

ADDIS ABABA UNIVERSITY
SCHOOL OF GRADUATE STUDIES

**THE STUDY OF THE ELECTRONIC THERMAL
CONDUCTIVITY OF SUPERCONDUCTING
MAGNESIUM DIBORIDE (MgB₂)**

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Dedicated to my late sister

Lombore Beyoro

who accidentally passed away while I was in my first year of this study

ABSTRACT

For magnesium diboride (MgB_2), some of the superconducting properties that have been studied are summarized. The energy dispersion relation is determined and it is used to determine the electronic thermal conductivity of MgB_2 . From that energy function, the expression for the electronic heat capacity of magnesium diboride in normal state has been determined. The general expression of the electronic thermal conductivity for MgB_2 in normal state is found. Then, by taking the energy gap parameter in to account the electronic thermal conductivity has been computed for the superconducting state of our material; that is below the transition temperature. Then, the electronic thermal conductivity of magnesium diboride has been plotted as a function of temperature with in the superconducting state. Moreover, the electrical conductivity of MgB_2 is calculated and the Wiedemann-Franz law is checked for normal state of a material. Finally, the general expression for electronic thermal conductivity of MgB_2 is determined in K - Space.

Key Words: Magnesium diboride, thermal conductivity, superconducting state

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1. GENERAL INTRODUCTION TO SUPERCONDUCTIVITY

1.1 Transition to the Superconducting State

While working in his low temperature laboratory in Leiden, Kamerlingh - Onnes, in 1911, discovered that at a certain temperature above absolute zero electrical resistivity ceased. That is, an electrical current could flow without any resistance. He gave a name "Superconductivity" to that new phenomena. Onnes observed in 1911 that the electrical resistance of pure mercury dropped abruptly while cooling it to a temperature below 4.2K. Hence, on account of its electrical properties he concluded that mercury has passed into a new state called superconducting state at a temperature value of 4.2K. Accordingly, the temperature at which a material passes from a normal state to a superconducting state is called a superconducting transition temperature (critical temperature) T_c of that material.

The following figure illustrates how mercury (Hg) made a transition from normal to superconducting state.

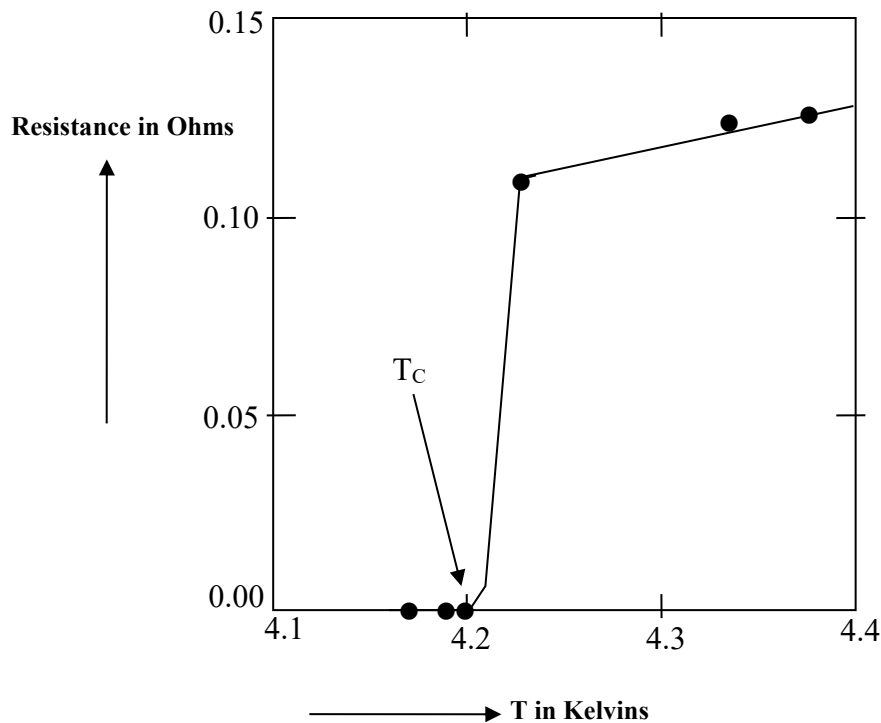


Fig. 1.1: The behavior of transition from normal to superconducting state in the first superconductor reported (Hg) by Onnes, with $T_c=4.2K$

Superconductivity could be defined as a complete absence of electrical resistance in a material and is observed in certain materials when they are cooled to below their superconducting

transition temperature. It is generally agreed that superconductivity relies on getting electrons to overcome their mutual Coulomb interaction and form Cooper pairs.

Superconductivity can occur in every pure element below some sufficiently low critical temperature. But it takes a long time to establish the state of superconductivity in such pure elements. For instance, a temperature should be lowered to about 0.1K to observe superconductivity in monovalent alkali metals. Superconductivity also exists in many alloys and binary compounds. From these we conclude that superconductivity occurs in any chemical material no matter whether it is element, compound or alloy.

The superconducting transition temperatures of some elements and compounds is given at the end of this chapter.

1.2 Developments in Superconductivity over years

Superconductivity as we have seen in the above section was discovered by Kamerlingh - Onnes in 1911 in mercury at a transition temperature of 4.2K. Kamerlingh noted that the superconducting state could be destroyed by applying large magnetic field, but a current induced in a closed conducting loop of wire persists for a long time.

A theory to explain a superconductivity phenomenon was not available for the next forty six years from its discovery. In 1957, a microscopic theory to explain the superconductivity phenomena was developed for the first time by Bardeen, Cooper and Schrieffer of University of Illinois. The theory is called BCS theory. The demonstration by Meissner that perfect diamagnetism being a basic property of superconductivity was done in 1934. The phenomenological description of superconducting flow was pointed in 1935 by London. Accordingly, superconductivity is a quantum phenomenon on a macroscopic scale; with the lowest energy state separated by a finite interval from the excited states and hence diamagnetism is a fundamental property of a superconductor. Nb₃Sn and Nb₃Ge were discovered as superconducting with T_c of 18K and 23K respectively in 1973. The T_c of 23K remained unbeaten for decades. Finally, a new era in superconductivity opened in 1986. Then, Bednorz and Mueller discovered a sharp drop of resistance at a relatively high temperature than before in La₂Ba_xCuO_{4-δ}. Accordingly, a sharp drop of resistance was observed in a material Lanthanum - Barium - Copper - Oxide (La_{2-x}Ba_x CuO₄) at an approximate temperature of 30K. This opened door to the study of high temperature superconductivity. With in a month time Chu of the University of Houston and Wu of the University of Alabama in collaborations discovered another high temperature superconductors namely, Yttrium -

Barium - Copper - Oxide ($\text{YBa}_2\text{Cu}_3\text{O}_7$) possessing a transition temperature of about 90K. Following these discoveries more studies were done and more high temperature superconductors with still high T_c were discovered. Currently the critical temperature has reached a maximum of 125K in Thallium (Tl) based system and 160K in Mercury (Hg) based system under pressure.

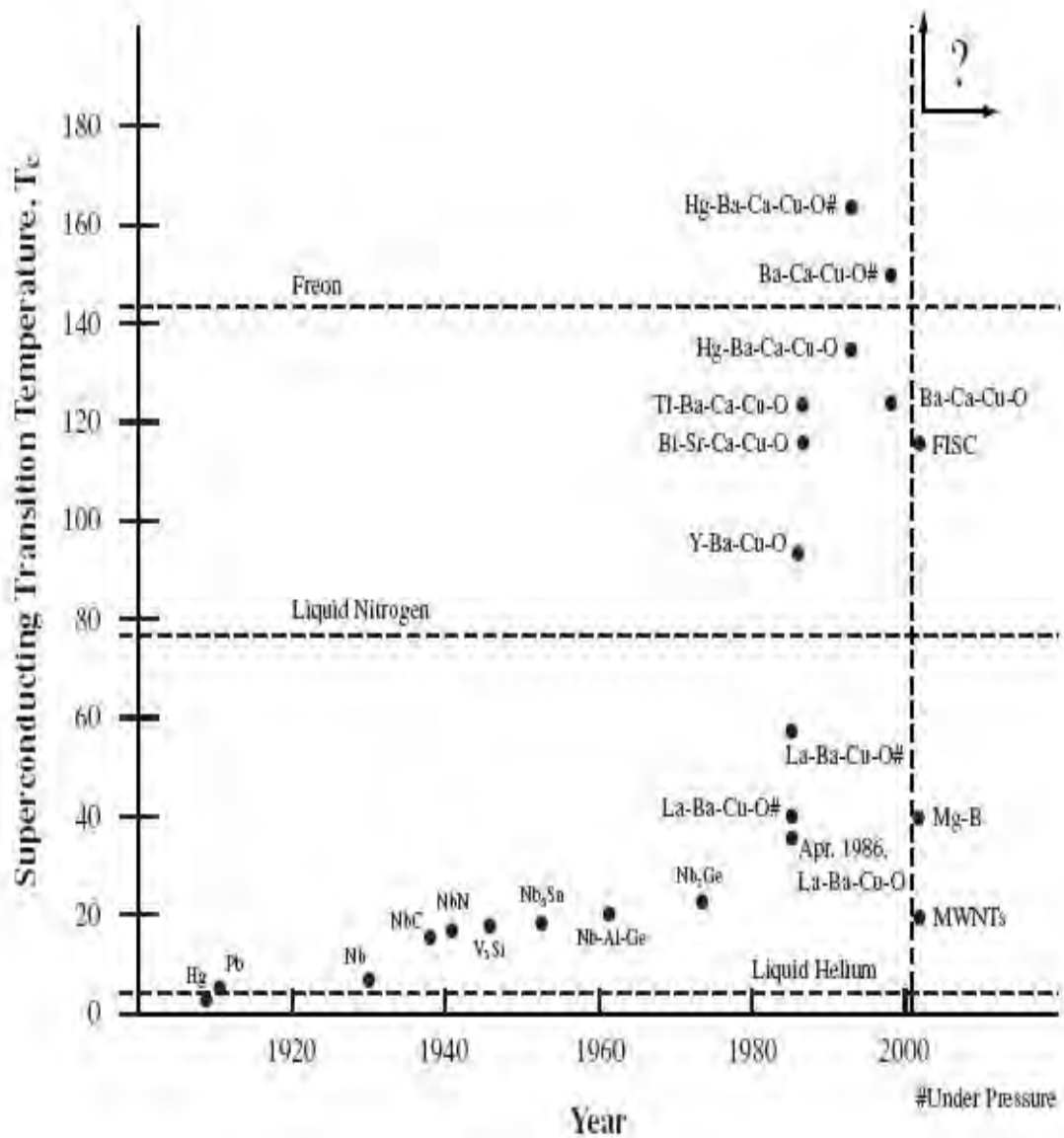


Figure 1.2 Resistivity development in regard to T_c over years

1.3 Superconductivity and Magnetic Field

Onnes have recognized that a superconducting state can again be changed to normal state by passing excessive current through the wire. He then recognized that the magnetic field induced by this current is making the wire to come back to its normal conducting state. Superconductivity is manifested only if the external field is less than the critical value H_c . The critical value of the magnetic field H_c is the minimum value of external magnetic field at which superconductivity is destroyed from a material. For most superconducting materials the critical value H_c varies with temperature from H_0 at $T=0$ to zero at a critical temperature T_c . The dependence of H_c on temperature can be demonstrated by Tuyn's law given by the following equation.[20]

$$H_c = H_0 \left(1 - \left(\frac{T}{T_c} \right)^2 \right)$$

In addition to this, the superconductor expels a magnetic field from its interior. Meissner and Ochsenfeld have tried to show that the state of a superconductor is independent of any previous magnetic environment, that is a material cooled through the superconducting transition temperature expels all magnetic field lines (flux lines) from its interior. The following figure illustrates the behavior of a superconductor in a magnetic field.

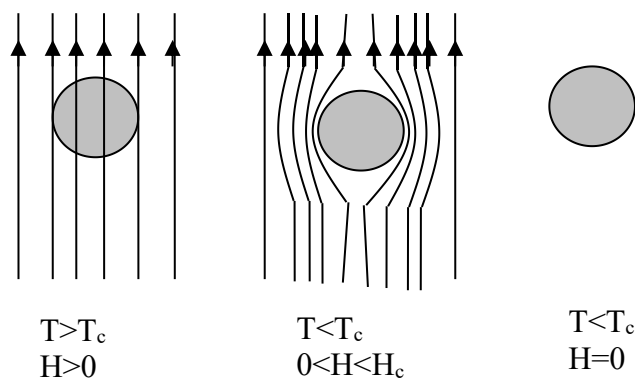


Figure 1.3 The Illustration of the behavior of a superconductor in a magnetic field showing that it expels a magnetic flux if $T < T_c$ and $0 < H < H_c$

1.4 BCS Theory and Its Contributions

BCS theory developed by Bardeen, Cooper and Schrieffer explains the properties of superconductors including the mechanism of superconductivity. According to BCS theory, what is responsible for the transition of a material to the superconducting state is an effective attraction between pairs of electrons of opposite spin and momentum. Below the superconducting transition temperature, T_c (in superconducting state), the electron pairs form a condensate, a macroscopically occupied single quantum state, which flows with no resistance and acts to screen out modest external magnetic fields, thus bringing about the perfect diamagnetism measured in the Meissner effect. At low temperatures, it requires a finite amount of energy, $\Delta \approx 1.75k_B T_c$, to split up one of the pairs in the condensate; this is the energy gap. Its impact on superconducting properties had been worked out phenomenologically by Bardeen in the years immediately preceding to the development of the microscopic theory (BCS theory). Therefore, the superconducting state is characterized by two distinct components: a superfluid (the condensate), and a normal fluid made up of the single particle excitations which result from the break up of the condensate pairs at finite temperatures. The excited quasiparticles which make up the normal fluid behave display certain coherent effects in response to external fields, coherence phenomena which are a signature of the BCS pairing theory, but otherwise behave normally, in that they collide with one another, with phonons, and with the walls of their container. The characteristic length over which coherent behavior can occur, that is the coherence length, is of the order of a thousand times the interparticle spacing. The BCS superconducting transition is basically different from what might happen if the pairs had formed well above T_c , and then condensed. In this case, the coherence length would be of the order of the interparticle spacing, and the energy gap would not be related to T_c .

