



PARAMETRIZATION OF FERROMAGNETIC PHASE TRANSITION IN FE

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Abstract

The paper looks about phase transition and the thermodynamic property of Iron. The Thermodynamic functions are studied and parametrized. These parameters, which control the phases, one can often make the jumps arbitrarily small and thus produce continuous phase transitions. This kind of phase transitions are abrupt changes in the equilibrium behavior of the materials because the materials can be considered to be made up of an effectively infinite number of particles.

The property of ferromagnetic substance is that the atomic magnets tend to be brought into parallel orientation not only by an applied magnetic field but also by an inner field. The inner field is due to electrostatic interactions, which are related to the orientation of the magnetic moments of electrons through the Pauli principle because of that the spins generate magnetic fields.

The spin Hamiltonian for iron has been derived from electronic structure calculations using Ising model. The Coupling interactions J_{ij} depend on the surrounding magnetic order. The exchange interactions are expected in general to tend to cause the atomic moments on adjacent atoms to align themselves in the antiparallel orientation. If these interactions are less important than the interactions that stabilize the parallel orientation of the atomic moments, the substance will be ferromagnetic at low temperature.

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Chapter 1

Introduction

A magnetic material involves Different forms of magnetic behavior and symmetry consideration. Classification of the different types of magnetism is accomplished by considering the response of the material to a magnetic field,the magnitude and orientation of magnetic moments in the unit cell.

Magnetic behavior of most materials can be classified as diamagnetism, paramagnetism, ferromagnetism,antiferromagnetism or ferrimagnetism.A simple approach to finding the symmetry for these structures is possible by considering the intersection of the atomic crystal structure with the symmetry of the magnetic moments by taking into account their spins orientations.

Differences in magnetic behavior arise from differences in exchange interactions for different materials. The exchange interactions are quantum mechanical phenomena required by the Pauli exclusion principle.For strong exchange,the magnetic moments have a strong coupling to one another[1].

1.1 Properties of Ferromagnetism

Ferro is,the Latin word for iron,a material which displays strong magnetic properties.Electrons produce a small magnetic field as they spin and orbit the nucleus of an atom.For many atoms,the combinations of electrons in their orbits cancel each other out.In ferromagnetic materials, however,the electron fields in the atoms do not cancel out,so they exhibit a

long-range ordering phenomenon at the atomic level, which causes unpaired electron spins to line up parallel with each other in a region called a domain[2].

Ferromagnetism is due to the ordered array of magnetic moments caused by the interaction of atomic spin moments occurring in certain conditions. It is a typical phenomenon occurring in materials such as iron, cobalt, nickel, and many alloys containing these elements. The ferromagnetic phase appears when a small external magnetic field yields a large magnetization inside the material, due to the alignment of the spin magnetic moments[3].

Ferromagnetic substances are made of atoms with permanent magnetic dipole moments. The electrons in these atoms naturally place the system in a state of lower energy by having neighboring atomic dipole moments aligned with each other. This alignment of moments results in large net magnetization even in the absence of an external magnetic field, known as spontaneous magnetization.

Below a certain critical temperature, T_c , an increasing magnetic field applied to the ferromagnetic substance will cause increasing magnetization to a limiting value, called the saturation magnetization. This occurs when the domains themselves are forced to rotate and align with the external magnetic field. Thermal agitation above the Curie temperature converts the material from a ferromagnetic substance to a weak paramagnetic one[4].

The magnetic properties of solids originate in the motion of the electrons and in the permanent magnetic moments of the atoms and electrons. Ferromagnetism, which is very strong, occurs when quantum mechanical exchange interactions align adjacent magnetic moments in the same direction. If the exchange interaction aligns the moments in opposite directions, and only one type of moment is present, cancellation occurs and the material is called anti-ferromagnetic. Above some critical temperature, a phase transformation occurs. The magnetic moments in a ferromagnet have the tendency to become aligned parallel to each other under the influence of a magnetic field. However, unlike the moments in a paramagnet, these moments will then remain parallel when a magnetic field is not

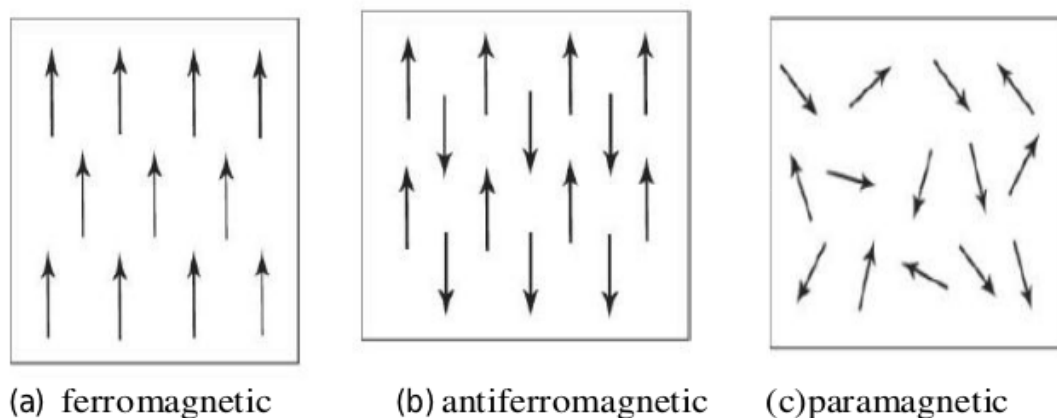


Figure 1.1: Schematic diagram showing the magnetic dipole moments randomly aligned applied. An example is Fe[5].

If the iron heat in the presence of B and then remove the field after the iron has cooled to room temperature, then it obtain a permanent magnet. In an ideal paramagnet, each microscopic magnetic dipole is affected only by external magnetic fields, not by one another. In an applied magnetic field these dipoles start to align parallel to the field such that the magnetisation of the material is proportional to the applied field[5].

1.2 Ferromagnetic Materials

The iron ions each have a magnetic moment and due to a complicated interaction with each other and with the conduction electrons, they tend to line up with each other. At sufficiently low temperatures, the moments can be aligned by an external magnetic field and produce a net magnetic moment or magnetization, which remains even if the magnetic field is removed. Materials that retain a non-zero magnetization in zero magnetic field are called ferromagnetic.

Ferromagnetic materials will respond mechanically to an impressed magnetic field, changing length slightly in the direction of the applied field. This property, called magnetostriction. The relatively high magnetizability comes from the ferromagnetic character of the individual domains. However, the very different way in which the domains interact with each

other helps in gaining an appreciation for the magnetization of ferromagnetic polycrystalline solids[6].

At high enough temperatures there is enough energy to destroy the magnetization, and the iron is said to be in the paramagnetic phase. Ferromagnetism is a property not just of the chemical make-up of a material, but of its crystalline structure and microscopic organization. This ordered state may not be explained by classical magnetic interaction between the constant magnetic moments, because the magnetic dipole-dipole interaction energy. Like iron, behave like paramagnets at high temperature, but below a certain temperature T_c , acquire a spontaneous magnetization. That is, they have a finite value of M , even when $B=0$. In these materials, long-range interactions between the dipoles create a mean internal field that can bootstrap an overall dipole alignment.

When the temperature is high, the thermal motion of the dipoles prevents this ordering. As the temperature cools, small regions of dipoles become susceptible to fluctuations, which can create small, aligned domains. As cooling continues, these domains are subject to larger aligning fluctuations, the susceptibility χ grows very large, and at T_c a global alignment locks in. We may say that at the critical temperature, an infinite χ multiplies a zero B to yield finite M [7].

1.2.1 characteristic of the ferromagnetic materials

1. They can often support a very strong magnetic field, because neighboring atoms tend to align their spins and their magnetic moments interact. Thus a small applied magnetic field is strongly enhanced by the behavior of the material itself. The enhancement is larger at low temperatures and smaller at high temperatures. The higher temperatures tend to literally shake up the aligned spins and substantially reduce their alignment. For temperatures above the critical temperature, when the field is zero, the alignment is also zero[7,8,9].

