Research Article

Thermal and Electronic Conductivity in Normal and Superconducting Erbium Nickel Borocarbide (ErNi$_2$B$_2$C)

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In this work, the total electronic energy, the electronic thermal conductivity, and the heat capacity of erbium nickel borocarbide, ErNi$_2$B$_2$C, in the normal and superconducting states are calculated using Boltzmann transport equations (BTEs) and energy dispersion relation function. Results from the electronic thermal conductivity versus temperature ($T$) are presented. From the result, electrical and thermal conductivity at low temperature obey the Wiedemann–Franz law. Moreover, at the normal state, the electronic thermal conductivity of ErNi$_2$B$_2$C is directly proportional to the temperature ($T$) and reaches its maximum (kink) at the transition temperature, $T_c$. After the superconducting transition temperature, the electronic thermal conductivity begin to decrease. The drop in electronic thermal conductivity beyond its peak (kink) value is due to the formation of energy gap and the absence of Cooper pairs.

1. Introduction

The phenomenon of superconductivity has a rich and interesting history, starting in 1911 when Kamerlingh Onnes discovered that upon cooling elemental mercury to very low temperature, the electrical resistance suddenly and completely vanished below a critical temperature, $T_c$, of 4.2 K [1, 2] (Figure 1). This resistance-less state enables persistent currents to be established in circuits to generate enormous magnetic fields and to store and transport energy without dissipation.

Superconductors have other unique properties such as the ability to expel and screen magnetic fields (Meissner effect) and quantum oscillations controlled by the magnetic field that provide extraordinary measurement sensitivity [2, 3].

Electrons of materials at normal state are free to move and provide electrical conduction, but collisions with other electrons, lattice vibrations, impurities, and defects in the material cause resistance and thus energy dissipation in the material. Unlike normal metals, superconducting materials allow the passage of electricity through them without almost any electrical resistance and this was mystery at that time.

Although phenomenological models with predictive power were developed in the 30s and 40s to explain this mystery, the microscopic mechanism underlying superconductivity was not discovered until 1957 by three American physicists John Bardeen, Leon Cooper, and John Schrieffer through their BCS theory to explain the mystery in superconductors [3, 4].

According to the theory, at very low temperature, two electrons with equal and opposite speeds are glued together in a coordinated fashion, so collisions are not possible, and they move through the material without any resistance [3–5].

In this work, concepts of superconductivity and the general properties of ErNi$_2$B$_2$C in its normal and superconducting states are explained. Using Boltzmann transport equations (BTEs) and energy dispersion relation function, the electronic thermal conductivity and heat capacity of ErNi$_2$B$_2$C in both the normal and superconducting states are calculated.

1.1. Formation of Energy Gap Parameter and Critical Temperature of ErNi$_2$B$_2$C. Superconducting energy gap is a
2. Methods

In this work, Boltzmann transport equations (BTEs) and energy dispersion relation function were used to calculate the electronic thermal conductivity and heat capacity of ErNi$_2$B$_2$C in both the normal and superconducting states.

3. Electronic Thermal Conductivity of ErNi$_2$B$_2$C in Its Normal and Superconducting States

Metals possess both phonon thermal conductivity and electronic thermal conductivity. So, the total thermal conductivity is the sum of both phonon thermal conductivity, $K_p$, and electronic thermal conductivity, $K_e$ [10–12].

3.1. Heat Current Density ($J_Q$). The heat current density ($J_Q$) is defined as

$$E_K = \frac{1}{\Omega} \sum (E_K - E_F) \omega f_k K,$$

where $\Omega$ is the volume of the metallic material to be crossed by the electrons, $f_k$ is the Fermi–Dirac distribution function, $\omega_k$ is the group velocity, $E_k$ is the energy at a state $k$, and $E_F$ is the Fermi energy [13, 14].

The Fermi–Dirac distribution at $k$-mode is given by [15]

$$f_k^O = \frac{1}{\exp(E_k - \mu/k_B T) + 1},$$

where $k_B$ is Boltzmann’s constant, $T$ is the temperature, $\mu$ is the chemical potential, and the superscript in $f_k$ indicates the thermal equilibrium.

From the Fermi–Dirac distribution function at the thermal equilibrium, we have relations for partial derivative of $f_k$.

$$\frac{\partial f_k^O}{\partial E_k} = \frac{1}{k_B T} \left[ f_k^O(1 - f_k^O) \right],$$

$$\frac{\partial f_k^O}{\partial T} = \frac{E_k - \mu}{T} \frac{\partial f_k^O}{\partial E_k},$$

$$\frac{\partial f_k^O}{\partial \mu} = -\frac{\partial f_k^O}{\partial E_k}.$$

Assume that $f_k$ characterizes local equilibrium in such a way that the special variation of $f_k$ arises from the temperature, $T$, and chemical potential, $\mu$:

$$\frac{\partial f_k}{\partial \tau} = \frac{\partial f_k^O}{\partial T} \nabla_T + \frac{\partial f_k^O}{\partial \mu} \nabla \mu.$$

Substituting equations (9) and (10) into equation (11), we get

$$\frac{\partial f_k}{\partial \tau} = \frac{E_k - \mu}{T} \nabla_T f_k^O - \frac{\partial f_k^O}{\partial E_k} \nabla \mu.$$
But, \[
\frac{\partial f_k}{\partial t} = \frac{\hbar}{\mu} \frac{\partial f_k^O}{\partial E_k} \mu_k + \frac{1}{\hbar} \frac{\partial E_k}{\partial t} F = -eE. \tag{13}
\]

The description of quasi-particles as wave packet allows one to introduce the non-equilibrium distribution function \( f(k, r) \) which is the average occupation number for a state \( k \) at a point \( r \). In the absence of interactions and external fields, the function is equal to the equilibrium, \( f k 0 \); otherwise, it becomes time dependent [16].

