are overlaid by a theoretical Mössbauer spectrum.

the transitions are not allowed due to the photon having spin 1. The six allowed transitions cause Mössbauer spectra to exhibit a sextet instead of a singlet which is observed in the absence of magnetic ordering. In our case the magnetic field on the nucleus comes from radial spin polarization of the s-orbitals, which in turn come from uncompensated spin of the outermost electrons[5].

The strength of the hyperfine field on the nucleus can be seen in Mössbauer spectra as the resolution of the sextet. A strong hyperfine field produces a clear sextet whereas a singlet indicates a weak hyperfine field. The normalized temperature dependence of the hyperfine field is a Brillouin function that can be seen in Figure 5, where $M/M_0$ is normalized magnetization and $T/T_c$ is normalized temperature. The exact shape of the Brillouin curve depends on magnetic moment of the atoms[6].

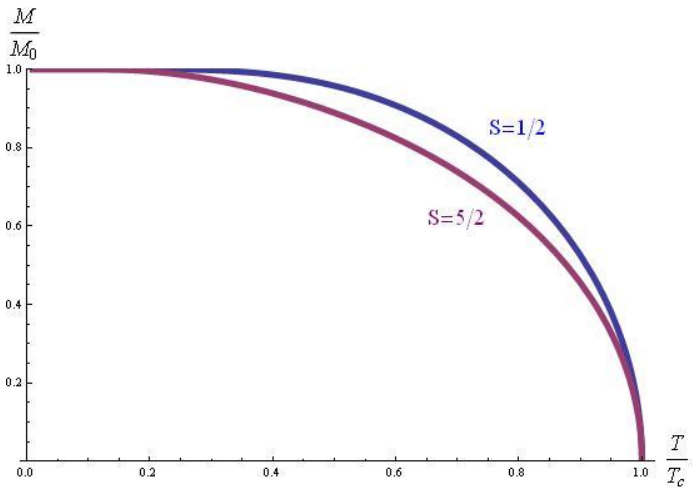


Figure 5: Normalized temperature dependence of hyperfine field of atoms with 5/2 and 1/2 spin.

## 2. Results

Amorphous $BaFe_2As_2$ crystal is crushed into a powder with particle size on the order of a micron before Mössbauer spectra are taken. Debye temperature is determined by measuring the temperature dependence of the isomer shift. Figure 6 shows the theoretical curve of a material with Debye temperature equal to 257K.

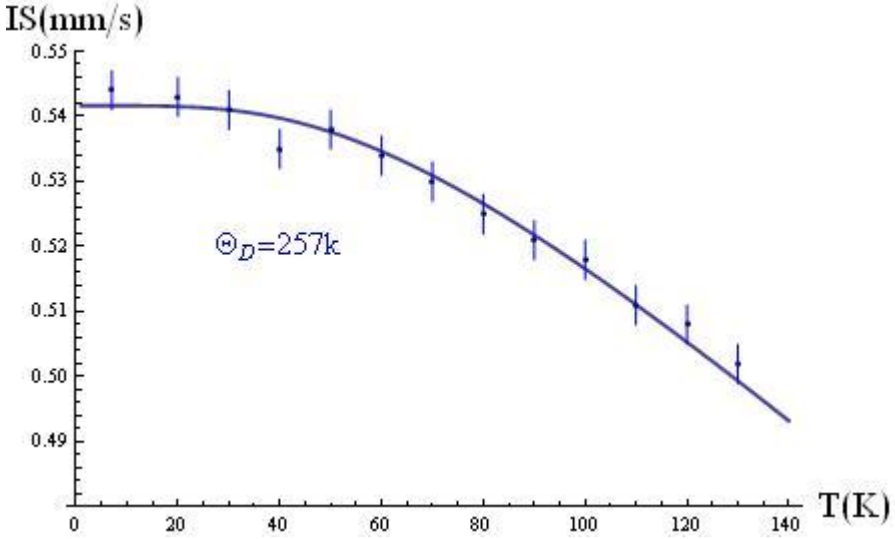


Figure 6: An attempt to fit data with a single Debye temperature.