2. Are Materials possess a permanent magnetic moment,result from atomic magnetic moments due to uncancelled electron spins as a consequence of the electron structure,in the absence of an external field,and manifest very large and permanent magnetizations. permanent magnetic moments are located in atoms or molecules and originate from;
 - the circling of the electrons around the nuclei(orbital moments)
 - from the spin of the electrons themselves(spin moments)
 - coupling interaction arise from the electronic structure of metal cause to net spin magnetic moments of adjacent atoms align with one another[9].

3. In ferromagnetic materials,mutual interaction is important that atoms can be so closely spaced for the magnetic field due to the moment of one atom to have a significant effect on the orientation of another.

Macroscopic magnetization occurs when a field is applied to a solid,because those domains that have a magnetic dipole moment nearly aligned with the applied field grow at the expense of domains whose magnetic dipole moments are less aligned with the applied field.

The maximum possible magnetization(saturation magnetization) of a ferromagnetic material represents the magnetization that results when all the magnetic dipoles in a solid piece are mutually aligned with the external field at lower temperature.

1.2.2 Property of Magnetic domains

when a ferromagnetic material seemingly does not possess a permanent magnetic moment we find that regions called magnetic domains.in each of these domains all magnetic moments are parallel,but in the lowest lying energy state of the system,the orientation of the magnetic moments of these domains are random therefore no macroscopic magnetic moment is observed.When such a material is put in a strong enough external magnetic

field the magnetic moments of the domains interact with it.

This interaction results in the magnetization of the material: the domain walls will move, reorienting the domains so more of the dipoles are aligned with the external field. The domains will remain aligned when the external field is removed, creating a magnetic field of their own extending into the space around the material, thus creating a permanent magnet. The domains do not go back to their original minimum energy configuration when the field is removed because the domain walls tend to become joined or snagged on defects in the crystal lattice, preserving their parallel orientation [10].

When an external H field is applied to a ferromagnet with unordered domains, the domain structure changes. At lower field strengths the change in the domain structure is a reversible one, i.e. switching the field off again the original structure will reassert itself. As the magnetic field increases domain walls may move and rotate irreversibly as they must pass through lattice defects (that the material will not return to its macroscopically non-magnetic state). even after we switch off the magnetic field, a non zero M_{rem} magnetization remains in it. If the external magnetic field strength is increased more and more domains will turn to be parallel with it. There exists a saturation field strength H_{sat} which turns all magnetic moments in the same direction. Further increase in the magnetic field cannot produce larger magnetization [11].

From considering the hysteresis curves, the magnetization can be much less than the saturation magnetization and even equal to zero b/c of magnetic domains. Within each domain the magnetization is uniform and equal to the spontaneous magnetization. However different domains are magnetized in different directions. Now if we calculate the average magnetization of this sample it will not be equal to the spontaneous magnetization. The average magnetization will be than M_s and could even be zero (if we have the appropriate domain configuration). why ferromagnetic materials are subdivided into domains rather than be uniformly magnetized? We know than a system will always be in a state in which its energy is minimum. We have to explain therefore why a subdivided state has a

smaller energy than a uniformly magnetized state. There are several types of energy which contribute to the total energy of the material[12].

Exchange energy

This is the energy which is responsible for ferromagnetism of magnetic materials. The exchange coupling between nearest neighbors is significant and results in parallel alignment of the magnetizations in ferromagnetic materials.

Magnetostatic energy

A magnetic material should not always be uniformly magnetized like as a ferromagnet in a state of uniform magnetization. The state of uniform magnetization has the lowest possible exchange energy, since all adjacent spins are parallel to each other. However, the exchange energy is not the only type of energy that a magnetic material has. This state costs a large amount of magnetostatic energy.

1.2.3 Arrangement of Magnetic moments in domains

It can be explain in terms of the alignment of many atomic scale magnetic moments. However, with ferromagnetism there is an important modification: one finds that the moments of many atoms or molecules tend to be aligned in small regions.

- randomly arranged atomic moments before H is applied.

In paramagnetic materials, the moments are randomly arranged until an external field comes along and aligns them. If you were to look at the magnetic moment layout of a typical ferromagnetic materials, you would find something like this: Enough atomic scale moments are aligned that definite regions or domains of magnetization exist. Each domain is fairly small, and each is randomly oriented with respect to its neighbor; the material as a whole has no net magnetization.

- After H is removed the atoms will oriente in the same direction.

If this material is placed into a strong enough external magnetic field, the domains

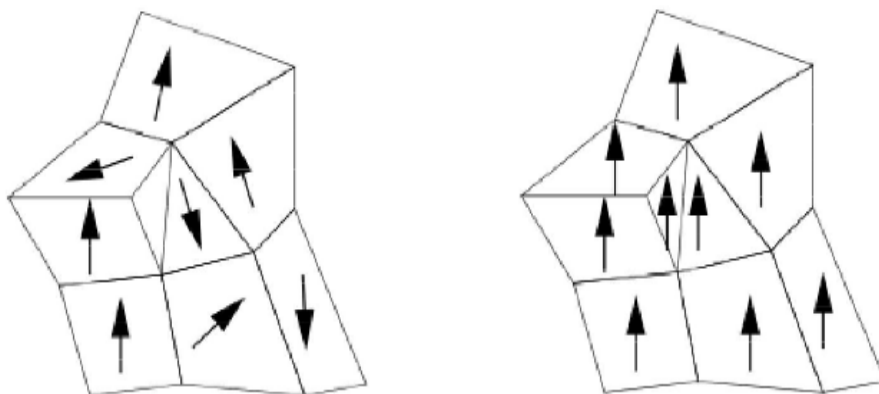


Figure 1.2: randomly arranged atomic moments before H is applied(left),and removed the atoms will orient in the same direction(right)

are re-aligned all point in the same direction. Once the external magnetic field is removed, it turns out to be energetically favorable for these domains to remain pointing in this direction. The domains are fixed with this magnetization then permanent magnet is made[12].

1.3 Magnetization curve and Hysteresis Loop

If we apply a magnetic field to a previously demagnetized ferromagnetic material, magnetization will gradually increase. Starting from point O , of the graph shown below, the magnetization increases relatively fast at first, then the increase becomes slower, until it reaches a constant value at point A . At this point, the specimen is saturated. This curve is the initial magnetization curve. The saturation magnetization, M_s , is equal to the spontaneous magnetization.

If the field H is now decreased, M does not retrace the initial magnetization curve, but decreases more slowly and when H reaches zero, M still has a non-zero value M_r . This is the largest magnetization we can get in zero field. It is called the remanent magnetization or remanence.

In order to decrease M further, we must apply a field in the opposite direction. When the

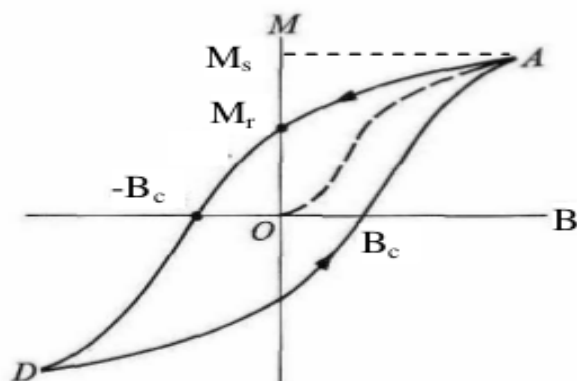


Figure 1.3: Hysteresis loop and the magnetization curve. The coercivity field B_c is the reverse field that reduces M to zero. The remanence M_r is the value of M at $B=0$. The saturation magnetization M_s is the limit of M at large value of B .

reverse field is sufficiently large, M passes through zero. The reverse field needed to bring the magnetization to zero from remanence is called the coercive field or coercivity H_c .

A further increase of the reverse field results in increasing M in the direction in which H is now applied. Eventually, M reaches the saturation value M_s again. If we continue to change H between large values in opposite directions, M will vary repeatedly along the closed loop. This loop is called the hysteresis loop [13].

1.3.1 Hysteresis and Remanence

Within the domain, the magnetic field is intense, but in a bulk sample the material will usually be unmagnetized because the many domains will themselves be randomly oriented with respect to one another. But when that material is exposed to a magnetic field, the magnetic fields will line up with each other and the material will be magnetized.