BCS theory had a significant impact on many other fields of physics. It predicts that any system of interacting fermions could undergo a superconducting, or in the case of fermions with no charge, a superfluid transition, provided one had a net fermion attractive interaction in some angular momentum channel. For instance, after the initial publication of the BCS results, Bohr, Mottelson and Percus, working together in Copenhagen in the summer of 1957, showed that neutrons or protons in the atomic nucleus would pair as a result of their mutual attraction, and that one could explain in this way many hitherto puzzling nuclear phenomena, Nambu in Chicago explored the consequences of BCS pairing for the high energy phenomena found in elementary particle physics. The presence of neutron and proton superfluids in the

newly discovered pulsars, rotating neutron stars, was invoked in 1969 (by Baym, Pethick, Ruderman and Percus) as the explanation for the observed long time decay of the glitches (sudden jumps in the pulsar rotational period) which were discovered in the Vela and Crab pulsars in March and September of 1969. Since ^3He atoms are fermions and possess a long range attraction, it was widely expected that liquid ^3He would undergo a transition to the superfluid state, and the low temperature physics community searched seriously for signs of that transition, a search which proved successful for Osheroff, Lee, and Richardson who discovered in 1972 that ^3He became a superfluid at a temperature of some three millidegrees above absolute zero.

Inspired by the BCS theory, condensed matter experimentalists sought new classes of superconducting metals and searched intensively for materials which would become superconducting at substantially higher temperatures than the transition temperatures $\leq 20\text{K}$ which seemed to characterize normal superconducting metals. Hence there appeared to be a ceiling to the superconducting transition temperatures and new superconductors were determined, which could mainly be associated with the phonon-induced interaction mechanism responsible for superconductivity. Currently superconductors with much higher superconducting transition temperature have been determined.

1.5 Type I & Type II Superconductivity

Superconductivity is quenched when the material is exposed to a sufficiently high magnetic field as observed in all superconductors. This magnetic field, H_c , is called the critical field. In the early superconductors, including all of the elemental superconductors except niobium, the superconductivity is quenched in relatively low magnetic fields. The superconductors having one critical field are therefore called type I superconductors.

On the other hand, type II superconductors have two critical fields. The first is a low-intensity field H_{c1} , which partially suppresses the superconductivity. The second is a much higher critical field, H_{c2} , which totally quenches the superconductivity. The upper critical field of type II superconductors tends to be two orders of magnitude or more above the critical fields of a type I superconductor. Therefore, it is the existence and discovery of the type II superconductors that the manufacturing of superconducting magnets of high strength became possible. Let's see some points on both type I and type II superconductors separately in the following sub sections.

1.5.1 Type I Superconductors

The Type I superconductors are mainly comprised of metals and metalloids that exhibit some conductivity at room temperature. They require incredible cold to slow down molecular vibrations sufficiently to facilitate unimpeded electron flow in accordance with what is known as BCS theory. BCS theory suggests that electrons form themselves in Cooper pairs in order to help each other to overcome molecular obstacles. Physicists call this process phonon-mediated coupling because of the sound packets generated by the flexing of the crystal lattice.

Type I superconductors are characterized to be the "soft" superconductors. They were discovered first and they need the coldest temperatures to become superconductive. They exhibit a very sharp transition to a superconducting state and they also exhibit a "perfect" diamagnetism.[26]

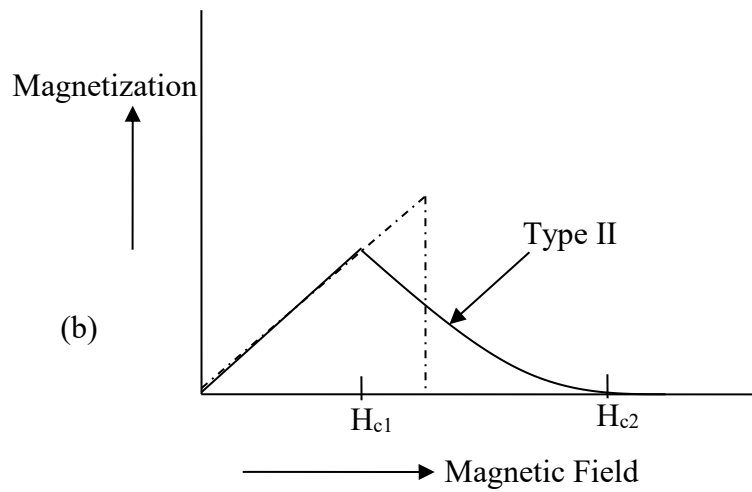
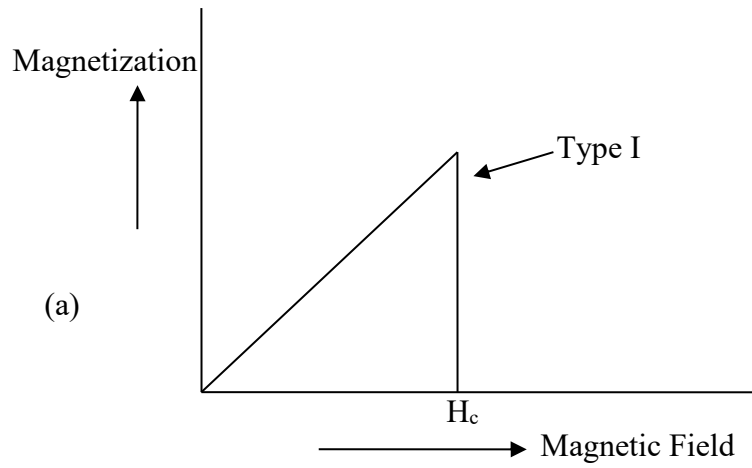


Figure 1.4: The magnetization versus magnetic field graph to differentiate (a) Type I superconductors, from (b) Type II superconductors

Some of the known type I superconductors are given in table 1.1 together with the corresponding critical temperature T_c . A periodic table is attached as an appendix to refer this type I superconductors.

Superconductor	Critical Temperature (T_c)
Lead (Pb)	7.196 K
Lanthanum (La)	4.88 K
Tantalum (Ta)	4.47 K
Mercury (Hg)	4.15 K
Tin (Sn)	3.72 K
Indium (In)	3.41 K
Palladium (Pd)	3.3 K
Chromium (Cr)	3 K
Thallium (Tl)	2.38 K
Rhenium (Re)	1.697 K
Protactinium (Pa)	1.40 K
Thorium (Th)	1.38 K
Aluminum (Al)	1.175 K
Gallium (Ga)	1.083 K
Molybdenum (Mo)	0.915 K
Zinc (Zn)	0.85 K
Osmium (Os)	0.66 K
Zirconium (Zr)	0.61 K
Americium (Am)	0.60 K
Cadmium (Cd)	0.517 K
Ruthenium (Ru)	0.49 K
Titanium (Ti)	0.40 K
Uranium (U)	0.20 K
Hafnium (Hf)	0.128 K
Iridium (Ir)	0.1125 K
Beryllium (Be)	0.023 K
Tungsten (W)	0.0154 K
Platinum (Pt)	0.0019 K
Rhodium (Rh)	0.000325 K

Table 3.1 Some Type I Superconductors

1.5.2 Type II Superconductors

The Type II category of superconductors is comprised of metallic compounds and alloys, except for the elements vanadium, technetium and niobium. The recently discovered superconducting metal-oxide ceramics that normally have a ratio of 2 metal atoms to every 3 oxygen atoms called perovskites belong to the category of type II superconductors. Type II superconductors have higher T_c 's than Type I superconductors by a mechanism that is still not completely understood. The highest T_c attained at ambient pressure currently is 138K. Some theorists predict an upper limit of about 200K for the critical temperature of layered cuprates but others assert that there is no limit.

The first superconducting Type II compound, an alloy of lead and bismuth, was fabricated in 1930 by de Haas and Voogd but recognized after the discovery of Meissner effect. Shubnikov at the Kharkov Institute of Science and Technology in the Ukraine then identified this in 1936 when he found the two distinct critical magnetic fields (known as H_{c1} and H_{c2}) in $PbTl_2$.

Type II superconductors are hard superconductors and they differ from Type I superconductors in that their transition from a normal to a superconducting state is not sharp, instead it is gradual across a region of mixed state behavior. Since a Type II will allow some penetration by an external magnetic field into its surface.

The recently discovered copper oxide superconductors are type II superconductors and early research indicated upper critical fields that appear to be at least as high as anything yet discovered. For instance, the upper critical field of yttrium-barium-copper-oxide is 14T at liquid nitrogen temperature (77 K) and at least 60T at liquid helium temperature. The similar rare earth copper oxide, thulium-barium-copper-oxide, was reported to have a critical field of 36T at liquid nitrogen temperature and 100T or greater at liquid helium temperature. These values of the critical field are much greater than the strongest household magnets. It is apparent that if the problems of working with these brittle ceramic materials can be overcome, magnets of incredible strength can be made for a multitude of potential applications.

Some of the currently known type II superconductors are given in table 1.2 together with the corresponding critical temperature T_c . [25]

Compound/Alloy	Critical Temperature (T _c)
Hg _{0.8} Tl _{0.2} Ba ₂ Ca ₂ Cu ₃ O _{8.3}	138 K
Hg ₃ Ba ₂ Ca ₂ Cu ₃ O ₈	133-135K
HgBa ₂ Ca ₂ Cu ₃ O ₈	125-126K
HgBa ₂ Ca ₃ Cu ₄ O ₁₀₊	123-125K
HgBa ₂ Ca _{1-x} Sr _x Cu ₂ O ₆₊	94-98K
HgBa ₂ CuO ₄₊	127-128 K
Tl ₂ Ba ₂ Ca ₂ Cu ₃ O ₁₀	126 K
Tl _{1.6} Hg _{0.4} Ba ₂ Ca ₂ Cu ₃ O ₁₀₊	123 K
TlBa ₂ Ca ₂ Cu ₃ O ₉₊	118-120K
Tl _{0.5} Pb _{0.5} Sr ₂ Ca ₂ Cu ₃ O ₉	118 K
Tl ₂ Ba ₂ CaCu ₂ O ₆	112 K
TlBa ₂ Ca ₃ Cu ₄ O ₁₁	103 K
TlBa ₂ CaCu ₂ O ₇₊	95 K
Tl ₂ Ba ₂ CuO ₆	96 K
NdBa ₂ Cu ₃ O ₇	95 K
Y ₂ Ba ₄ Cu ₇ O ₁₅	94 K
GdBa ₂ Cu ₃ O ₇	92 K
YBa ₂ Cu ₃ O ₇	90 K
TmBa ₂ Cu ₃ O ₇	89 K
YbBa ₂ Cu ₃ O ₇	39 K
MgB ₂	30 K
Ba _{0.6} K _{0.4} BiO ₃	23.2 K
Nb ₃ Ge	19 K
Nb ₃ Si	18.1 K
Nb ₃ Sn	18 K
Nb ₃ Al	17.1 K
V ₃ Si	17 K
Ta ₃ Pb	16.8 K
V ₃ Ga	14.5 K
Nb ₃ Ga	13.9 K
V ₃ In	

Table 1.2 Some Type II Superconductors

1.6 Excitations in crystals

A material can make a transition to its superconducting state if electrons Cooper pairs. Forming Cooper pairs may be possible by different mechanisms involving excitations of solid. There are a number of excitations including phonon, magnons, plasmons, polarons etc which may mediate Cooper pair formation [20], [23].

1.6.1 Phonons:

The phonon is defined as the quantized units of lattice vibration, a periodic displacement of the atoms from the equilibrium positions that can be characterized by its energy and momentum, as well as a velocity, wavelength and wave vector.

1.6.2 Magnons or Spin Waves

Magnons are defined as the low-lying excitations that occur in ordered magnetic materials introduced by Bloch in 1930. Accordingly, Some of the spins are observed as deviating slightly from the alignment of their ground state and this disturbance propagates with a wave like behavior through the solid Spins as we know are properly described by quantum mechanical operators. Therefore, spin waves are quantized with the basic quantum called magnon. It is analogous to phonon for quantized lattice vibrations.

1.6.2 Plasmons

Plasmons are defined as the coupled plasma oscillations of the electrons or holes in crystal lattices. Plasmons cannot be formed thermally in metals because most metals melt at very small thermal energy of order 0.1eV.

1.6.3 Polarons

A term polaron comes from polar (charge). The electron together with its accompanying cloud of phonons is termed polaron. The name polaron arises because the positive ions are attracted towards the electron and polarize lattice.

1.6.4 Exciton

Exciton is defined to be an electron in combination with a hole in a crystal solid. The electron has gained sufficient energy to be in an excited state and is bound by electrostatic attraction to the positive hole. Exciton is formed from an electron from the bottom of the conduction band and a hole from near the top of the valence band. The exciton may migrate through the solid and eventually the hole and electron recombine with emission of a photon. Then the wave function of exciton spreads over many inter atomic spacings and the exciton is well described by the theory of hydrogen atom.