The single Debye temperature model clearly does not work because of the anomalous behavior near 40K. Figure 7 shows data fit with two Debye temperatures, indicating that the Debye temperature changes from 257K to 120K when the sample is cooled below 40K. It should be noted that each data point represents a

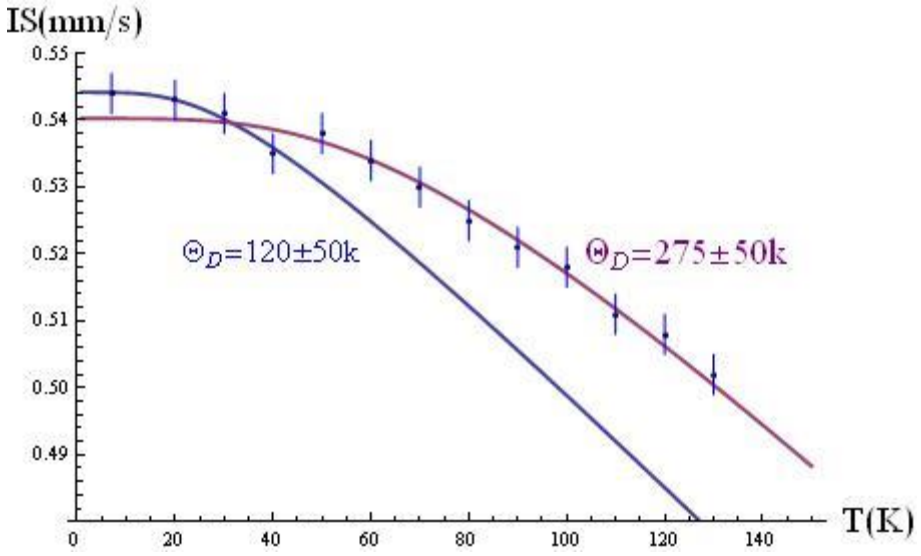


Figure 7: Debye temperature changes from 275K to 120K when cooled below 40K.

Mössbauer spectrum that was fitted with a two sextet model. Figures 8 and 9 show the justification for using the two sextet model. While the two sextet model fits our data better, it raises interesting questions about the structure of the $BaFe_2As_2$ lattice.

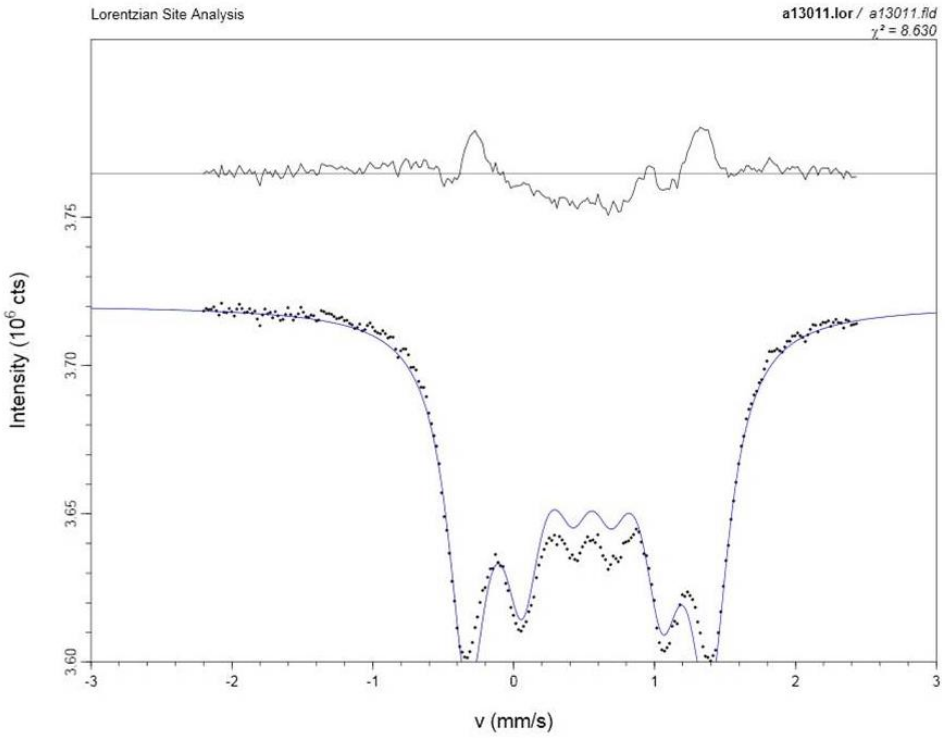


Figure 8: Mössbauer spectrum at 20K fit using one sextet.