Ferromagnets will tend to stay magnetized to some extent after being subjected to an external magnetic field. This tendency to "remember their magnetic history" is called hysteresis.

Permanent magnetization is one result of hysteresis, can be the basis for the storage of information on tapes. When we develop a picture of energy dissipation, it will be clear

that hysteresis also implies the generation of heat, and this can impose limits on the use of magnetizable materials. Liquids having significant magnetizabilities have been synthesized by permanently suspending macroscopic particles composed of single ferromagnetic domains.

The fraction of the saturation magnetization which is retained when the driving field is removed is called the remanence of the material, and is the basis of data storage on audio and video tapes and computer hard drives.

Chapter 2

Ferromagnetic Phase Transition and Property

2.1 Phase and Phase transition

A common definitions of phase;

- 1) It is A portion of the system whose properties and composition are homogeneous which is physically distinct from other parts of the system.therefore,the transition from the state of paramagnetic to ferromagnetic change is indeed a phase change,since a paramagnetic phase has different magnetic properties than a ferromagnetic phase and there is a change in symmetry during the transition.
- 2) Which has a set of order parameters, n_1, n_2, n_3 ..which specify its physical properties and describe the the over all activity of the system.
- 3) Is An assembly of atoms or molecules which has attained equilibrium under specified external constraints consists of one or more homogeneous and physically distinct regions.These regions of each type may be distinguished by a common set of parameters defining such intrinsic properties and they constitute a phase of the assembly.Two phases are distinguishable if they represent different states,different structural arrangements and have different compositions.

A phase transition can be driven as a result of some variation in externally imposed conditions like temperature, pressure, chemical composition, magnetic or electric field etc and the systems undergo a process what is called a phase transition. If the driving parameter is temperature, the high temperature phase is almost has a higher symmetry. due to these cases, phase transitions entail a change in the entropy of the system [14]

The term phase transition has been used broadly to cover several types of phase changes [15]. among these the followings are some.

- a) structural transitions of the solid state ,
- b) transitions related to the change in the state of matter,
- c) transitions related to changes in composition,
- d) metallurgical transitions,
- e) transitions related to changes in the electronic structures of crystals,
- f) Transitions that change thermodynamic properties or the disorder of a system.

2.2 Ferromagnetic phase transition and Critical Phenomena

The picture for the second order phase transitions has completely two phases differing by a certain symmetry. One phase possesses this symmetry, and in the other phase, this symmetry is broken [10]. For instance, for the ferromagnetic phase transition this is the time-reversal symmetry: It exists in the non-magnetic phase, but is broken in the magnetic phase. Thus, second-order phase transition is a spontaneously symmetry breaking [15]. Because of this, the two phases do not coexist at any temperature except for T_c . What happens we describe first with an example of the ferromagnetic phase transition, where the low-symmetry ferromagnetic phase is characterized by the magnetization.

The magnetization decreases with increasing the temperature and turns to zero at the

temperature T_c . Thus, at the transition temperature the ferromagnetic phase becomes paramagnetic above the transition temperature, the magnetic moment equals zero. The low-temperature phase transforms into the high-temperature phase continuously. This continuous transformation can be generalized to any species of the second-order phase transition.

A ferromagnetic substance, such as iron, can carry a permanent magnetization. Above a certain temperature T_c the magnetization vanishes. This change in magnetic properties is associated with a change in the internal order of the crystal. Many condensed matter systems undergo transitions from one phase to another as a function of temperature, pressure, composition and other thermodynamic variables.

2.3 Terms in phase transition

2.3.1 Order parameter

It is a quantity characterizing the transition and the symmetry of the phases. It contains all the information about the degree of order or extent of deformation in the low-temperature phase.

In a ferromagnet the order parameter is the magnetization describing the orientation and size of the material and its resulting magnetic field since the spins generate magnetic fields, pointing in some particular direction. This alignment is seen as a large time-independent magnetic field vector [16].

But, the order parameter, to account for the continuous nature of for our case of the ferromagnetic transition is zero in the high-symmetry phase, finite in the low-symmetry phase, and a continuous function of temperature turns to zero at the transition point.

2.3.2 Curie temperature, T_c

Is a temperature that takes place a phase transition or phase change occurs. If the temperature is above T_c , the random motion of the magnetic moments is so strong that they can

never become aligned. Just a tiny bit below, though, and they can align [15]. The magnitude of the Curie temperature varies from material to material; for example, for iron, cobalt and nickel the respective values are 1043, 1394 and 631 K.

Ferromagnetic materials exhibit a long-range ordering phenomenon at the atomic level which causes the unpaired electron spins to line up parallel with each other in a region called a domain. The long range order which creates magnetic domains in ferromagnetic materials arises from a quantum mechanical interaction at the atomic level. This interaction is remarkable in that it locks the magnetic moments of neighboring atoms into a rigid parallel order over a large number of atoms in spite of the thermal agitation which tends to randomize any atomic-level order [17, 18].

The Influence of Temperature on Magnetic Behavior

A phase transition is marked by abrupt macroscopic changes as external parameters are changed, such as an increase of temperature. Raising the temperature of a solid results in an increase in the magnitude of the thermal vibrations of atoms. The atomic magnetic moments are free to rotate. Hence, with rising temperature, the increased thermal motion of the atoms tends to randomize the directions of any moments that may be aligned.

For ferromagnetic system the atomic thermal motions counteract the coupling forces between the adjacent atomic dipole moments, causing some dipole misalignment. This results in a decrease in the saturation magnetization (that was maximum at 0 K) at which temperature the thermal vibrations are a minimum [17].

With increasing temperature, the saturation magnetization diminishes gradually and then abruptly drops to zero at Curie temperature. At the mutual spin coupling forces are completely destroyed, such that for temperatures above ferromagnetic materials is paramagnetic.

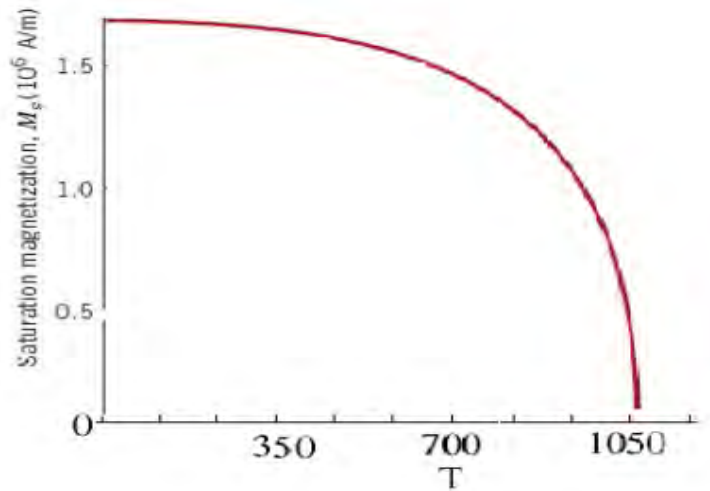


Figure 2.1: Plot of saturation magnetization of iron as a function of temperature

2.3.3 Symmetry in system

When the external field coupling to the order parameter is zero, one often expects the free energy to be symmetric as a function of the order parameter [18]. This is not true in general, since a vanishing external field only requires that the first order derivative is zero. But if we consider this simple symmetric case the free energy of the system without field is the same for a given value of the order parameter and for the opposite value.

The most symmetric situation therefore will have a value of zero for the order parameter. This does often, but not necessarily, correspond to the state of the system at high temperatures. For example, $M = 0$ at high temperatures. There is no preferred direction of the magnetization. When we apply a magnetic field we will have in general that $M \neq H$.

Broken symmetry of Iron

At the coexistence curve the system chooses one of the possible ground states, and breaks the symmetry between the possible values of the order parameter by choosing a particular one. In that case the broken symmetry is forced by external constraints.

When a crystal changes its symmetry, it is a process of going from one phase to another. We therefore speak of a phase transition entailing a change of symmetry. Ferromagnetic crystals are

those crystals which involve at least one phase transition which changes the directional symmetry of the crystal[19].