2. A REVIEW ON THE STUDY OF SUPERCONDUCTING MAGNESIUM DIBORIDE (MgB₂)

2.1 Introduction to High T_c Superconductivity

Superconductivity is defined as a complete resistanceless state of a material and it is observed in some materials when cooled below some fixed temperature called superconducting transition temperature. Initially superconductivity was observed in 1911 by H. Kamerlingh Onnes in Leiden Laboratory in mercury at a temperature of 4.2K. The first theory to explain Superconductivity phenomena was developed in 1957 by John Bardeen, Leon Cooper and Robert Schrieffer in the University of Illinois. Superconductivity relies on getting electrons to overcome their mutual coulomb repulsion interaction and form Cooper pairs. In the BCS theory of low temperature superconductivity, electrons are held together as a result of their interactions with phonons or lattice Vibrations. That is BCS theory completely explains the low temperature superconductivity.

A new era in superconductivity study opened in 1986 when Bednorz and Mueller of IBM laboratory discovered a sharp drop in the resistance of La_{2-x}Ba_xCuO₄ at a temperature of approximately 30K, which was recorded as a superconducting transition temperature of a material. Following this a number of researches were carried out and more materials were found even with higher critical temperature T_c than before. Currently, the maximum T_c attained is 120K in Tl based systems and 160K in Hg based systems under pressure. All shared a feature that is responsible for the occurrence of high T_c superconductivity that is the presence of planes containing Cu and O atoms separated by the planes. Currently high T_c superconductivity is the subject of immense interest because of the following.

1. Its interdisciplinary nature (material scientists, chemists & physicists).
2. Potential application of materials with T_c greater than temperature at which nitrogen liquefies (77K).
3. Applications in cellular phone systems, superconducting transmission lines, microwave systems, etc.
4. The possibility of finding a superconductor at room temperature.

High Tc superconductors are characterized by common properties that they are ceramic, flaky oxides, poor metals at room temperature and highly isotropic electrical and magnetic properties that are sensitive to oxygen content. In low temperature superconductors their mutual repulsion of electrons or holes can be overcome with lattice vibrations or phonons. But in high Tc superconductors the binding mechanism is still in debate.[27]

In the present chapter, we write a brief review of studies on magnesium diboride (MgB_2) superconductor starting with its physical and chemical properties and along with its anomalous superconducting properties will be presented.

2.2. Properties of Magnesium diboride

2.2.1 The Crystal Structure of MgB_2

Magnesium diboride consists of hexagonal planes, of boron atoms that are separated by magnesium planes, where magnesium is centered above and below the boron hexagons. This structure is very similar to structure of graphite where each carbon atom is bonded to three others and occupies all planar bonding states named the σ - bonds. The remaining one electron moves in orbitals above and below the plane to form π - bands boron atoms have less valence electrons than carbon so that not all of the σ bands are occupied. Therefore, the lattice vibrations in MgB_2 are much larger due to the strong electron pairs formation.

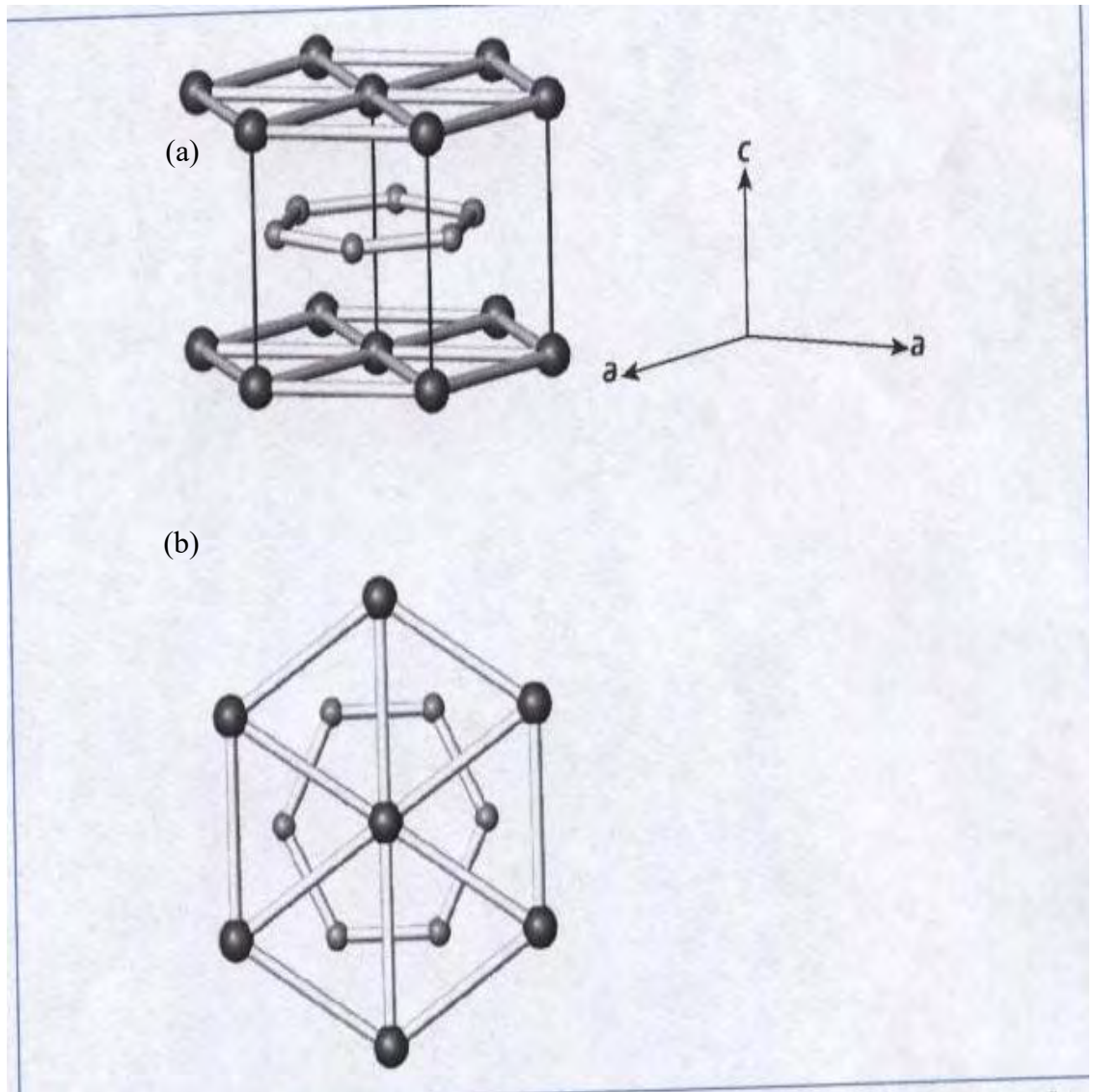


Figure 2.1: The crystal structure of MgB₂, where

- a) Magnesium planes consisting of only magnesium and B₂ planes containing only boron layered alternatively along the c - axis**
- b) The view from above, where the Mg layers consist of triangular lattice planes and B₂ layers consist of a hexagonal honeycomb lattice planes similar to those of graphite.**

2.2.2 Some physical properties of MgB₂

The major physical properties that characterize a material of my interest, magnesium diboride (MgB₂), are listed below.

1. The superconducting transition temperature of magnesium diboride is approximately 39K.
2. No other borides have comparable superconducting transition temperature yet.
3. It is a very good metal even better than some pure metals with resistivity ratio $\frac{R(300K)}{R(40K)} > 15$ and at 300K, R= 9 to 10 $\mu\Omega$ but at 40K: R= 0.38 $\mu\Omega$. [17]
4. The magnetic penetration length is about 850Å.
5. Its coherence length is estimated to be 50Å. [17]
6. The electronic mean free path at 40K is estimated as 600Å.
7. Magnesium Diboride (MgB₂) is an isotropic material.
8. Unlike other superconductors it has been verified that MgB₂ has two energy gaps. [13]

2.2.3 Superconductivity in MgB₂

Intermetallic superconductors are referred to as Bardeen-Cooper-Schrieffer (BCS) based superconductors. In such superconductors that do not contain copper oxide the superconducting transition temperature has so far been arrived around a maximum of 30K. Therefore no superconductors have been found to have higher T_C than this transition temperature. However the intermetallic compound magnesium diboride (MgB₂) exhibits superconductivity with transition temperature T_C of 39K, which is the highest yet recorded temperature in its group (in intermetallic compounds). This material differs from other ordinary metallic superconductors in many important ways such as: the failure of conventional models to predict its unusually high transition temperature, the isotope substitution effect on T_C and its anomalous specific heat. Its anomalous properties are explained by the fact that electronic states dominated by the boron plane couple strongly to specific modes of phonon that makes pair formation favorable. This can explain the high transition temperature, more than one energy gap and anomalous structure in specific heat.

Magnesium diboride is classified under type II superconductors; since it is comprised of metallic materials. As we have seen in the chapter one of this thesis, type II superconductors achieve higher T_C 's than type I superconductors. In addition to this, the transition from normal to superconducting state for type II superconductors is gradual across a region of a mixed state. Superconductivity gets destroyed in type II superconductors above the upper critical field (H_{C2}) unlike type I superconductors that need relatively lower critical field for destroying their superconductivity. The electronic structure studies of MgB_2 suggest that electron phonon interaction plays an essential role in the occurrence of superconductivity in this material.

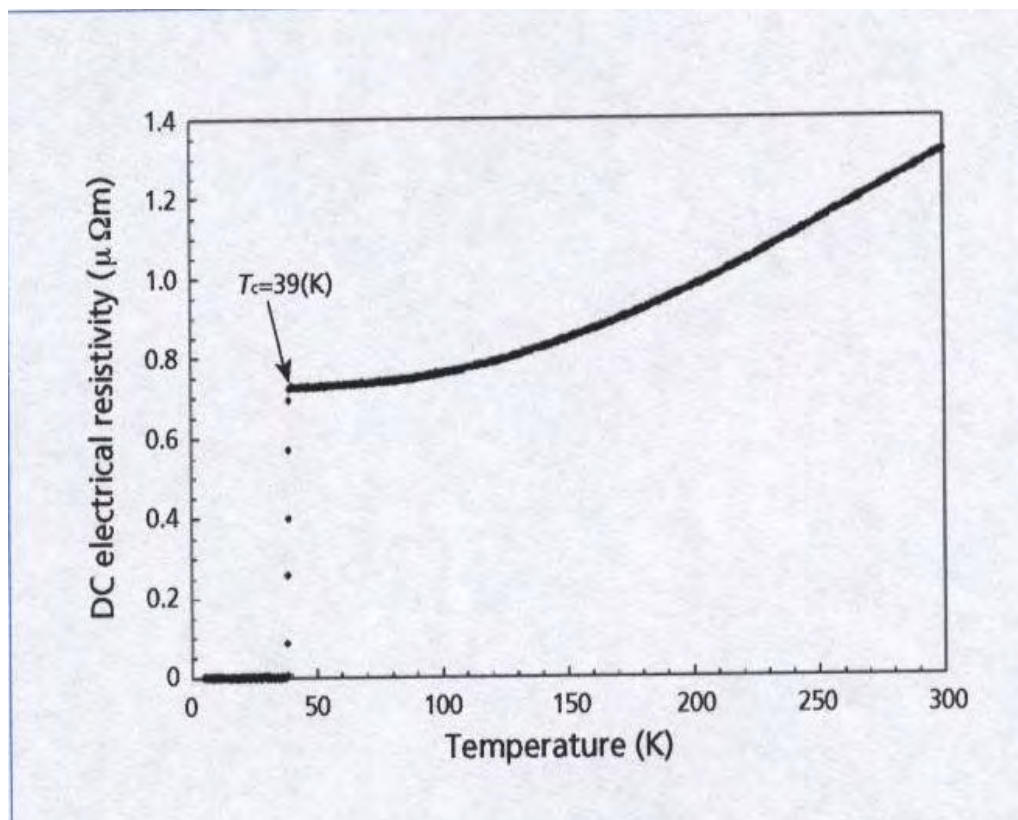


Figure 2.2: The temperature dependence of resistivity in MgB_2 [17]

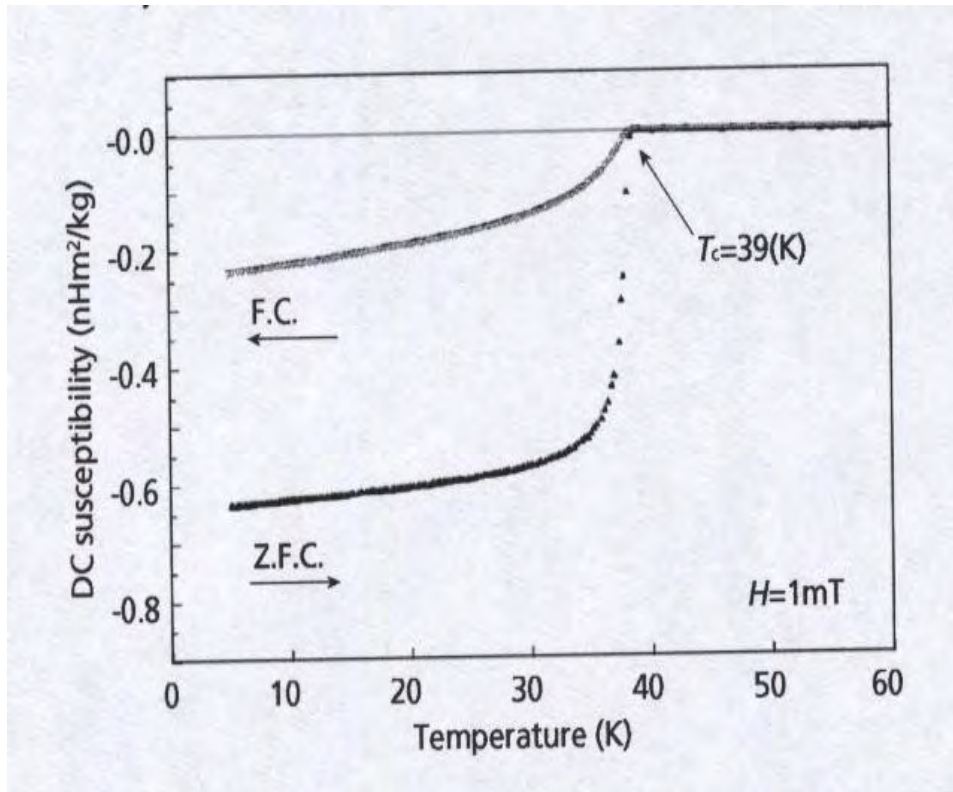


Figure 2.3: The temperature variation of susceptibility in MgB₂ [17]

As we can see from figure 2.2 the electrical resistivity decreases linearly from room temperature down to about 150K, below which it decreases in proportion to the second or third power of temperature. The resistivity then drops sharply at a temperature of 39K becoming zero at 38K.