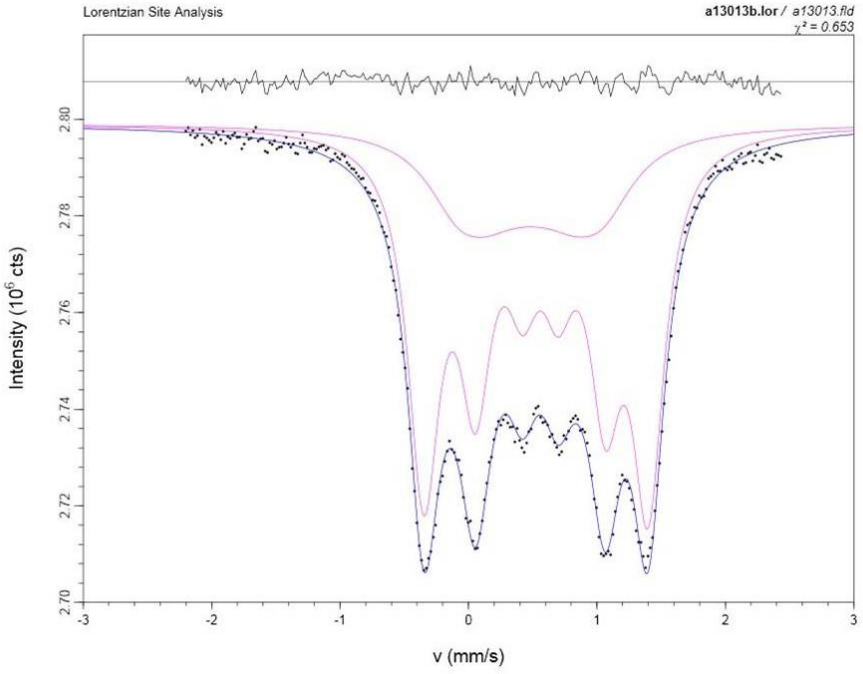


Figure 9: Mössbauer spectrum at 40K fit using two sextet model.

## 3. Discussion

Mössbauer spectra fit with two sextets are clearly superior to the one sextet model. However this raises an important question as to where the second sextet comes from. Fitting spectra with two sextets implies that there are two distinct iron sites, each contributing to one of the sextets[7]. Symmetry of the lattice suggests that all iron sites should have the same chemical environment. Figure 10 shows the unit cell of $BaFe_2As2$ and four arsenic atoms surround each iron atom. The two sextet fit can be explained by an incommensurate

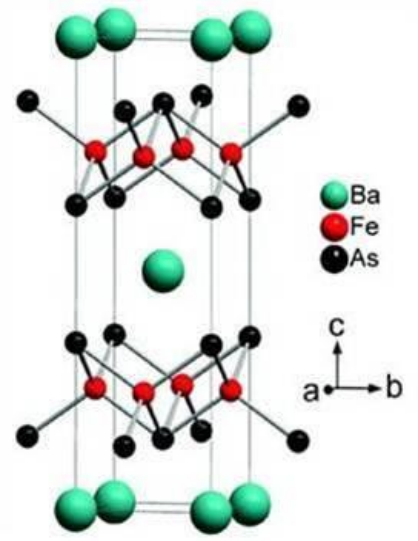


Figure 10: The unit cell of $BaFe_2As_2$.

spin density wave in $BaFe_2As_2$[8]. A spin density wave is spatial spin polarization of electron density. A non-uniform distribution of uncompensated electron spin would cause various iron sites in a symmetric lattice to experience different values of hyperfine field on the nucleus[9]. Figure 11 shows a one dimensional model of an incommensurate spin density wave. The amplitude of the wave corresponds to amount of spin polarization, which determines the strength of the magnetic field on the nucleus.

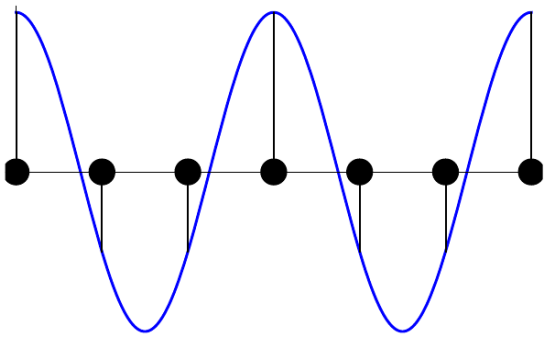

Figure 11: An incommensurate spin density wave leads to two distinct iron sites.

## 5. Acknowledgements

Thanks to Dr. Airat Khasanov for his help on this continuing project, and to the Undergraduate Research Program at UNC Asheville.

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