Let us consider a crystal of iron. At high enough temperatures, it is a paramagnetic phase. Application of a magnetic field to it induces a response in the form of a magnetic moment, and the magnitude of the magnetic moment induced by the applied field is proportional to the magnitude of the field applied. The response function in this case is a single-valued function. There is a unique value for the induced magnetization for every value of the field applied. When a crystal of iron is cooled, there comes a temperature at which it makes a ferromagnetic phase transition. In this phase the crystal has a nonzero magnetic moment even when no external magnetic field is applied to it; we call this magnetic moment spontaneous magnetic moment or spontaneous magnetisation[19].

The existence of this spontaneous magnetisation also implies that the crystal has a lower directional symmetry (a lower pointgroup symmetry) compared to that of its paramagnetic phase. There can be at least two such equivalent directions. Some regions of the crystal may have their spontaneous magnetic moment pointing in a particular direction, and some others may have it pointing in the opposite direction. Ferromagnetic materials possess symmetry, and sometimes undergo a change of symmetry spontaneously when environmental conditions are changed [20].

Chapter 3

Models and Thermodynamic property for studying Ferromagnetic phase transition in Iron

3.1 Ising Model

Certain metals spontaneously develop a finite magnetization at ordinary temperatures. Above T_c , these systems exhibit randomly oriented spins. Only below this temperature is a permanent spontaneous magnet formed. The Ising model displays a finite temperature phase transition between a ferromagnetically ordered phase at low temperatures, and a paramagnetic phase at high temperatures. It is developed to understand the orientation of spins, magnetic property in the study of solids in the studies of phase transitions at finite temperature [21].

Ferromagnetism is an interesting phenomenon in solids, like Fe and Ni, are observed to acquire a finite magnetization below a certain temperature. It is a fundamentally quantum mechanical effect, and arises when electron spins spontaneously align along a certain direction. The Ising model provides a simple way of describing how a magnetic material responds to thermal energy and an external magnetic field. In this model, each domain has a corresponding spin assigned as ± 1 [21, 22].

The spins must take interactions in order to understand transitions between phases. In the Ising model, the interactions in a ferromagnet tend to align a single spin with its neighbors

of the Hamiltonian(the total energy)has the form;

$$E_i = -J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i \quad (3.1.1)$$

Here,we have assigned an energy J for each pair of neighboring spins,depending on alignment. J is a coupling constant expressing the strength of the interaction between neighboring spins.If J is positive then the states $\uparrow\uparrow$ and $\downarrow\downarrow$ are energetically favourable and each element of the lattice has parallel alignment,indicating the material is ferromagnetic. B is an external magnetic field interacting with the magnetic moment set up by the spins.when $B = 0$,the lowest energy states are obtained by choosing all spins to be either up or down. If J is negative,the states $\uparrow\downarrow$ and $\downarrow\uparrow$ are energetically favourable and the material will be antiferromagnetic. the symbol $\langle ij \rangle$ indicates that we sum over nearest neighbors only with $S_i = \pm 1$, N is the total number of spins,.

This feature leads to,at low enough temperatures,a cooperative phenomenon called spontaneous magnetization.That is,through interactions between nearest neighbors,a given magnetic moment can influence the alignment of spins that are separated from the given spin by a macroscopic distance. These long range correlations between spins are associated with a long-range order in which the lattice has a net magnetization in the absence of a magnetic field[23].

3.2 Assumptions in Ising Model

The Ising model postulates a lattice with a magnetic dipole or spin on each site.

- 1.The spins takes only two values,+1 for up spin \uparrow or -1 for a down spin \downarrow .Since each spin can take one of two values, there are a total of possible states for a size lattice.
- 2.The model actually mimics real magnetic materials exchange interactions of spins,doing so by including terms in the Hamiltonian (the equation that defines the total energy) proportionalto the products of the spins $S_i S_j$.In the simplest case, the interactions are only between spins on sites which are nearest neighbours on the lattice[24,25].

3.It identifies the partition function (Z),for the canonical ensemble,defined over all microstates N ,and the probability (P) of finding the system in a given configuration of the thermodynamic limit.

The partition function(Z) of the model is the sum:

$$Z = \sum_{i=1} e^{-\beta E_i} \quad (3.2.1)$$

$$P_i = \frac{e^{-\beta E_i}}{Z} = \frac{e^{-\beta E_i}}{\sum_{i=1} e^{-\beta E_i}}$$

$$P_i = \frac{e^{-\beta E_i}}{\sum_{i=1} e^{-\beta E_i}} \quad (3.2.2)$$

where E_i is the total energy of a state i while Z is the partition function for the canonical ensemble defined as where the sum extends over all microstates N .

$$Z = \sum_{i=1} e^{-\beta E_i} \quad (3.2.3)$$

$$= \sum_{i=1} e^{-\beta(-J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i)}$$

$$Z = \sum_{i=1} e^{\beta(J \sum_{\langle ij \rangle} S_i S_j + B \sum_i S_i)} \quad (3.2.4)$$

In the thermodynamical limit where N goes to large,the partition function is given by;

$$Z = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \dots \sum_{s_N} e^{\beta(J \sum_{\langle ij \rangle} S_i S_j + B \sum_i S_i)} \quad (3.2.5)$$

or we can conclude in the general form as;

$$Z_N = \sum_{s_i=\pm 1} \Pi_{i=1}^N e^{\beta(J \sum_{\langle ij \rangle} S_i S_j + B \sum_i S_i)} \quad (3.2.6)$$

3.3 Spin Interactions and phase transitions

In studies of phase transitions we are interested in minimizing the free energy by varying the average magnetization(order parameter).The magnetization disappears at T_c .

Here the local magnetization is treated as a constant and all effects from fluctuations are

neglected. Stated differently, we reduce a complicated system of many interacting spins to a set of equations for each spin. Each spin sees now a mean field which is set up by the surrounding spins [26]. A way to achieve this is to rewrite the interaction between two spins at sites i and j by adding and subtracting the mean value of the spin $\langle S \rangle$, that is

$$S_i S_j = (S_i - \langle S \rangle + \langle S \rangle)(S_j - \langle S \rangle + \langle S \rangle) \quad (3.3.1)$$

this gives

$$S_i S_j = (S_i - \langle S \rangle)(S_j - \langle S \rangle) + \langle S \rangle^2 + \langle S \rangle (S_i - \langle S \rangle) + \langle S \rangle (S_j - \langle S \rangle)$$

because of that all effects from fluctuations are neglected, we have ignored terms of the order $(S_i - \langle S \rangle)(S_j - \langle S \rangle)$. These are the terms which lead to correlations between neighbouring spins. then;

$$S_i S_j = (\langle S \rangle^2 + \langle S \rangle (S_i - \langle S \rangle) + \langle S \rangle (S_j - \langle S \rangle)) \quad (3.3.2)$$

Then the total energy will be from the above equations, we have from

$$E_i = -J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i$$

and substitute the value of $S_i S_j$, we obtain

$$E_i = -J \sum_{\langle ij \rangle} ((\langle S \rangle^2 + \langle S \rangle (S_i - \langle S \rangle) + \langle S \rangle (S_j - \langle S \rangle)) - B \sum_i S_i) \quad (3.3.3)$$

$$\begin{aligned} E_i &= -J \sum_{\langle ij \rangle} \langle S \rangle^2 - J \sum_{\langle ij \rangle} \langle S \rangle ((S_i - \langle S \rangle) \\ &\quad + \langle S \rangle (S_j - \langle S \rangle)) - B \sum_i S_i \end{aligned} \quad (3.3.4)$$

then,

$$E_i = zJ \langle S \rangle^2 - (B + zJ \langle S \rangle) \sum_i S_i \quad (3.3.5)$$

where z is the number of nearest neighbours for a given site i . Let us define an effective field which of all spins by,

$$E_{eff} = (B + zJ \langle S \rangle) \quad (3.3.6)$$

By substituting the above expressions, the partition function will be now;

$$Z = \sum_{S_i}^N \Pi_i e^{-(\beta(zJ\langle S \rangle^2 - E_{eff} \sum_i S_i))} \quad (3.3.7)$$