The susceptibility graph that we see in figure 2.3 shows that cooling MgB₂ below its T_c results in an increase in magnitude of susceptibility. But cooling in an external magnetic field (F.C) results in a slow change in susceptibility than in the case of zero field cooling (Z.F.C.). Moreover, we also observe that the susceptibility changes sharply at a critical temperature T_c similar to that of resistivity.

2.3 Studies carried out on some superconducting properties of Magnesium diboride (MgB_2)

2.3.1 MgB_2 energy gaps and temperature dependence

The energy gap is the energy needed to break the pairs apart. Energy gap determines the thermodynamic properties of a superconductor and is directly related to superconducting transition temperature of the material. Studies reveal that magnesium diboride has two energy gaps unlike most other superconductors. According to calculations made by Louie, Cohen and co-workers the energy gaps correspond to transition temperatures of 15K and 45K that combined to give an overall transition temperature of 39K. []

According to Badr, of the Menofiya University using the tunneling spectra shows that the major peak Δ_1 occurs at around 2meV that is smaller than BCS value. The larger gap Δ_2 appears at around 9meV. The two energy gaps depend on temperature. With temperature both energy gaps follow the BCS behavior and they survive up to $T_C=39K$. $\Delta_1(0)$ and $\Delta_2(0)$ are observed to be 1.8meV and 8.2meV respectively and the ratio Δ_2/Δ_1 is about 4.5 throughout the temperature range from 0 to 40K. [13]

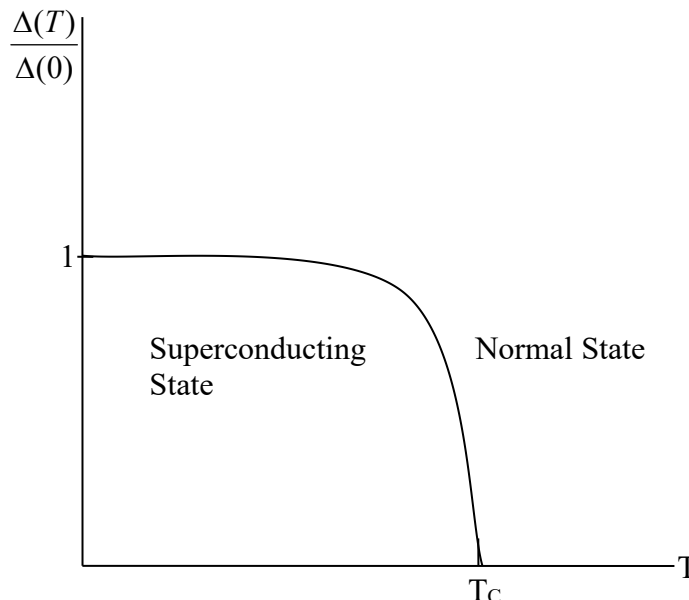


Figure 2.4 The energy gap parameter Δ decreases as temperature is raised from zero and comes to zero at transition temperature T_c [23]

2.3.2 The Effect of pressure on T_C of MgB_2

Almost all the superconducting metallic materials show a decrease in T_C with pressure. The measurements of pressure influence on the transition temperature and critical field gives information about the interaction that causes superconductivity. The binary compound MgB_2 superconductor under pressure behaves exactly like other metallic materials. Several groups have studied the effect of pressure on MgB_2 superconductor's properties. But all have observed that a transition temperature T_C decreased with increasing pressure. This relationship is well explained by Ummarino with the framework of the two bands Eliashberg theory. [9]

2.3.3 Upper critical field (H_{C2}) of magnesium diboride

The upper critical field is very important magnetic superconductivity parameter. Therefore starting from its discovery as a superconducting material a lot of researches were carried out on the analysis of upper critical field (H_{C2}) of magnesium diboride. Recently, the upper critical field $H_{C2}(T)$ for magnesium diboride was analyzed in terms of single and multiband Eliashberg models. The upper critical field was investigated by transport, ac susceptibility and dc magnetization measurements in magnetic fields of up to 16T with in temperature range $T=3K$ and $T_C=39K$. So far a complete $H_{C2}(T)$ curve was reported for MgB_2 wire showing high residual resistivity ratio of about 25. Accordingly the relatively high value of $H_{C2}(0)$ of about 13T to 18T has been recorded if a strongly coupled subgroup of heavy quasiparticles is involved in superconductivity. A peculiarity of the $H_{C2}(T)$ dependence on temperature is its recognized positive curvature near its T_C . This is similar to a typical feature of non-magnetic rare earth borocarbides. Studies are still being carried out and very interesting results that enhanced upper critical field observations were reported. Accordingly if carbon is doped with MgB_2 thin films $H_{C2}(0) > 50T$; that is improved H_{C2} . Such high critical field suggests that magnesium diboride could be appropriate to be used as a high field magnet conductor. On average bulk samples of carbon and magnesium diboride powders subject to hot isostatic pressing and Mg vapor have achieved critical fields in excess of 32T and critical current exceeding $10^6 A/cm^3$. This implies that doping it with carbon enhances the upper critical field of magnesium diboride superconductor. [12]

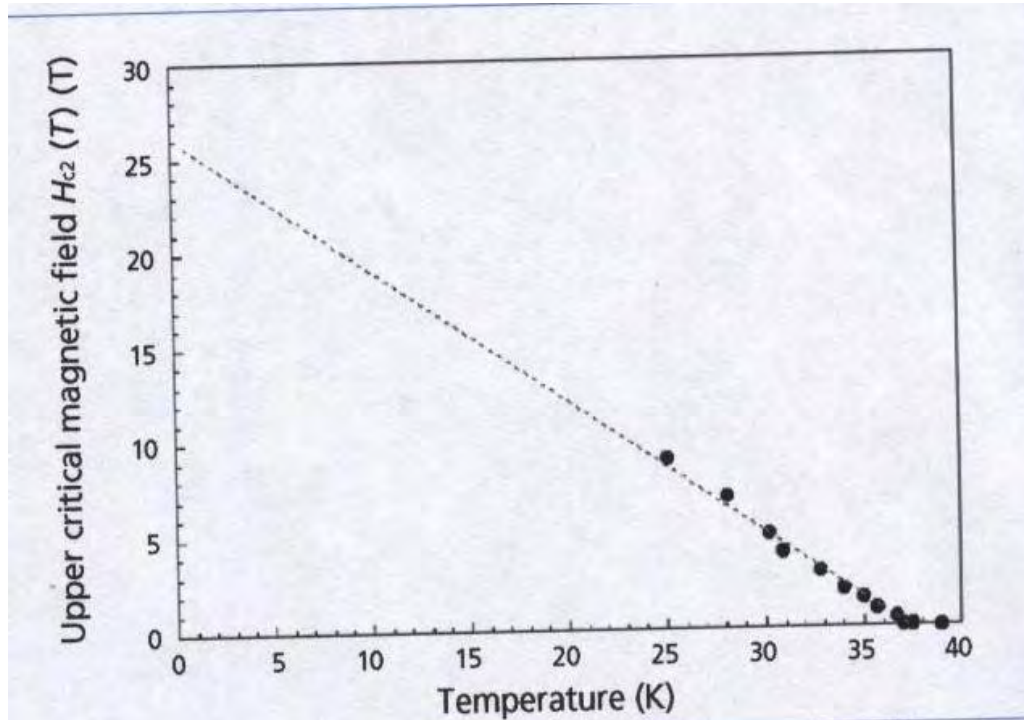


Figure 2.5: Upper critical field H_{c2} plotted at different temperatures below 40K [17]

2.5 Thermal Conductivity Study of MgB_2

Our material of interest exhibits phonon mediated s-wave superconductivity. Thermal conductivity studies of superconducting MgB_2 have been carried out both in the superconducting and the normal state region. The normal state thermal conductivity is equally determined by the contributions of both the electronic and lattice parts of the thermal conductivity. Whereas the superconducting state thermal conductivity is dominated by the lattice part of the thermal conductivity.

Thermal conductivity is one of the transport coefficients that exhibit non-zero values in both the normal and the superconducting states. The most important interactions in a given superconductor can be distinguished by the temperature dependence of thermal conductivity. The magnitude of thermal conductivity $K(T)$ explains how the electrons and phonons interact in a superconductor.

A lot of studies were made on the thermal conductivity of MgB_2 and investigations were also made to show how it affects the superconductivity in MgB_2 . That is the temperature effects in transport measurements have been studied. A paper published before a year in collaboration of Bauer, Paul, Berger, Majumdar, Giovannini and Saccone; [10] a lot of investigations have been made and accordingly in superconducting state of MgB_2

electron scattering on static imperfections dominates the thermal conductivity. According to more studies made in this property:

1. The temperature dependent thermal conductivity has a typical behavior of intermetallic compound.
2. As metals the thermal conductivity of MgB_2 comes from both electronic and lattice contributions such that: $K=K_e+K_l$
Where K stands for thermal conductivity, K_e electronic thermal conductivity and K_l for lattice thermal conductivity.
3. Using Wiedemann Franz law:
 $K_e=L_0T/\rho(T)$, where $L_0=2.45 \times 10^{-8} \text{W}\Omega\text{k}^{-2}$ is Lorenz number
Over a large temperature range the contribution of both K_e and K_l is of the same size.
4. The measurement of the thermal conductivity showed no anomaly at T_c . This implies that electron or hole scattering in static imperfections dominate in magnesium diboride.

Experimental studies show that below T_c , the thermal conductivity shows a peak or shoulder depending on whether the heat current is dominated by electrons or phonons and a more complex behavior is exhibited if both contributions are important. It is usual that below T_c quasiparticle condensation causes a decrease of the electron contribution to the thermal conductivity K_e and an increase in a phonon contribution. Despite this studies show that lattice vibrations give negligible contributions to the thermal transport in superconducting state. [10]
In our present work we try to study the electronic thermal conductivity of magnesium diboride theoretically. For our work we take the already accepted energy dispersion relation for a material in question. On the way to the thermal conductivity, several concepts like specific heat, mean free path, etc are also discussed.

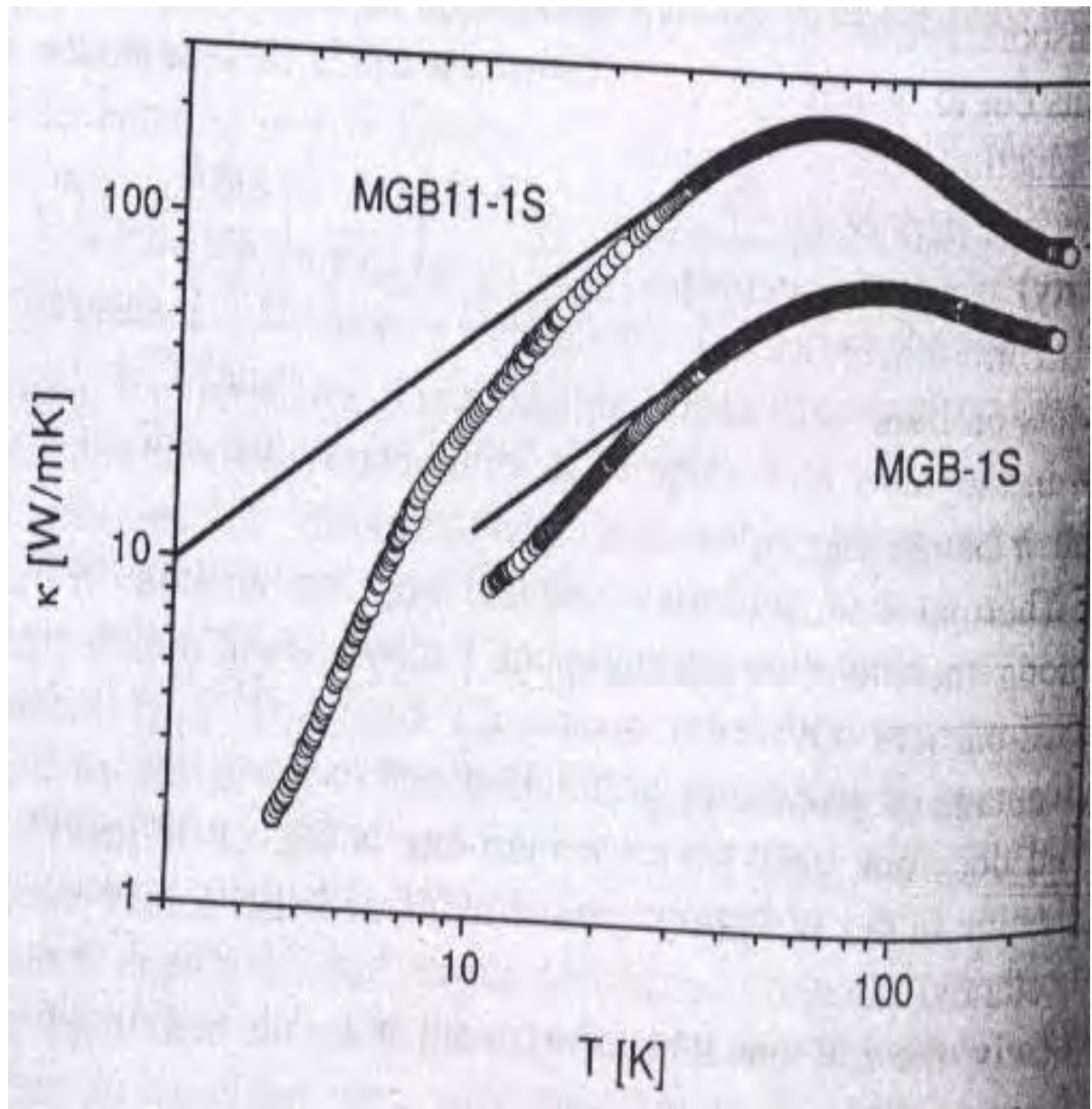


Figure 2.6 Thermal conductivity values of the sample in experiment conducted from 10 to 250K. [10]