For $i=1,2,\dots,N$ items the expression is;

$$Z_N = e^{-zN\beta J\langle S \rangle^2} \sum_{S_1} \dots \sum_{S_N} \times \Pi_i e^{\beta E_{eff} S_i} \quad (3.3.8)$$

expand for all values of N ;

$$\begin{aligned} Z_N &= e^{-zN\beta J\langle S \rangle^2} \times \sum_{S_1} e^{\beta E_{eff} S_1} \times \sum_{S_2} e^{\beta E_{eff} S_2} \dots \\ &\dots \sum_{S_N} e^{\beta E_{eff} S_N} \end{aligned} \quad (3.3.9)$$

let define the expansion of;

$$\sum_{S_1} e^{\beta E_{eff} S_1} \times \sum_{S_2} e^{\beta E_{eff} S_2} \dots \sum_{S_N} e^{\beta E_{eff} S_N}$$

represent by series of

$$\begin{aligned} \frac{e^{\beta E_{eff} S_1}}{1 - e^{\beta E_{eff} S_N}} &= e^{\beta E_{eff}} + e^{-\beta E_{eff}} = 2\cosh(\beta E_{eff}) \\ Z_N &= e^{-zN\beta J\langle S \rangle^2} (2\cosh(\beta E_{eff}))^N \end{aligned} \quad (3.3.10)$$

so, the Free energy will be;

$$\begin{aligned} F &= -KT \ln Z = -KT \ln(e^{-zN\beta J\langle S \rangle^2} (2\cosh(\beta E_{eff}))^N) \\ &= -NKT \ln(2) + zNJ \langle S \rangle^2 - NKT \ln \cosh(\beta E_{eff}) \end{aligned} \quad (3.3.11)$$

and minimizing F with respect to $\langle S \rangle$, i.e., $\frac{\partial F}{\partial S} = 0$, we get

$$\langle S \rangle = \tanh(2\cosh(\beta E_{eff})) \quad (3.3.12)$$

Then expand F in powers of $\langle S \rangle$ and using $\langle M \rangle = N \langle S \rangle$ at Close to the phase transition we expect $\langle S \rangle$ to become small and eventually vanish. use the identity;

$$\cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{8!} + \dots \text{ and}$$

$$\tanh x = x - \frac{x^3}{5} + \frac{2x^5}{15} + \dots \text{ Then,}$$

$$\tanh(\cosh x) = \cosh x - \frac{\cosh x^3}{5} + \frac{2\cosh x^5}{15} + \dots$$

Rewrite the free energy;

$$F = -NKT \ln(2) + zNJ \langle S \rangle^2 - NKT \ln \cosh(\beta((B + zJ \langle S \rangle))) \quad (3.3.13)$$

by expanding the $\ln \cosh(\beta E_{eff})$ term we get;

$$\begin{aligned} &= \left(\frac{1}{2} \langle S \rangle^2 + \frac{1}{3} \frac{\langle S \rangle^4}{4} + \frac{1}{4} \frac{\langle S \rangle^6}{6} \dots \right) \\ &= \frac{1}{2} \langle S \rangle^2 + \frac{1}{12} \langle S \rangle^4 + \frac{1}{24} \langle S \rangle^6 + \dots \end{aligned}$$

Therefore;

$$\begin{aligned} F &= -NKT \ln(2) + zNJ \langle S \rangle^2 - NKT - BN \langle S \rangle + NKT \left(\frac{1}{2} \langle S \rangle^2 \right. \\ &\quad \left. + \frac{1}{12} \langle S \rangle^4 + \frac{1}{24} \langle S \rangle^6 + \dots \right) \end{aligned} \quad (3.3.14)$$

$$\begin{aligned} F &= -BN \langle S \rangle + zNJ \langle S \rangle^2 - NKT \left[\ln(2) + 1 + \left(\frac{1}{2} \langle S \rangle^2 + \frac{1}{12} \langle S \rangle^4 \right. \right. \\ &\quad \left. \left. + \frac{1}{24} \langle S \rangle^6 + \dots \right) \right] \end{aligned} \quad (3.3.15)$$

combine like terms

$$\begin{aligned} F &= -NKT(\ln 2 + 1) - BN \langle S \rangle + \frac{(2zJ - KT)}{2} N \langle S \rangle^2 - \\ &\quad \left[\frac{KT}{4} N \frac{\langle S \rangle^4}{3} - \frac{KT}{6} N \frac{\langle S \rangle^6}{4} + \dots \right] \end{aligned} \quad (3.3.16)$$

using $\langle M \rangle = N \langle S \rangle$ and, $F_0 = -NKT(\ln 2 + 1)$ and the new constants a, b and c by; $a = \frac{2zJ - KT}{N}$, $b = \frac{KT}{3N^3}$, $c = \frac{KT}{4N^4}$ we can rewrite the Free energy as;

$$F = F_0 - B \langle M \rangle + \frac{1}{2} a \langle M \rangle^2 + \frac{1}{4} b \langle M \rangle^4 + \frac{1}{6} c \langle M \rangle^6 \dots \quad (3.3.17)$$

3.4 Studing The Property of The Function Near Phase Transition

3.4.1 Landau Theory

Arguably the first reasonably successful and general approach to understanding phase transitions goes back to Landau in the 1930s. The basic idea here that we can write the free energy (F) as a smooth function of a measurable order parameter describing the transition and it can be expressed as a low-order Taylor expansion in terms of the order parameter, together with terms that couple the order parameter with other physical quantities [27].

Landau free energy, F , which describes the energetics of the system in the vicinity of a phase transition, is a real quantity and depends on temperature, pressure, electric or magnetic field and stress, etc. The free energy expresses the two important principles, the energy minimization and the entropy maximization as the temperature increases. A higher entropy may be interpreted as a larger degree of disorder. When equilibrium is reached at a given temperature, we have a balance between these two principles [28].

For a given set of external parameters, the stable state of the system is the one for which the Landau free energy is minimal as a function of all internal degrees of freedom.

Assumptions Using Landau Theory

Landau theory has been widely applied in the solid state sciences for many reasons.

- The Landau theory gives an equation for the order parameter as a function of the environmental parameters that is universal: It only depends upon the kind of symmetry reflected in the ordering [28, 29].
- It is a general approach to phase transitions that is phenomenological in nature and applies only to the neighbourhood of a critical point, where the order parameter is small.

- The free energy as a function of the order parameter is the important state function to parameterize, since all other relations follow from a knowledge of it and that the free energy does not depend on the direction of the magnetization M but only on its value[29]
- It describes the systematic lowering of the symmetry of the system from a high-symmetry state, which is almost the high-temperature state. In this state, all the order parameters are small. Therefore,

$$F = F_o + \Delta F(m^i) \quad (3.4.1)$$

where F_o does not depend on the order parameter and therefore has no influence on the phase transition while $\Delta F(m^i)$ is small in the vicinity of the phase transition.

The Taylor expansion of the Landau free energy

Having recognized that F is small near the phase transition, where all the order parameters go to zero, the next natural step is to perform a Taylor expansion in powers of m^i . At each temperature, the order parameter m is determined from the minimization of the free energy. By the order parameter, the expansion will look like this:

$$\begin{aligned} F(T, m) &= -mH + \frac{b}{2}m^2 + \frac{c}{3}m^3 + \frac{d}{4}m^4 + O(m^5) \\ &= [-VH + F_1]m + F_2m^2 + F_3m^3 + F_4m^4 + \dots \end{aligned} \quad (3.4.2)$$

The odd-power terms are never present in the free energy of the high-symmetry phase at the transition because of the symmetry we imposed we have $F(T, m) = F(T, -m)$ and an expansion of the free energy F only contains even powers of M .

If the minimum of the free energy occurs at a non zero value of M , there will always be two minima $+M$ and $-M$ [12].

Because of time reversal invariance, the free energy does not change if we reverse the

direction of the field, $F(H) = F(-H)$. This implies that from the symmetry;

$$\begin{aligned} m(H) &= -\frac{\partial F(H)}{\partial H} = \frac{-\partial F(-H)}{\partial H} \\ &= \frac{\partial F(-H)}{\partial(-H)} \\ m(H) &= -m(H) \end{aligned} \tag{3.4.3}$$

so that it seems that the zero-field magnetization density must vanish.

$$m(H) = \frac{M(H)}{V}$$

3.4.2 The Coefficients In the expansion

The linear and Cubic terms

In the Landau free energy there is never any linear term in the order parameters that does not couple to the external fields. because of ΔF must be invariant by all elements of the high-symmetry group and in each term of the expansion. However, if m were to be invariant by all symmetry operator, then the corresponding mode could not break any symmetry and could not be involved in a symmetry breaking transition.

but mVH describes the energy contribution originating from the external field. Applying an external magnetic Field H to the free energy, the linear coupling term to an external field is permitted only if m is translationally invariant. Finally, m must transform by rotation in such a way that $-mH$ is an invariant. If these conditions are met, the phase transition is ferroic (Ferromagnetic, Ferroelectric and Ferroelastic transitions)[29]. In these cases, we can write the Magnetization in ferromagnetic phase transition as;

$$M = -\frac{\partial F}{\partial H} \tag{3.4.4}$$

and the Free energy as written above;

$$F(T, m) = -mH + \frac{a}{2}m^2 + \frac{c}{3}m^3 + \frac{b}{4}m^4 + \dots$$

This is called the Landau condition for continuity.

The quartic term and higher-order terms

In the absence of higher-order terms, the quartic term is essential in producing a well-conditioned free energy, this is satisfied if $b > 0$, is a constant that close to the transition has to be taken temperature independent. Higher order term are Usually not needed External field term For Curie transition, F_4 must be positive at all temperatures (otherwise no equilibrium order parameter): Indeed, if it happens to be negative, the minimization of the energy would yield infinite order parameter at any rate, outside the range of validity of Landau theory. The energy also has to be proportional to the volume of the system V , $F_4 = \frac{bV}{4}$.

The quadratic term

This term is always allowed and has the following structure:

$$\sum_i k^i (m^i)^2$$

where all the m^i 's have different symmetries (we do not have bilinear terms like $m^i m^j$). To ensure that the high-symmetry phase is the stable phase at high temperature, one must have $k^i > 0$ for $T > T_c$ (so that all the second derivatives are positive for $m=0$).

In the Landau theory, phase transitions occur when one of the coefficients of the quadratic term in the order parameter expansion changes sign (from positive to negative, e.g., as a function of temperature), whilst all the other coefficients remain positive.

If the driving parameter is temperature, the sign-changing term is usually written as $\alpha(T - T_c)m^2$. Clearly, the simultaneous change of two or more coefficient in the expansion of the above equation can only be accidental. This is because only a single mode (or more precisely a single symmetry) drives each phase transition.

F_2 - must vanish at the transition temperature. For $F_2 > 0$, the only energy minimum is at $m=0$ this corresponds to the high-symmetry phase. For $F_2 < 0$ one has two minima at finite m and a maximum at $m=0$. This corresponds to the low-symmetry phase: Indeed, the

energy is even in m , but the minima are located at the finite value of the order parameter, indicating broken symmetry. then $F_2 = \frac{\alpha(T-T_c)V}{2}$, $\alpha > 0$.

Since the order parameter turns to zero at the transition point, close to the transition it is small. Then one can expand the free energy in the powers of the order parameter up to the fourth as,

$$\begin{aligned} F(m) &= -mHV + F_2m^2 + F_4m^4 + \dots \\ &= -mVH + \frac{\alpha(T - T_c)V}{2}m^2 + \frac{bV}{4}m^4 + \dots \end{aligned} \quad (3.4.5)$$

Let us define the free energy per unit volume $f(m) = \frac{F(m)}{V}$ as a function of the average magnetization density, $m = \frac{M}{V}$. The advantage of a formulation in terms of energy and magnetization densities is that it does not depend on the size of the system. Then

$$\begin{aligned} f(m) &= \frac{F(m, T)}{V} \\ &= \frac{\alpha(T - T_c)}{2}m^2 + \frac{b}{4}m^4 + \dots \end{aligned} \quad (3.4.6)$$

Usually $F(m)$ only contains terms with even powers of m or $F(m) = F(-m)$. But there are some cases, however, when $F(m) \neq F(-m)$, then terms with odd powers of m must be included in the above Equation.

3.5 Analysis of the thermodynamic parameters

3.5.1 The Free Energy

Having defined an appropriate order parameter, and assume the free energy of the low temperature phase can be written as a power series in the order parameter m , the Landau free energy without the odd-order terms had from the previous expressions;

$$F(m, T) = \frac{\alpha(T-T_c)}{2}m^2 + \frac{b}{4}m^4 + ..$$

This form of Landau free energy describes a continuous phase transition. but Our purpose is to extract a few relevant thermodynamic parameters both above and below the phase transition.

3.5.2 Magnetization

Magnetization (M), Is the magnetic dipole moment per unit volume of a material. It is the vector field that expresses the density of permanent or induced magnetic dipole moments in a magnetic material.

The origin of the magnetic moments responsible for magnetization can be

- microscopic electric currents resulting from the motion of electrons in atoms.
- the spin of the electrons or the nuclei.

$$M = \frac{\text{magnetic moment}}{\text{volume}} = \frac{\mu}{V} = \frac{\text{current} \cdot \text{area}}{\text{length}^3} = \frac{\text{current}}{\text{length}} = \frac{A}{m} \quad (3.5.1)$$

Magnetization describes how a material responds to an applied magnetic field as well as the way the material changes the magnetic field, and can be used to calculate the forces that result from those interactions. By minimizing F with respect to m and put Zero we obtain: $M = -\frac{\partial F}{\partial m} = 0$

$$-\frac{\partial}{\partial m} \left(\frac{\alpha(T-T_c)}{2}m^2 + \frac{b}{4}m^4 \right) = 0 \quad (3.5.2)$$

we get $\alpha(T-T_c)m + bm^3 = 0$, then

$m=0$ for $T > T_c$ and

$$m = \left[\frac{\alpha}{b}(T_c - T)\right]^{1/2}, T < T_c \quad (3.5.3)$$

3.5.3 Magnetic Susceptibility

The magnetic susceptibility, χ , is a measure of the change of the magnetization due to the change in the external magnetic field. Also it is a parameter that shows how much an extensive parameter changes when an intensive parameter increases. Thus, the magnetic susceptibility tells us how much the magnetization changes by increasing the temperature. It can also be calculated from the Landau free energy by differentiating

$$F(m, T) = \frac{\alpha(T - T_c)}{2}m^2 + \frac{b}{4}m^4 + ..$$

with respect to m , one finds the general formula:

$$\begin{aligned} \chi &= \frac{\partial M}{\partial H} = \left(\frac{\partial^2 F}{\partial m^2}\right)^{-1} \\ &= \alpha(T - T_c) + 3m^2b = \alpha(T - T_c) + 3b\left[\frac{\alpha}{b}(T_c - T)\right] \end{aligned} \quad (3.5.4)$$

It can be evaluated for all values of the field, but it is particularly easy to calculate at $H=0$ (low-field susceptibility), where it produces different temperature dependences above T_c ($m=0$) and below T_c ($m = \frac{\alpha}{b}(T_c - T)^{1/2}$) by inserting the value of m , we get the following relations as;

$$\chi = \frac{1}{2\alpha(T_c - T)}, T < T_c \quad (3.5.5)$$

Note that the zero-field susceptibility diverges at the critical temperature.

$$\chi = \frac{1}{\alpha(T - T_c)}, T > T_c \quad (3.5.6)$$

3.5.4 Heat Capacity

The specific heat tells us, how much the energy changes with increasing temperature. The plot of the measured specific heat versus the temperature proves the expectation well in

zero magnetic field[30].

It is easy to see that, within Landau theory, the entropy below the phase transition is from the free energy we insert the value of $m = 0$ for $T > T_c$ and $m = \frac{\alpha}{b}(T_c - T)^{1/2}$ for $T < T_c$, we get the final expression of F as

$$F = 3\frac{\alpha^2}{4b}(T_c - T)^2 \quad (3.5.7)$$

then the specific heat below the critical point ($T < T_c$) is:

$$C_v = -T \frac{\partial^2 F}{\partial T^2} = 3\frac{\alpha^2}{2b}T, T < T_c \quad (3.5.8)$$

The specific heat curve shows the peak at 1042 K due to the need to increase the energy supplied to the material to continue to heat it up. this is related to the fact that the ordered spins of the antiferromagnetic FCC γ Fe and of the ferromagnetic BCC α Fe must be randomized to change these phases into their respective paramagnetic states.