2.4 Current Development of Application areas & Summary

Compared to other high T_c superconductors, MgB_2 itself being a high T_c superconductor has its own unique properties. Some of the properties are its simple crystal structure, large coherence length, high critical current densities, high upper critical fields and the existence of two superconducting energy gaps. The largest critical current densities $>10MA/cm^2$ and critical fields of 40T are achieved for thin films of MgB_2 . From upper critical field measurements, the anisotropy ratio being reported is between 1.2 and 9. [17]

The study of superconductor MgB_2 is interesting because of several reasons. For instance, problem of cost is one, or in other words it is economical. That is both magnesium and boron are common materials, cheap and easy to work with & can be bought from chemical companies. MgB_2 is a material that is very easy to synthesize and is stable. Its T_c is greater than that of conventional metallic superconductors and current studies indicate that naturally occurring grain boundaries do not significantly inhibit current flow leading to another significant advantage over the cuprate superconductors. Moreover its cooling is also possible by electric refrigerators rather than using liquid helium because of its higher superconducting transition temperature. With all these and other applications magnesium diboride is a high T_c superconductor being studied extensively. Much research has to be done in order to improve the industrial prospects of superconductivity and in our point of view MgB_2 is going to be the best material in promoting technologies mainly in material science and engineering fields. [5]

3. ELECTRONIC THERMAL CONDUCTIVITY STUDY OF MAGNESIUM DIBORIDE (MgB₂)

3.1 Introduction

It is obvious that metals are characterized by high electrical conductivity. In addition to this, from our day-to-day experience, metals are also high conductors of heat. This is because electrons play a leading role in electrical conductivity as well as thermal conductivity. It is possible to say this since metals are characterized by excess electrons that are free to move in metals. Even though electron gas is characterized by small heat capacity, electrons are important for heat (thermal) conduction because they have long mean free paths and move with high velocity.

3.2 A Heat Current Density Calculation and its Relation to Thermal Conductivity

For a heat energy flow in metallic materials like magnesium diboride, the heat energy current density or the power per unit area due to the flow of electrons is defined to be:

$$\frac{dQ}{dt/A} = U = \Omega^{-1} \sum_k (\varepsilon_k - \varepsilon_F) v_k f_k \quad \dots\dots\dots (3.1)$$

where ε_F stands for Fermi energy,

f_k stands for Fermi Dirac distribution function with $f_k \cong f_k^0 + f_k^1$ and

$$f_k^0 = \frac{1}{1 + e^{(\varepsilon_k - \varepsilon_F)/k_B T}} \quad \dots\dots\dots (3.2)$$

and Ω stands for the volume of a metallic material to be crossed by the electrons, v_k be electron velocity, ε_k be energy and ε_F for Fermi energy.

From the linearized form of Boltzman equation we get:

$$\left(\frac{\partial f_k^1}{\partial t}\right)_{collisions} = \frac{e}{\hbar c} \vec{v}_k \times \vec{H} \cdot \frac{\partial f_k^1}{\partial k} + \vec{v}_k \cdot \left(\vec{\nabla} T \frac{\partial f_k^0}{\partial T} + e\vec{E} \frac{\partial f_k^0}{\partial \varepsilon} \right) \dots\dots\dots (3.3)$$

where \vec{E} stands for the electric field and \vec{H} stands for the magnetic field with general case of assumption of existence of these fields.

The above equation holds true for a heat flow resulting from any combination of fields and gradient of temperature.

For thermal conductivity calculation; both \vec{E} and \vec{H} are taken to be zero. Hence the above eq. (3.3) reduces to:

$$\left(\frac{\partial f_k^1}{\partial t}\right)_{collisions} = \vec{v}_k \cdot \vec{\nabla} T \frac{\partial f_k^0}{\partial T} \dots\dots\dots (3.4)$$

But thermal conductivity (K) is defined by the following equation.

$$U = -K \cdot \vec{\nabla} T \dots\dots\dots (3.5)$$

$$\text{But } \frac{\partial f_k^0}{\partial \varepsilon_k} = \frac{\partial}{\partial \varepsilon_k} \left(\frac{1}{1 + e^{(\varepsilon_k - \varepsilon_F)/k_\beta T}} \right)$$

$$\Rightarrow \frac{\partial f^0}{\partial \varepsilon_k} = \frac{1}{k_\beta T} (f_k^0 (1 - f_k^0)) \dots\dots\dots (3.6)$$

Since, in low temperature case $\frac{\partial f_k^0}{\partial \varepsilon_k}$ is approximated to $-\delta(\varepsilon_k - \varepsilon_F)$;

where δ is the Kronecker delta function.

Let us define a vector **mean free path** \vec{l}_k as follows.

$$f_k^1 = (\varepsilon_k - \varepsilon_F) \frac{\vec{\nabla} T}{T} \cdot \vec{l}_k \frac{\partial f^0}{\partial \varepsilon} \dots\dots\dots (3.7)$$

But;

$$\frac{\partial f_k}{\partial T} = - \left(\frac{\varepsilon_k - \varepsilon_F}{T} \right) \frac{\partial f^0}{\partial \varepsilon_k} \dots\dots\dots (3.8)$$

Therefore, considering only elastic scattering and from the above equations we get:

$$U = \frac{1}{\Omega} \sum_k (\varepsilon_k - \varepsilon_F)^2 \vec{v}_k \frac{\vec{\nabla} T}{T} \cdot \vec{l}_k \frac{\partial f_k^0}{\partial \varepsilon} \dots\dots\dots (3.9)$$

3.3 Calculation of Total Energy of Electrons in magnesium diboride (MgB₂)

For the material of our interest namely; Magnesium diboride (MgB₂) we try to obtain an expression for thermal conductivity and electrical conductivity. Before that we recall some of the properties of MgB₂.

The crystal of magnesium diboride comprises of alternative stacking of a honeycomb lattice Boron B₂ layers and triangular lattice Magnesium (Mg) layers. It is verified by band calculations that the magnesiums are fully ionized and the Fermi level bands are characterized mainly by Boron 2p characters. There are four Fermi surfaces where two in 2p_z bands and the rest in 2p_{x,y} bands. The 2p_z bands are derived from the intra-layer π bonding orbitals where as 2p_{x,y} bands are derived from the intra-layer σ bonding orbitals. The 2p_{x,y} bands have a quasi two dimensional hole character where as the 2p_z bands have the inter-layer coupling between adjacent atomic orbitals in the c - axis direction.

The tight binding approximation can be applied to the band structure calculations for magnesium diboride (MgB₂). This shows that the 2p_z bands are well reproduced by the nearest neighbor (n.n) hopping model on a layered honeycomb lattice of Boron sites in which the following dispersion relation; [11].

$$\varepsilon_k = 2t_{xy}\gamma_{xy}(k) - 2t_z \cos k_z \dots\dots\dots (3.10)$$

holds true, where

$$\gamma_{xy}(k) = \sqrt{\frac{3}{4} + \frac{1}{2} \cos k_x + \cos\left(\frac{1}{2}k_x\right) \cos\left(\frac{\sqrt{3}}{2}k_y\right)} \dots\dots\dots (3.11)$$

Where t_{xy} (t_z) denotes the intra-layer (inter-layer n.n. electron hopping energy, while γ_{xy} is the structure factor of the intra-layer electron hopping to the n.n sites on the honeycomb lattice.

For small values of x, cosine function can be expanded into Taylor series as follows.

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots\dots$$

Hence, for values of k_x, k_y and k_z very small, that is:

For $k_x \ll 1$
 $K_y \ll 1$ and
 $K_z \ll 1$

Using the conditions given and the mathematical identity; we have

$$\begin{aligned} \cos k_x &\approx 1 - \frac{k_x^2}{2} = 1 - \frac{k_x^2}{2} \\ \cos\left(\frac{1}{2}k_x\right) &\approx 1 - \frac{\left(\frac{1}{2}k_x\right)^2}{2} = 1 - \frac{k_x^2}{8} \\ \cos k_z &\approx 1 - \frac{k_z^2}{2} = 1 - \frac{k_z^2}{2} \\ \cos\left(\frac{\sqrt{3}}{2}k_y\right) &\approx 1 - \frac{\left(\frac{\sqrt{3}}{2}k_y\right)^2}{2} = 1 - \frac{3k_y^2}{8} \end{aligned}$$

Therefore,

$$\begin{aligned} \gamma_{xy}(k) &= \sqrt{\frac{3}{4} + \frac{1}{2}\left(1 - \frac{k_x^2}{2}\right) + \left(1 - \frac{k_x^2}{8}\right)\left(1 - \frac{k_y^2}{8}\right)} \dots\dots\dots (3.12) \\ \Rightarrow \gamma_{xy}(k) &= \sqrt{\frac{3}{4} + \frac{1}{2} - \frac{k_x^2}{4} + 1 - \frac{3k_y^2}{8} - \frac{k_x^2}{8} + \frac{3k_x^2 k_y^2}{64}} \end{aligned}$$

But since both k_x and k_y are very small:

$$\begin{aligned} k_x^2 k_y^2 &\rightarrow 0 \\ \Rightarrow \gamma_{xy}(k) &= \sqrt{\frac{3}{4} + \frac{2}{4} + \frac{4}{4} - \frac{2k_x^2}{8} - \frac{k_x^2}{8} - \frac{3k_y^2}{8}} \dots\dots\dots (3.13) \\ \Rightarrow \gamma_{xy}(k) &= \sqrt{\frac{9}{4} - \frac{3}{8}(k_x^2 + k_y^2)} \\ \Rightarrow \gamma_{xy}(k) &= \sqrt{\frac{9}{4}\left(1 - \frac{1}{6}(k_x^2 + k_y^2)\right)} \\ \Rightarrow \gamma_{xy}(k) &= \frac{3}{2}\sqrt{1 - \frac{1}{6}(k_x^2 + k_y^2)} \end{aligned}$$

$$\Rightarrow \gamma_{xy}(k) = \frac{3}{2} \left[1 - \frac{1}{6} (k_x^2 + k_y^2) \right]^{\frac{1}{2}} \dots\dots\dots (3.14)$$

For small value of x, Taylor expansion of $(1+x)^a$ gives:

$$(1+x)^a = 1 + ax + \frac{a(a-1)}{2!} x^2 + \frac{a(a-1)(a-2)}{3!} x^3 + \dots\dots$$

And for $x \ll 1$, the terms of order two and above will approach to zero.

Hence, $x^2, x^3, x^4, \dots\dots \rightarrow 0$

$$\Rightarrow (1+x)^a \approx 1 + ax; \text{ for small } x$$

Therefore, in the above expression for $\gamma_{xy}(k)$ of eq. (3.14), k_x^2 and k_y^2 are very small that:

$$\Rightarrow \frac{1}{6} (k_x^2 + k_y^2) \ll 1$$

From eq. (3.14) above we have:

$$\gamma_{xy}(k) = \frac{3}{2} \left[1 - \frac{1}{6} (k_x^2 + k_y^2) \right]^{\frac{1}{2}}$$

To expand this equation using Taylor expansion we use the following substitution.

Let, $u = -\frac{1}{6} (k_x^2 + k_y^2) \dots\dots\dots (3.15)$

$$\Rightarrow \gamma_{xy}(u) = \frac{3}{2} (1+u)^{\frac{1}{2}} \dots\dots\dots (3.16)$$

Then expanding eq. (3.16) we get:

$$\gamma_{xy}(u) = \frac{3}{2} \left(1 + \frac{1}{2} u \right) \dots\dots\dots (3.17)$$

Then substituting the expression of u from eq. (3.15) into eq. (3.17) we get:

$$\begin{aligned} \gamma_{xy}(k) &= \frac{3}{2} \left[1 + \frac{1}{2} \left(-\frac{1}{6} (k_x^2 + k_y^2) \right) \right] \\ \Rightarrow \gamma_{xy}(k) &= \frac{3}{2} \left(1 - \frac{1}{12} k_x^2 - \frac{1}{12} k_y^2 \right) \end{aligned}$$

$$\Rightarrow \gamma_{xy}(k) = \frac{3}{2} - \frac{1}{8}k_x^2 - \frac{1}{8}k_y^2 \dots\dots\dots (3.18)$$

In addition to this; we have:

$$\cos k_z \approx 1 - \frac{k_z^2}{2} = 1 - \frac{k_z^2}{2}$$

Therefore, the energy in K - space will be:

$$\begin{aligned} \varepsilon_k &= 2t_{xy}\gamma_{xy}(k) - 2t_z \cos k_z \\ \Rightarrow \varepsilon_k &= 2t_{xy} \left[\frac{3}{2} - \frac{1}{8}k_x^2 - \frac{1}{8}k_y^2 \right] - 2t_z \left[1 - \frac{k_z^2}{2} \right] \dots\dots\dots (3.19) \end{aligned}$$

But, the tight binding approximation fit of the states close to the Fermi level as obtained from ab-initio band structure calculation gives the values of the parameters t_{xy} and t_z .

Accordingly, [28]

$$\begin{aligned} t_{xy} &\approx 1.6eV \\ t_z &\approx 1.25eV \end{aligned}$$

Therefore, using these values of t_{xy} and t_z ; and substituting them in the expression for energy in k-space given in equation (3.19) we get:

$$\begin{aligned} \varepsilon_k &= 2(1.6) \left[\frac{3}{2} - \frac{1}{8}k_x^2 - \frac{1}{8}k_y^2 \right] - 2(1.25) \left[1 - \frac{k_z^2}{2} \right] \\ \Rightarrow \varepsilon_k &= 3.2 \times \frac{3}{2} - 3.2 \times \frac{1}{8}k_x^2 - 3.2 \times \frac{1}{8}k_y^2 - 2.5 + 1.25k_z^2 \\ \Rightarrow \varepsilon_k &= 4.8 - 2.5 - \frac{2}{5}k_x^2 - \frac{2}{5}k_y^2 + \frac{5}{4}k_z^2 \\ \therefore \varepsilon_k &= 2.3 - \frac{2}{5}k_x^2 - \frac{2}{5}k_y^2 + \frac{5}{4}k_z^2 \dots\dots\dots (3.20) \end{aligned}$$

This can be taken as the dispersion relation. From this dispersion relation the total energy can be calculated and then the specific heat and finally; the thermal conductivity can be calculated.

3.4 Heat Capacity Calculation for Magnesium Diboride (MgB₂)

The calculation of heat capacity is necessary to express the thermal conductivity of magnesium diboride in terms of its heat capacity.

The heat capacity of a material is defined to be the amount of energy transferred per unit change in temperature. Or mathematically, it is a partial derivative of the total energy with respect to absolute temperature.

Thus;

$$C = \frac{\partial E}{\partial T} \dots\dots\dots (3.21)$$

where C stands for a heat capacity; and

E stands for the total energy transferred.

As we have seen in the above section, we have a dispersion relation of energy. Then using this dispersion relation the total energy in K - space is given by:

$$E = \sum_k f_k^0 \varepsilon_k \dots\dots\dots (3.22)$$

Using the above expression for the total energy and the definition of heat capacity we calculate the heat capacity by taking the occupancy of the electronic state.

To take the occupancy of electronic states, let's start by finding $\Delta \varepsilon$, that:

$$\Delta \varepsilon = \varepsilon(T) - \varepsilon(0)$$

$$\Rightarrow \Delta \varepsilon = \int_0^{\infty} \varepsilon D(\varepsilon) f_k^0(\varepsilon) d\varepsilon - \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon$$

Using the identity:

$$N = \int_0^{\infty} D(\varepsilon) f^o(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon \dots\dots\dots (3.24)$$

$$\text{But; } \int_0^{\infty} D(\varepsilon) f^o(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} D(\varepsilon) f^o(\varepsilon) d\varepsilon + \int_{\varepsilon_F}^{\infty} D(\varepsilon) f^o(\varepsilon) d\varepsilon$$

Therefore,
$$\Delta \varepsilon = \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) f^0(\varepsilon) d\varepsilon + \int_{\varepsilon_F}^{\infty} \varepsilon D(\varepsilon) f^0(\varepsilon) d\varepsilon - \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon - \int_0^{\varepsilon_F} \varepsilon_F D(\varepsilon) f^0(\varepsilon) d\varepsilon$$

$$- \int_{\varepsilon_F}^{\infty} \varepsilon_F D(\varepsilon) f^0(\varepsilon) d\varepsilon + \int_0^{\varepsilon_F} \varepsilon_F D(\varepsilon) d\varepsilon$$

Hence simplifying the above expression we get:

$$\Delta \varepsilon = \int_{\varepsilon_F}^{\infty} (\varepsilon - \varepsilon_F) D(\varepsilon) f^0(\varepsilon) d\varepsilon + \int_0^{\varepsilon_F} \varepsilon_F D(\varepsilon) (1 - f^0(\varepsilon)) d\varepsilon - \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) (1 - f^0(\varepsilon)) d\varepsilon$$

$$\Rightarrow \Delta \varepsilon = \int_{\varepsilon_F}^{\infty} (\varepsilon - \varepsilon_F) D(\varepsilon) f^0(\varepsilon) d\varepsilon + \int_0^{\varepsilon_F} (\varepsilon_F - \varepsilon) (1 - f^0(\varepsilon)) D(\varepsilon) d\varepsilon \dots\dots\dots (3.25)$$

$$\therefore \Delta \varepsilon = \int_{\varepsilon_F}^{\infty} (\varepsilon - \varepsilon_F) D(\varepsilon) f^0(\varepsilon) d\varepsilon + \int_0^{\varepsilon_F} (\varepsilon_F - \varepsilon) D(\varepsilon) d\varepsilon$$

The first integral term in the above expression is required to bring a conduction electron from ε_F to the energy greater than ε_F and the second term is to promote an electron from 0 to ε_F .

Therefore the electronic heat capacity at constant volume is computed as follows.

$$C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T} \left[\int_{\varepsilon_k}^{\infty} (\varepsilon - \varepsilon_F) D(\varepsilon) f^0(\varepsilon) d\varepsilon + \int_0^{\varepsilon_F} (\varepsilon_F - \varepsilon) D(\varepsilon) d\varepsilon \right]$$

$$\Rightarrow C = \int_0^{\infty} (\varepsilon - \varepsilon_F) \frac{df^0}{dT} D(\varepsilon) d\varepsilon$$

Taking $D(\varepsilon_F)$ to be constant, we take it out of the integral. Hence we get:

$$\Rightarrow C = D(\varepsilon_F) \int_0^{\infty} (\varepsilon - \varepsilon_F) \frac{df^0}{dT} d\varepsilon$$

$$\Rightarrow C = D(\varepsilon_F) \frac{\pi^3 k_B^2 T}{3} \dots\dots\dots (3.26)$$

We can further simplify the energy dispersion relation given in eq. (3.20) as follows:

$$\varepsilon_k = 2.3 - \frac{2}{5} k_x^2 - \frac{2}{5} k_y^2 + \frac{5}{4} k_z^2$$

$$\Rightarrow \varepsilon_k = 2.3 - \frac{2}{5} [k_x^2 + k_y^2 + k_z^2] + \frac{2}{5} k_z^2 + \frac{5}{4} k_z^2$$

$$\Rightarrow \varepsilon_k = 2.3 - \frac{2}{5} k^2 + \frac{33}{20} k_z^2$$

Where, $k_x^2 + k_y^2 + k_z^2 = k^2$

$D(\varepsilon_F)$ can easily be computed for the case when;

$$\varepsilon_k \propto k^2$$

Then for the contribution of the middle term in energy dispersion relation containing k^2 term, since

$$D(\varepsilon_F) = \frac{3N}{2\varepsilon_F} \dots\dots\dots (3.27)$$

Substituting eq. (3.27) in eq. (3.26) in place of $D(\varepsilon_F)$ gives:

$$C' = \frac{\pi^2 N k_\beta^2}{2\varepsilon_F} T \dots\dots\dots (3.28)$$

where C' standing for the k^2 contribution of specific heat of magnesium diboride in normal state.

But at the Fermi level; $\frac{3}{2} k_\beta T_F = \frac{1}{2} m v_F^2 = \varepsilon_F$

Hence, the specific heat can be rewritten in terms of Fermi velocity as follows.

$$\therefore C' = \frac{\pi^2 N k_\beta^2}{2 \left(\frac{1}{2} m v_F^2 \right)} T$$

$$\Rightarrow C' = \frac{\pi^2 N k_\beta^2}{m v_F^2} T \dots\dots\dots (3.29)$$

The contribution of k_z^2 can be approximated to one third of the contribution of k^2 .

Hence,

$$C = \frac{\pi^2 N k_\beta^2}{m v_F^2} T + \frac{1}{3} \times \frac{33}{20} \times \frac{\pi^2 N k_\beta^2}{m v_F^2} T$$

$$\Rightarrow C_{el} \approx \frac{31\pi^2 Nk_B^2}{20mv_F^2} \dots\dots\dots (3.30)$$

The above expression (eq. 3.30) gives electronic heat capacity of magnesium diboride in normal state.

3.5 Calculation of Thermal Conductivity of Magnesium Diboride

In section 3.2 we have tried to generally express a thermal current density U and we have also tried to see how the two quantities namely; thermal current density and thermal conductivity are related to each other. In this section we will try to derive the expression for thermal conductivity from the previous equations.

A superconductor is characterized by an energy gap. Our aim is to derive the expression for thermal conductivity of magnesium diboride both at normal and superconducting state. Here under, we derive the expression for normal state, where $\Delta \rightarrow 0$. Finally, we also derive the thermal conductivity of the superconducting state by including the energy gap parameter Δ .

Hence, from eq. (3.5) we have: $U = -K \bullet \vec{\nabla}T$

And from eq. (3.9) we have:

$$U = \frac{1}{\Omega} \sum_k (\epsilon_k - \epsilon_F)^2 \vec{v}_k \frac{\vec{\nabla}T}{T} \bullet \vec{l}_k \frac{\partial f_k^0}{\partial \epsilon} \dots\dots\dots (3.31a)$$

Rearranging terms in eq. (3.31a) we get:

$$U = \frac{1}{\Omega T} \sum_k (\epsilon_k - \epsilon_F)^2 \vec{v}_k \vec{l}_k \frac{\partial f_k^0}{\partial \epsilon} \bullet \vec{\nabla}T \dots\dots\dots (3.31b)$$

Comparing eq. (3.31b) with eq. (3.5), we get the expression for thermal conductivity to be as follows.

$$K = -\frac{1}{\Omega T} \sum_k v_k l_k (\epsilon_k - \epsilon_F)^2 \frac{\partial f_k^0}{\partial \epsilon} \dots\dots\dots (3.32)$$

For small thermal energy's limit as compared to the Fermi energy,

$$\frac{\partial f_k^0}{\partial \epsilon} \rightarrow -\delta(\epsilon_k - \epsilon_F).$$

And we can change the summation over the allowed k values to integration over k - space using the relation for any function F(k) as follows:

$$\sum_k F(k) = \frac{2\Omega}{(2\pi)^3} \iint F(k) d\varepsilon \frac{dS_k}{\hbar v_k} \dots\dots\dots (3.33)$$

Where $\hbar v_k = \frac{\partial \varepsilon}{\partial k}$ and $dS_k \equiv$ the area element in k - space of constant energy ε .

The summation in eq. (3.33) can then be changed to an integral by taking the function in the summation to be $F(k)$ and separate the integrals since ε is constant over dS_k .

Hence:

$$K = -\frac{1}{4\pi^3 T} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k \int (\varepsilon - \varepsilon_F)^2 \frac{\partial f^0}{\partial \varepsilon} d\varepsilon \dots\dots\dots (3.34)$$

But the second integral in the above expression can be integrated by extending the limits of integration from $-\infty$ to $+\infty$ as follows.

$$\int_{-\infty}^{+\infty} (\varepsilon - \varepsilon_F)^2 \frac{\partial f^0}{\partial \varepsilon} d\varepsilon = \frac{(\pi k_\beta T)^2}{3} = \frac{\pi^2 k_\beta^2 T^2}{3} \dots\dots\dots (3.35)$$

Substituting this result for the second integral in eq. (3.34) gives:

$$K = \frac{k_\beta^2 T}{12\pi} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k \dots\dots\dots (3.36)$$

But from the relation of mean free path to the electron velocity we have:

$$\vec{l}_k = \vec{v}_k \tau \dots\dots\dots (3.37)$$

where \vec{l}_k stands for the vector mean free path; and τ denotes the average time between two collisions of electrons.

Moreover, the momentum in k - space gives; $\hbar k = m v_k$. Hence $\hbar = \frac{m v_k}{k}$.

Substituting the value of \hbar and simplifying the terms in the integral of eq. (3.36) gives:

$$\int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k = \frac{\tau}{m} \int k dS_k = \frac{4\pi^3 \tau}{m} \dots\dots\dots (3.38)$$

Combining eqs. (3.36) and (3.38) and after simplifying, we arrive at the following result, which is the expression for thermal conductivity.

$$K' = \left(\frac{k_\beta^2 T}{12\pi} \right) \left(\frac{4\pi^3 \tau}{m} \right) = \frac{1}{3} \frac{\pi^2 k_\beta^2 \tau T}{m} \dots\dots\dots (3.39)$$

K' in eq. 3.39 stands for the energy containing k^2 term's contribution to thermal conductivity of magnesium diboride as in the case of a heat capacity.