3.6 Role of Magnetism and Temperature on Phase stability of Fe

The allotropic transformations in Fe are interesting examples of important contributions to structural stability from magnetic effects that can bring about phase changes in a unary system. At room temperature the stable form, called ferrite (α iron) has a BCC crystal structure[30].

Facts about the stability and the influence of the magnetic transitions on thermodynamics of Fe are;

1. The BCC(α phase) of Fe is stable at the low temperature. Because
 - At 0 K the ferromagnetic ordering in the BCC α phase causes the internal energy and enthalpy of that phase to be lower than the internal energy and enthalpy of the antiferromagnetic and paramagnetic FCC phase.
 - The large exchange energy of the aligned magnetic moments of the ferromagnetic BCC Fe greatly reduces its internal energy[6].
2. The BCC Fe phase transforms on heating to the FCC(γ) phase at about 910 C. because, on heating a more open structure, which therefore has higher vibrational entropy should be the more stable phase.
3. The FCC(γ) phase transforms on heating to the BCC(δ) phase at about 1400 C. this transformation in Fe has important contributions to structural stability from magnetic effects that can bring about phase changes.

However, there the specific heat curve the peak at 1042 K for the α phase due to the need to increase the energy supplied to the material to continue to heat it up. this is related to the fact that the ordered spins of the antiferromagnetic FCC γ Fe and of the ferromagnetic BCC α Fe must be randomized to change these phases into their respective paramagnetic states.

The ferromagnetic to paramagnetic change which occurs on heating takes place by what is known as a higher order transition. Changes in properties such as specific heat occur over a range of temperatures as can be seen from the large peak in the specific heat curve for α Fe corresponding to the magnetic disordering[30].

Therefore, a change of phase occurs when one or more of its order parameters changes discontinuously from one value to another or from zero to a non-zero value (or vice versa). Thus, when a ferromagnetic phase changes to a paramagnetic phase, a phase change has occurred, since the magnetic order parameter, the magnetization of the material, changes from a nonzero value to zero on passing through the Curie temperature on heating. There really is a β Fe phase, which is the paramagnetic BCC α phase!

Chapter 4

Result and Discussion

From the expansion of the free energy we can conclude that;

- The equilibrium value of the order parameter m is given by the minimum of the free energy close to the phase transition. that is from the graph we can see as the magnetization increases the Free energy will increase. this indicates the increasing or decreasing of the Free energy come from the proportional value of magnetization.

At high temperatures ($T > T_c$), there is a single minimum at $m=0$. At low temperatures ($T \ll T_c$) the free energy has a maximum at $m=0$ and minima at non-zero values of m . For the free energy F to represent a phase transition, it is necessary that the value of a change sign at the transition temperature.

- From the graph of the magnetization one can see that, at transition, the magnetization rapidly decreases. Thus the magnetic susceptibility should show a fast increase to infinity.
- With increasing temperature, the magnetization diminishes gradually and then abruptly drops to zero at Curie temperature. At the mutual spin coupling forces are completely destroyed, such that for temperatures above T_c , the ferromagnetic materials will be paramagnetic.
- One can note also that at site first nearest neighbor magnetic susceptibility will be order dropping (i.e. after the point T_c).

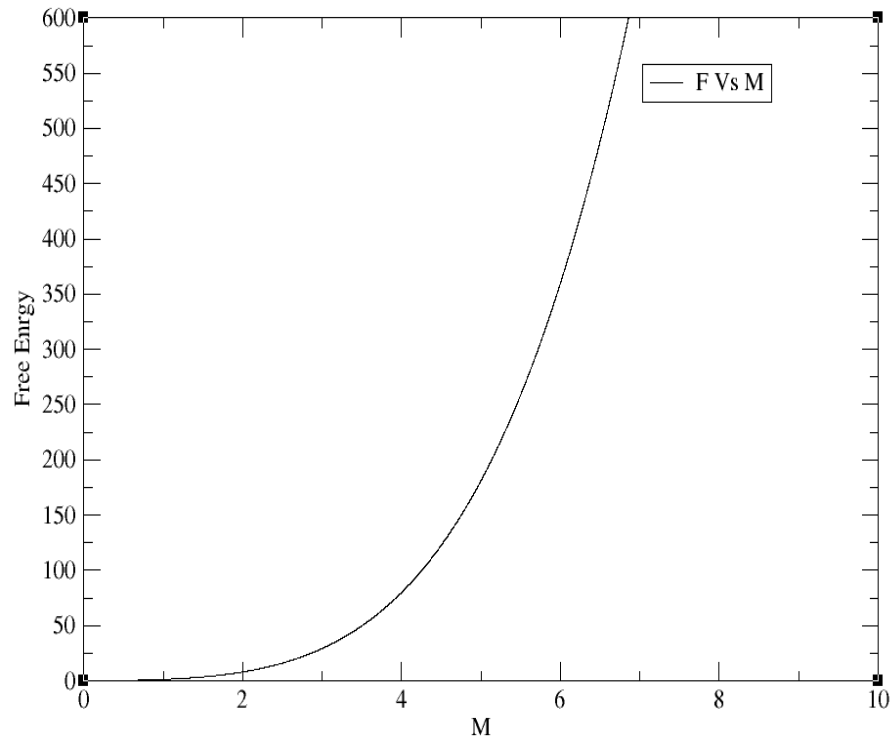


Figure 4.1: graph of The Free energy vs magnetization

- The susceptibility still diverges as $1/T$, but the singularity moves up to T_c . A permanent magnetization begins to grow at T_c , and increases with cooling. Below T_c the susceptibility continues to follow the Curie-Weiss law.
- As the temperature T approaches T_c from below, the susceptibility approaches infinity.
- Above T_c the susceptibility becomes suddenly negative, i.e. the material becomes paramagnetic.
- Near critical point, singularities are very easy to observe and measure, the susceptibility is infinite.

The ferromagnetic to paramagnetic change which occurs on heating takes place by a higher order transition. Changes in properties such as specific heat occur over a range of temperatures as can be seen from the large peak in the specific heat curve for α Fe

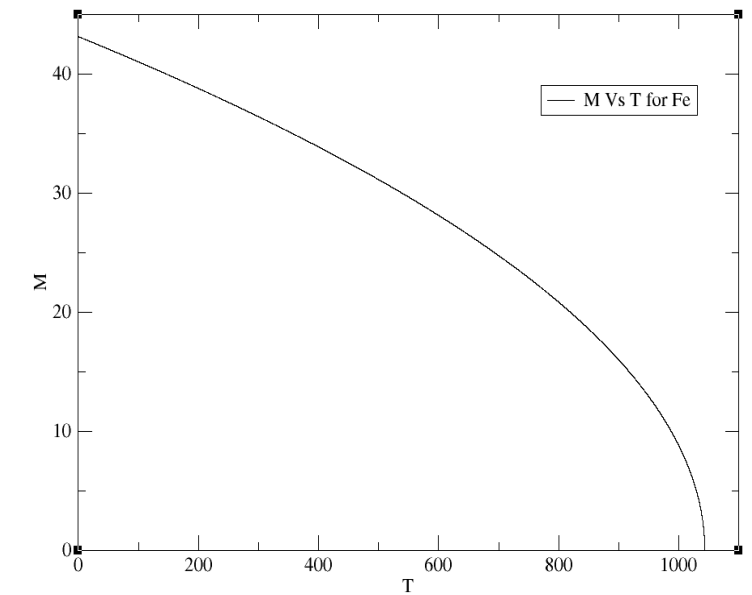


Figure 4.2: The graph of Magnetization versus temperature of Fe. at transition, the magnetization rapidly decreases

corresponding to the magnetic disordering associated with change of phase is by Curie temperature, T_c . Thus, this change in magnetic structure.