If N is the number of conduction electrons involved in a metal, the thermal conductivity will be:

$$K' = \frac{1}{3} \frac{N\pi^2 k_\beta^2 \tau T}{m} \dots\dots\dots (3.40)$$

The above expression of thermal conductivity holds true also as in a heat capacity if ; the energy varies as k^2 .

That is,

$$K = \frac{1}{3} \frac{N\pi^2 k_\beta^2 \tau T}{m} + \frac{1}{3} \times \frac{1}{3} \times \frac{33}{20} \times \frac{N\pi^2 k_\beta^2 \tau T}{m}$$

$$\Rightarrow K = \left(\frac{1}{3} + \frac{11}{60} \right) \frac{N\pi^2 k_\beta^2 \tau T}{m}$$

$$\Rightarrow K = \frac{31}{60} \frac{N\pi^2 k_\beta^2 \tau T}{m} \approx \frac{1}{2} \frac{N\pi^2 k_\beta^2 \tau T}{m} \dots\dots\dots (3.41)$$

$$\Rightarrow K \propto T$$

This gives the general expression of thermal conductivity of magnesium diboride in normal state.

In eq. (3.41), the coefficient of T is constant. Hence, the graph of K versus T will be linear with the following slope.

$$\frac{K}{T} = \frac{31}{60} \frac{N\pi^2 k_\beta^2 \tau}{m} \equiv \text{constant} \dots\dots\dots (3.42)$$

The above result, is obtained for normal state of a material magnesium diboride (MgB_2), that is in the case when, $\Delta \rightarrow 0$

Let us now consider significant but small value of the energy gap below T_c in superconducting state. That is nearly around the transition temperature.

In a superconducting state, the superconductor is characterized by an energy gap Δ where the energy dispersion relation is then given by:

$$\tilde{\epsilon}_k^2 = \epsilon_k^2 + \Delta^2 \dots\dots\dots (3.43)$$

$$\Rightarrow \tilde{\varepsilon}_k = \varepsilon_k \left(1 + \frac{\Delta^2}{\varepsilon_k^2} \right)^{1/2} \dots\dots\dots (3.44)$$

Since Δ is small, expanding using Taylor's series gives:

$$\Rightarrow \tilde{\varepsilon}_k = \varepsilon_k \left(1 + \frac{\Delta^2}{2\varepsilon_k^2} \right) = \varepsilon_k + \frac{\Delta^2}{2\varepsilon_k} \dots\dots\dots (3.45)$$

Then substituting $\tilde{\varepsilon}_k$ in place of ε_k of eq. (3.32) gives:

$$K = -\frac{1}{\Omega T} \sum_k \bar{v}_k \bar{l}_k (\tilde{\varepsilon}_k - \varepsilon_F)^2 \frac{\partial f^0_k}{\partial \varepsilon} \dots\dots\dots (3.46)$$

But from eq. (3.45),

$$\tilde{\varepsilon}_k = \varepsilon_k \left(1 + \frac{\Delta^2}{2\varepsilon_k^2} \right) = \varepsilon_k + \frac{\Delta^2}{2\varepsilon_k}$$

$$(\tilde{\varepsilon}_k - \varepsilon_F)^2 = \left(\varepsilon_k - \varepsilon_F + \frac{\Delta^2}{2\varepsilon_k} \right)^2$$

$$\text{Hence, } (\tilde{\varepsilon}_k - \varepsilon_F)^2 = (\varepsilon_k - \varepsilon_F)^2 + \frac{2\Delta^2(\varepsilon_k - \varepsilon_F)}{2\varepsilon_k} + \frac{\Delta^4}{4\varepsilon_k^2}$$

We ignore the fourth order term of the energy gap to avoid complications.

Hence,

$$(\tilde{\varepsilon}_k - \varepsilon_F)^2 = (\varepsilon_k - \varepsilon_F)^2 + \frac{2\Delta^2(\varepsilon_k - \varepsilon_F)}{2\varepsilon_k} \dots\dots\dots (3.47)$$

Substituting eq. (3.47), in eq. (3.46) of thermal conductivity, we get the following expression.

$$K = -\frac{1}{\Omega T} \sum_k \bar{v}_k \bar{l}_k \left((\varepsilon_k - \varepsilon_F)^2 + \frac{2\Delta^2(\varepsilon_k - \varepsilon_F)}{2\varepsilon_k} \right) \frac{\partial f^0_k}{\partial \varepsilon} \dots\dots\dots (3.48)$$

$$\Rightarrow K = -\frac{1}{\Omega T} \sum_k \bar{v}_k \bar{l}_k \left((\varepsilon_k - \varepsilon_F)^2 \right) \frac{\partial f^0_k}{\partial \varepsilon} + \sum_k \bar{v}_k \bar{l}_k \left(\frac{2\Delta^2(\varepsilon_k - \varepsilon_F)}{2\varepsilon_k} \right) \frac{\partial f^0_k}{\partial \varepsilon}$$

From the earlier calculations of thermal conductivity of the normal state the first term is

equal to $\frac{1}{2} \frac{N \pi^2 k_\beta \tau}{m} T$

$$\Rightarrow K = \frac{1}{2} \frac{N \pi^2 k_\beta \tau}{m} T + \frac{2\Delta^2}{(2\pi)^3 T} \iint \bar{v}_k \bar{l}_k \left(1 - \frac{\varepsilon_F}{\varepsilon_k} \right) \frac{\partial f^0_k}{\partial \varepsilon} \frac{\partial S_k}{\hbar v_k} d\varepsilon \dots\dots\dots (3.49)$$

$$\Rightarrow K = \frac{1}{2} \frac{N\pi^2 k_\beta \tau}{m} T + \frac{2\Delta^2}{(2\pi)^3 T} \int \vec{v}_k \vec{l}_k \frac{dS_k}{\hbar v_k} \int \frac{\partial f_k^0}{\partial \varepsilon} d\varepsilon - \frac{2\Delta^2}{(2\pi)^3 T} \int \frac{\varepsilon_F}{\varepsilon_k} \frac{\partial f_k^0}{\partial \varepsilon} d\varepsilon \int \vec{v}_k \vec{l}_k \frac{dS_k}{\hbar v_k}$$

But, the last integral contributes only if, $\varepsilon_k = \varepsilon_F$, otherwise it becomes zero. Since, $\varepsilon_k \neq \varepsilon_F$ we neglect the last integral. $\varepsilon_k \neq \varepsilon_F$

In addition to this,

$$\int \vec{v}_k \vec{l}_k \frac{dS_k}{\hbar v_k} = \frac{4\pi^3 \tau}{m}, \text{ from eq. (3.38) and}$$

$$\int \frac{\partial f_k^0}{\partial \varepsilon} d\varepsilon = 1$$

$$\Rightarrow K = \frac{1}{2} \frac{N\pi^2 k_\beta \tau}{m} T + \frac{2\Delta^2}{8\pi^3 T} \times \frac{4\pi^3 \tau}{m}$$

$$\Rightarrow K = \frac{1}{2} \frac{N\pi^2 k_\beta \tau}{m} T + \frac{\Delta^2 \tau}{m T}$$

$$\Rightarrow K = \alpha T + \Delta^2 \frac{\beta}{T} \dots\dots\dots (3.50)$$

This gives the general expression for thermal conductivity considering the energy gap to be non zero, which is in superconducting state.

The second term gives a kink in a curve of thermal conductivity versus temperature graph below transition temperature.

This results in the following graph that has a kink below and near T_c .

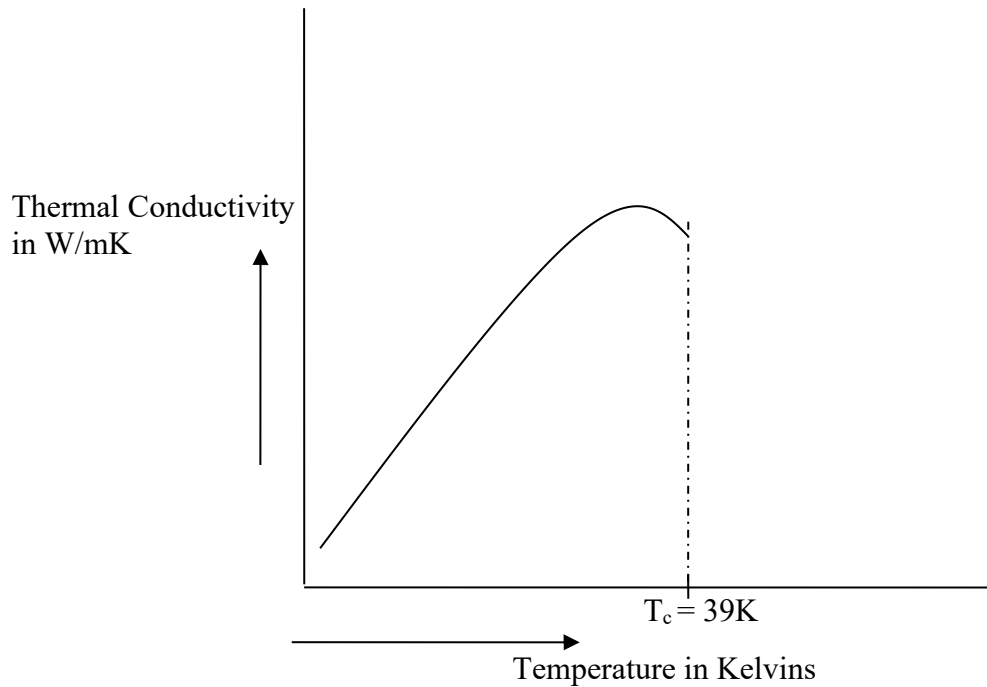


Figure 3.1 Thermal conductivity versus temperature graph

3.6 Electrical conductivity and Wiedemann - Franz Law

In the previous sections, we have tried to discuss the thermal conductivity of electrons in metals, especially in Magnesium Diboride. The result fits to the result for other metals. Electrical conductivity is another very important property that should be studied for the electrons to completely specify the electrons in a material.

We consider the electrical conductivity of a metal in which electrons are elastically scattered by random array of n impurities. In this case, we are interested with the result obtained for electrical conductivity since our aim is to relate thermal conductivity to electrical conductivity.

With the above assumptions the electrical conductivity σ is determined for any metallic material to be:

$$\sigma = -\frac{e^2}{\Omega} \sum_k v_k l_k \frac{\partial f_k^0}{\partial \epsilon} \dots\dots\dots (3.51)$$

Applying similar assertions of thermal conductivity, we get:

$$\sigma = -\frac{e^2}{4\pi^3} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k \int \frac{\partial f^0}{\partial \epsilon} d\epsilon \dots\dots\dots (3.52)$$

And also we recall that thermal conductivity is given by:

$$K = -\frac{1}{4\pi^3 T} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k \int (\varepsilon - \varepsilon_F)^2 \frac{\partial f^0}{\partial \varepsilon} d\varepsilon \dots\dots\dots (3.53)$$

Evaluating the integral gives:

$$\int_{-\infty}^{+\infty} -(\varepsilon - \varepsilon_F)^2 \frac{\partial f^0}{\partial \varepsilon} d\varepsilon = \frac{(\pi k_B T)^2}{3}$$

$$\int_{-\infty}^{+\infty} -\frac{\partial f^0}{\partial \varepsilon} d\varepsilon = 1 \dots\dots\dots (3.54)$$

Then substituting back these results in eqs. (3.44) and (3.45) gives eqs. (3.47) and (3.48) respectively:

$$\sigma = -\frac{e^2}{4\pi^3} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k \dots\dots\dots (3.55)$$

and

$$K = -\frac{1}{4\pi^3 T} \times \frac{(\pi k_B T)^2}{3} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k = -\frac{k_B^2 T}{12\pi} \int \frac{\vec{v}_k \vec{l}_k}{\hbar v_k} dS_k \dots\dots\dots (3.56)$$

Taking the ratio of the thermal to electrical conductivity we get:

$$\frac{K}{\sigma} = \frac{k_B^2 T / 12\pi}{e^2 / 4\pi^3} = \frac{\pi^2 k_B^2}{3e^2} T$$

$$\Rightarrow K = \sigma \left(\frac{\pi^2 k_B^2}{3e^2} \right) T \dots\dots\dots (3.57)$$

Eq. (3.57) relates the thermal conductivity to the electrical conductivity and the relation is called Wiedemann - Franz Law.

But since thermal conductivity was derived to be given by:

$$K \approx \frac{1}{2} \frac{N \pi^2 k_B^2 \tau T}{m} \dots\dots\dots \text{(For normal state)}$$

We then get the electrical conductivity from the relations given to be;

$$\sigma = \frac{3 N e^2 \tau}{2 m} \dots\dots\dots (3.58)$$

In this law (Wiedemann - Franz Law) of eq. 3.57, the expression in bracket is called Lorenz number and is denoted by L.

$$L = \frac{\pi^2 k_{\beta}^2}{3 e^2} \approx 2.45 \times 10^{-8} V^2 K^2 \dots\dots\dots (3.59)$$

Hence,

$$K = (L\sigma)T \dots\dots\dots (3.60)$$

3.7 The Expression of Thermal Conductivity of Magnesium Diboride in K - Space

The expression given by eq. (3.41) gives the general expression for thermal conductivity (K) using the given parameters for normal state. To write eq. (3.41) in terms of electronic heat capacity, we use the expression of the electronic heat capacity calculated in section 3.4.

Recalling the value of the electronic heat capacity of magnesium diboride calculated in section 3.4, the result given in eq. (3.30)

$$\Rightarrow C = \frac{31 \pi^2 N k_{\beta}^2}{20 m v_F^2} T$$

Therefore, in K - space; C_k is given by:

$$\Rightarrow C_k = \frac{31 \pi^2 N k_{\beta}^2}{20 m v_k^2} T \approx \frac{3 \pi^2 N k_{\beta}^2}{2 m v_k^2} T$$

Taking τ to be the scattering time or time between any two collisions, l to be a mean free path or average path length between two scattering events we have;

$$l_k = v_k \tau ;$$

From eq. (3.37)

$$l_k = v_k \tau$$

Then, recalling the expression for thermal conductivity given in eq. (3.41) we have;

$$K = \frac{31 N \pi^2 k_{\beta}^2 \tau T}{60 m}$$

Rearranging the parameters involved above we simplify the expression.

That is;

$$\begin{aligned}
 K &= \frac{31}{60} \frac{N\pi^2 k_\beta^2 \tau T}{m} \approx \frac{1}{2} \frac{N\pi^2 k_\beta^2 \tau T}{m} \\
 \Rightarrow K &= \frac{31}{60} \frac{N\pi^2 k_\beta^2}{m} \tau T \\
 \Rightarrow K &= \frac{31}{60} \frac{N\pi^2 k_\beta^2}{m} \left(\frac{l_k}{v_k} \right) T \left(\frac{v_k}{v_k} \right) \\
 \Rightarrow K &= \frac{1}{3} \left(\frac{31}{20} \frac{N\pi^2 k_\beta^2}{m v_k^2} T \right) l_k v_k \dots\dots\dots(3.61)
 \end{aligned}$$

But from eq. (3.30) the expression in bracket defines the specific heat C_k .

Hence, equation (3.41) can be written as;

$$K = \frac{1}{3} C_k l_k v_k \dots\dots\dots (3.62)$$

That is, $v = v_k$, $C = C_k$ and $l = l_k$ in K - space; to get the thermal conductivity by taking the summation over k giving the following general expression for thermal conductivity.

Therefore;

$$K = \frac{1}{3} \sum_k C_k l_k v_k \dots\dots\dots (3.63)$$

This is the general expression for the thermal conductivity of magnesium diboride in normal state condition in K - space, which is similar to the expression for most of the other metallic materials.

4. RESULTS, DISCUSSION AND CONCLUSION

4.1 Results and Discussion

We studied the behavior of a material; magnesium diboride (MgB_2), with respect to the study of its thermal conductivity. We determined the appropriate dispersion relation for magnesium diboride to be the following.

$$\varepsilon_k = 2.3 - \frac{2}{5}(k_x^2 + k_y^2) + \frac{5}{4}k_z^2$$
$$\Rightarrow \varepsilon_k = 2.3 - \frac{2}{5}k^2 + \frac{33}{20}k_z^2$$

On the way to the determination of thermal conductivity using the above dispersion relation, we determined the specific heat of a material in normal state. According to the calculation, the specific heat is determined to have the following expression.

$$C_{el} = \frac{31\pi^2 N k_\beta^2}{20 m v_F^2} T \approx \frac{3}{2} \frac{\pi^2 N k_\beta^2}{m v_F^2} T$$
$$\Rightarrow C_{el} = BT$$

where B is a constant

Similarly the calculation of electronic thermal conductivity resulted in the following expression that directly varies with temperature.

$$K = \frac{31}{60} \frac{N \pi^2 k_\beta^2 \tau}{m} T$$
$$K \approx \frac{1}{2} \frac{N \pi^2 k_\beta^2 \tau}{m} T$$

$$K = DT$$

where D is a constant.

But in experimental studies carried out and reviewed in chapter one, the curve of thermal conductivity versus temperature is more or less linear in superconducting state but shows some shoulder at a temperature immediately below the superconducting transition temperature. To explain this we used the energy gap in superconducting state since a superconductor is characterized by an energy gap. Therefore, once a material has performed transition to superconducting state, we modified the energy dispersion relation by including the energy gap, where:

$$\tilde{\varepsilon}_k^2 = \varepsilon_k^2 + \Delta^2$$

where Δ is energy gap and; $\varepsilon_k = 2.3 - \frac{2}{5}k^2 + \frac{33}{20}k_z^2$

$$\Rightarrow \tilde{\varepsilon}_k = (\varepsilon_k^2 + \Delta^2)^{1/2}$$

$$\Rightarrow \tilde{\varepsilon}_k = \varepsilon_k \left(1 + \frac{\Delta^2}{\varepsilon_k^2} \right)^{1/2}$$

Near the transition temperature, Δ is very small. That is, ($\Delta \rightarrow 0$). Therefore we can expand the above expression using Taylor expansion as follows.

$$\tilde{\varepsilon}_k = \varepsilon_k \left(1 + \frac{\Delta^2}{2\varepsilon_k^2} \right)$$

$$\Rightarrow \tilde{\varepsilon}_k = \varepsilon_k + \frac{\Delta^2}{2\varepsilon_k}$$

To study the superconducting state behavior of superconducting magnesium diboride, we used the above modified energy dispersion relation.

Then the result obtained for the thermal conductivity in superconducting state is:

$$K = \alpha T + \Delta^2 \frac{\beta}{T}$$

where β and α are constants.

Our graph of thermal conductivity versus temperature showed a shoulder below the superconducting transition temperature, that exactly fits what was already done experimentally. Since the first term is linear with temperature, we concluded that the second term in the above equation is responsible for the shoulder just below the transition temperature. If the energy gap goes to zero ($\Delta \rightarrow 0$), the result the thermal conductivity will be linear with temperature, hence is normal state.

Magnesium diboride in its normal state is also checked to obey Wiedemann Franz law given below as other metals.

$$\frac{K}{\sigma T} = \frac{\pi^2 k_B^2}{3\pi^2} = L_0 = 2.45 \times 10^{-8} V^2 K^2$$

where L_0 stands for Lorenz number.

This law is obeyed for normal state of a material since electrical conductivity is infinite in superconducting state.

We finally determined the thermal conductivity expression in K - space to be:

$$K = \frac{1}{3} \sum_k C_k l_k v_k$$

where C_k stands for heat capacity, l_k for mean free path and v_k for velocity in K - space.

4.2 Conclusions

The aim of this work was to calculate the thermal conductivity of superconducting magnesium diboride. From computations made we conclude that magnesium diboride acts as a pure metal near superconducting transition temperature.

As in most metals, Wiedemann Franz law is obeyed for magnesium diboride in normal state as it is not expected to be obeyed in superconducting state since electrical conductivity is infinite in superconducting state.

We calculated that electronic thermal conductivity is directly proportional to the temperature for magnesium diboride (MgB_2) at its normal state. We derived this starting with the energy dispersion relation that does not take the energy gap into account. Hence, the linear dependence is true only in the case when energy gap is not taken into account; i.e. in normal state. But if it were considered, the mode of dependence becomes different and contains $\frac{1}{T}$

term. Hence, a shoulder is formed just below T_c because of the effect of energy gap and inline with what was verified experimentally for superconducting state.

Moreover, the electronic heat capacity of magnesium diboride (MgB_2) also varies directly with temperature. The energy gap would have similar effect on a heat capacity as it has in thermal conductivity since their mode of dependence on temperature is similar, i.e. in normal state. In normal state, the energy gap is zero that it does not affect the heat capacity as well as the electronic thermal conductivity.

Finally, we recommend further studies on the effect of the energy gap parameter on thermal conductivity of MgB_2 to fully explain the behavior of thermal conductivity of a material. Since, MgB_2 is a recent superconductor much study on its superconducting properties has to be done to fully understand a material as a superconductor and to explain its anomalous properties.

REFERENCES

- [1] Y.Kong, O.V. Dolgov, O.Jepsen and O.K. Anderson, Physical Review B, Condmat/0102499 (2001)
- [2] S.V. Shulga, S.-L. Drechsler, , K. Winzer, M. Heinecke, K. Krug, K. Physical Review Letters 80, (1998) 1730.
- [3] E. Z. Kurmaev, I.I Lyakhovscaya, J, Kortus, A. Moewes, N. Niyata, M. Demeter, M. Neumann, M. Yanagihara, M. Watanabe, T. Muranaka, J. Akimitsu, Physical Review B 65, 134509 (2002)
- [4] J. Nakamura, N. Ymada, K. Kuroki, T. A. Callcott, D.L. EdererJ.D. Denlinger and R. C. C. Perera, Physical Review B 64, 174504 (2001)
- [5] H. Rosner, W.E. Picket, S. L. Dreschler, Physical Review B 66, 024521 (2002)
- [6] Jin Nakamura, Shin-ya Nasubida, Eiki Kabasawa, Hisashi Yamazaki, Nobuyoshi Yamada, Kazuhiko Kuroki, Department Of Applied Physics & Chemistry, University of Electro-Communications, Chofu, Tokyo, 182-8585, Japan (2003)
- [7] O. V. Dolgov, R.S. Gonnelli, G.A. Ummarino, A. A. Golubov, S.V. Shulga, J. Kortus, Physical Review B 68, 132503 (2003)
- [8] G. Profeta, A. Continenza, S. Massidda; Physical Review B 68 144508 (2003)
- [9] G. A. Ummarino, “ Pressure dependence of critical temperature in MgB₂ and two bands Eliashberg theory”, arXiv:cond - mat/0411603 V1 (2004)
- [10] E. Bauer, Ch. Paul, St. Berger, S. Majumdar, H. Michor, M. Giovannini, A. Saccone and A. Bianconi, “*Thermal conductivity study of magnesium diboride*”, arXiv:cond - mat/0104203 V2 (2001)
- [11] Nobuo Furukawa, “ Antiferromagnetism of a hubbard model on a layered honeycomb lattice”, arXiv:cond - mat/0103184 V3 (2001)
- [12] S.V Shulga, S.L Drechsler, H. Rosner and W. Picket, “The upper critical field problem in MgB₂”, arXiv:cond - mat/0103154 V1 (2001)
- [13] Mohammed H.Badr and K.W. Ng, Temperature and field dependence ofMgB₂ energy gaps”, arXiv:cond - mat/0206391 V1 (2002)
- [14] Milind N Kunchur, Sulg Ik Lee, and W.N. Kang; Physical Review. B 68, 064516 (2003)

- [15] H.Kitazawa, Y. Takano, J.Ye, K. Nishida,H. Abe, A.Matsushita and N.Tsujii; Applied Physics Letters, Volume 79, Number 17 (2001)
- [16] L. K. Yanson, mS. I. Beloborod'ko, Y. G. Naidyuk, O. V. Dolgov and A.A. Golubov; “ Self energy effect of superconducting energy gap in point contact spectra of MgB₂”, arXiv:cond - mat/310577 V2 (2003)
- [17] Yuji Zenitani and Jun Akimitsu, “Discovery of the new superconductor MgB₂ and its recent development”, JSAP International, Number 6 (2002)
- [18] M. Putti, V. Braccini, G. Galleani d' Agliano, F. Napoli, I. Pallecchi and A. S. Siri; Physical Review B 67 064505 (2003)
- [19] Frederick Rief, Fundamentals of statistical and thermal physics, McGraw - Hill Book Company, Inc (1965)
- [20] J. S. Blackmore, Solid State Physics, Second Edition, Cambridge University press 1985, (266 - 291)
- [21] A. B. Pipard, The Dynamics of Conduction Electrons, Gordon and Breach Science Publishers Inc, 1965 (1 - 81)
- [22] S. L. Soo, Analytical Thermodynamics, Prentice Hall Inc, 1962, (194 - 235)
- [23] Philip L. Taylor and Olle Heinonen, A Quantum Approach to Condensed Matter Physics, Cambridge University Press 2002
- [24] T. Tsuneto, Superconductivity and Superfluidity, Cambridge University Press 1998
- [25] Superconductivity.org, March 2005
- [26] Superconductivity.org, December 2004
- [27] Chu C.W., "High Temperature Superconductivity," *History of Original Ideas and Basic Discoveries in Particle Physics*, ed. H. B. Newman and T. Ypsilantis, Plenum Press, New York, 1996, 793.
- [28] G. Baskaran, “RVB contribution to superconductivity in MgB₂”, arXiv:cond - mat/0103308 V2 (2001)

Appendix

Periodic table to show Superconductive elements [26]

KNOWN SUPERCONDUCTIVE ELEMENTS

■ BLUE = AT AMBIENT PRESSURE
■ GREEN = ONLY UNDER HIGH PRESSURE

1	IA																										0
1	H	IIA																5	6	7	8	9	10	He			
2	3	4																	13	14	15	16	17	18			
3	Li	Be	III B IV B Y B YI B VII B VII — VII — IB IIB																B	C	N	O	F	Ne			
4	11	12	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36							
5	Na	Mg	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr							
6	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56							
7	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe									
8	55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86									
9	Cs	Ba	*La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn									
10	87	88	+Ac	104	105	106	107	108	109	110	111	112															
11	Fr	Ra		Rf	Ha	106	107	108	109	110	111	112															

SUPERCONDUCTORS.ORG

* Lanthanide Series

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu

+ Actinide Series

90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Declaration

I declare that, this thesis is my original work and has not been presented for a degree in this University or any other University.

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Approval

This thesis has been submitted for examination with my approval as University advisor.

Approved by:

Professor P. Singh