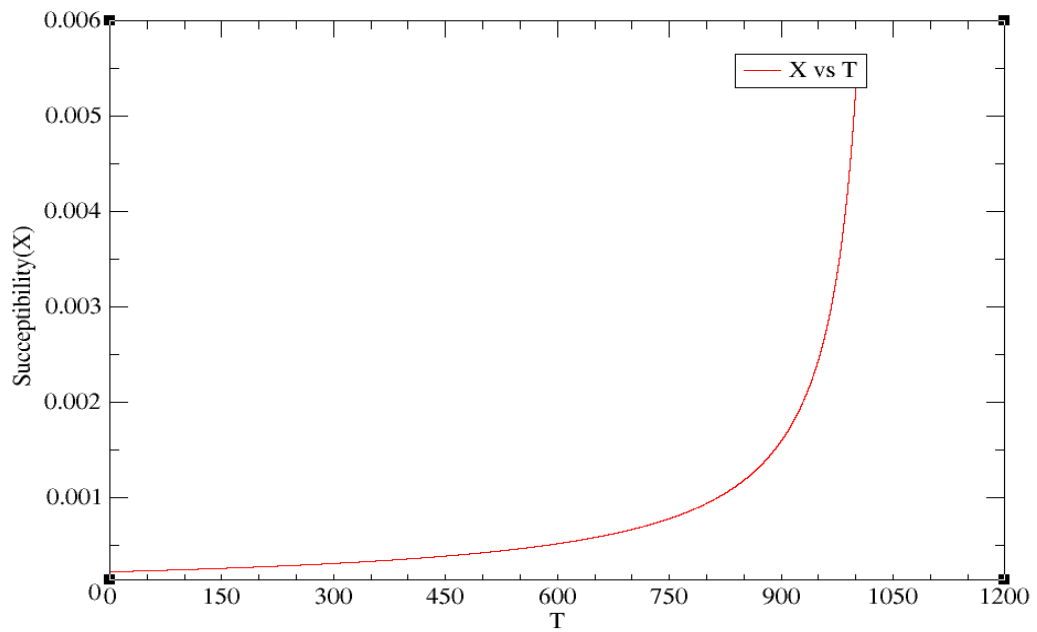
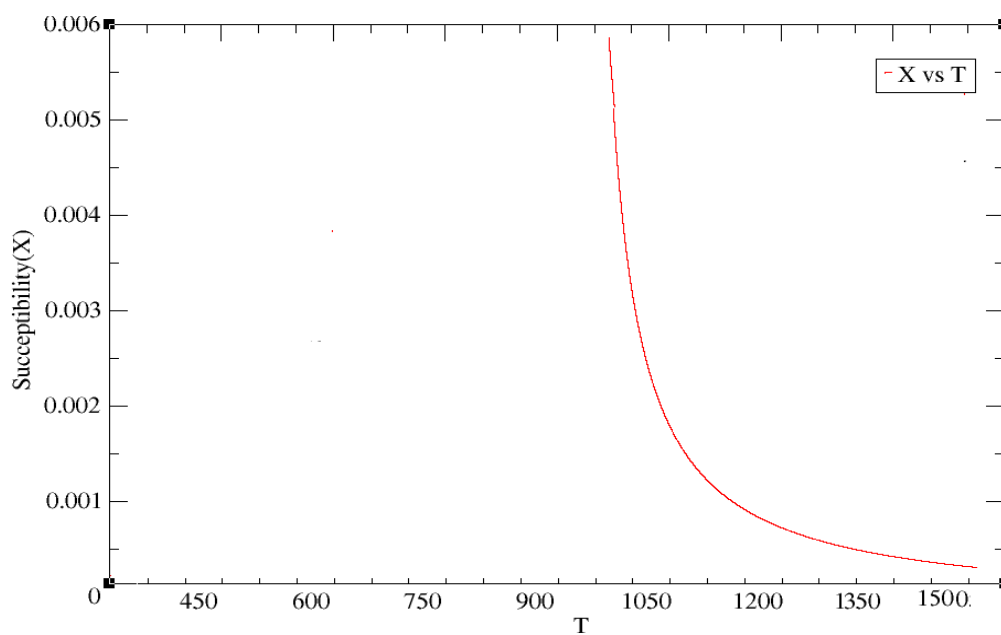
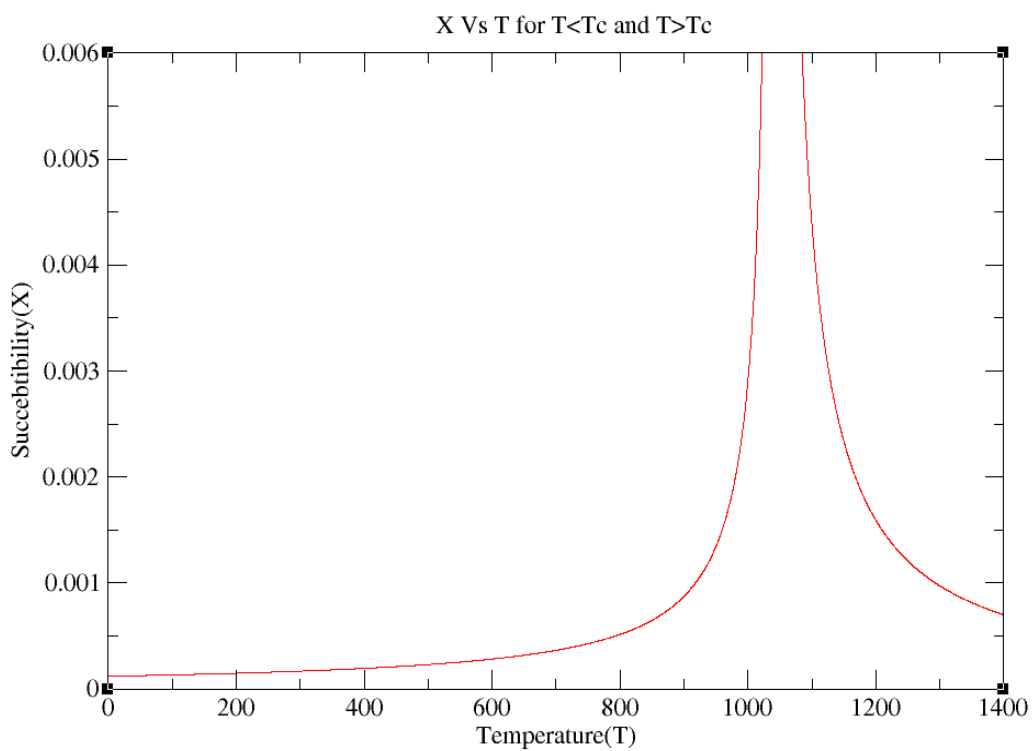


Figure 4.3: susceptibility versus Temperature For $T < T_c$. As the temperature T approaches T_c from below, the susceptibility approaches infinity. Above T_c the susceptibility becomes suddenly decreasing and became negative.

Figure 4.4: Succetbility for $T > T_c$ Figure 4.5: susceptibilty versus Temperature for below and above T_c .

Chapter 5

Conclusion

The properties of ferromagnetic substances is that the atomic magnets tend to be brought into parallel orientation not only by an applied magnetic field but also by an inner field which is proportional to the magnetization of the substance. The inner field is due to the electrostatic interactions, which are related to the orientation of the magnetic moments of electrons through the Pauli principle.

If these materials are placed into a strong enough external magnetic field, the domains are re-aligned in the same direction. even the external magnetic field is removed, it turns out to be energetically favorable for these domains to remain pointing in this direction. The domains are fixed with this magnetization and permanent magnets are made.

The change of phase occurs when one or more of the order parameters changes from one value to another or from zero to a non-zero value (or vice versa). when a ferromagnetic phase changes to a paramagnetic phase, a phase change has occurred, since the magnetization of the material changes. Iron, at high enough temperatures, it is a paramagnetic phase. Application of a magnetic field to it induces a response in the form of a magnetic moment which is proportional to the magnitude of the field applied.

The allotropic transformations in Fe has an important contributions to structural stability from magnetic effects that can bring about phase change. At room temperature the stable form, called ferrite (α iron) has a BCC crystal structure.

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Declaration

This Thesis is my original work has not been presented for a degree in any other University and that all the sources of the material used for this work have been dully acknowledged and specified.

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