Let us consider a system, in which only a temperature gradient exists and causes the electron to diffuse with the velocity, \( u \). Since the electron travels a distance \( d\veh \) after \( dt \), the electron distribution, \( f(r, k, t) \), at the position \( (r, k) \) in the phase space at a time \( t \) is expressed as

\[
f(r, k, t) = f(r - u_k dt, k + \frac{eE}{\hbar} dt, t - dt) + \frac{\partial f_k}{\partial t} \text{coll} dt. \tag{14}
\]

For small \( dt \), equation (14) can be expanded as [17, 18]

\[
f(r, k, t) = f(r, k, t) - u_k \nabla f + \frac{eE}{\hbar} \nabla f \frac{\partial f_k}{\partial t} + \frac{\partial f_k}{\partial t} \text{coll}, \tag{15}
\]

or

\[
\frac{\partial f_k}{\partial t} \text{coll} = u_k \frac{\partial f_k}{\partial t} + \frac{F}{\hbar} \frac{\partial f_k}{\partial k}. \tag{16}
\]

At the steady state \( \frac{\partial f_k}{\partial t} = 0 \), equation (16) becomes

\[
\frac{\partial f_k}{\partial t} \text{coll} = u_k \frac{\partial f_k}{\partial t} + \frac{F}{\hbar} \frac{\partial f_k}{\partial k}. \tag{17}
\]

Using equations (12) and (13) in equation (17), we get

\[
-\frac{E_k - E_T}{T} u_k \nabla T \frac{\partial f_k^O}{\partial E_k} \text{e}^{-\left(\frac{E}{\hbar} + \frac{1}{e} \nabla \mu\right)} u_k \frac{\partial f_k^O}{\partial E_k} = \frac{\partial f_k}{\partial t}. \tag{18}
\]

But,

\[
\frac{\partial f_k}{\partial t} = \frac{f_k - f_k^O}{\tau}, \tag{19}
\]

where \( \tau \) is the relaxation time. Hence, substituting equation (19) into equation (18) in the absence of magnetic field gives [19, 20]

\[
u_k \left(-\nabla T \frac{\partial f_k^O}{\partial T} \right) + e \nu_k \frac{\partial f_k^O}{\partial E_k} = \frac{f_k - f_k^O}{\tau}. \tag{20}
\]

The non-equilibrium part of distribution function with in the relaxation time approximation becomes

\[
f_k = f_k^O + e \nu_k \frac{\partial f_k^O}{\partial E_k} \text{e}^{-\left(\frac{E}{\hbar} + \frac{1}{e} \nabla \mu\right)} u_k \frac{\partial f_k^O}{\partial E_k} \tau \nabla T. \tag{21}
\]

Using equation (21) in equation (6), we get

\[
J_Q = \frac{1}{\Omega} \sum (E_k - EF) u_k \left[f_k^O + e \nu_k \frac{\partial f_k^O}{\partial E_k} \text{e}^{-\left(\frac{E}{\hbar} + \frac{1}{e} \nabla \mu\right)} u_k \frac{\partial f_k^O}{\partial E_k} \tau \nabla T \right]. \tag{22}
\]

It is convenient to change summation to integration.

In this case, the first term of equation (22) becomes zero, because the integration of even and odd function is zero, as \( u_k \) is odd and \( f_k \) is even function. So,

\[
J_Q = \frac{1}{\Omega} \sum (E_k - EF) \mu_k \frac{\partial f_k^O}{\partial E_k} \text{e}^{-\left(\frac{E}{\hbar} + \frac{1}{e} \nabla \mu\right)} u_k \frac{\partial f_k^O}{\partial E_k} \tau \nabla T. \tag{23}
\]

Introducing the new parameter called mean free path, \( l_k = \tau \mu \), equation (23) becomes

\[
J_Q = \frac{1}{\Omega} \sum (E_k - EF) \mu_k \frac{\partial f_k^O}{\partial E_k} \text{e}^{-\left(\frac{E}{\hbar} + \frac{1}{e} \nabla \mu\right)} u_k \frac{\partial f_k^O}{\partial E_k} \tau \nabla T. \tag{24}
\]

For thermal conductivity calculation, \( E \) and \( B \) are taken to be zero. Thus, equation (24) reduces to

\[
J_Q = \frac{1}{\Omega} \sum (E_k - EF) \mu_k l_k \left(\frac{\partial f_k^O}{\partial E_k} \tau \nabla T\right). \tag{25}
\]

3.2. Total Electron Energy. Using tight binding approximation, we can calculate the total electron energy of a given lattice structure. Consider a half-filled Hubbard model on a single layer honeycomb lattice with N-N hopping. The energy dispersion is given by \( E_k = 2t \sqrt{x^2 + y^2 + z^2} \), where \( t \) is the hopping energy and \( y \) is the energy scale. The energy dispersion has a particle-hole symmetry due to the bi-particle nature of lattice. Since borocarbide is an intermetallic compound, the tight binding fits to the band structure calculations of the following dispersion relation:

\[
E_k = \pm 2t \sqrt{x^2 + y^2 + z^2} \cos(k_x). \tag{26}
\]

where \( t \sqrt{x^2 + y^2 + z^2} \) denotes the interlayer N-N electron hopping energy and \( x, y \) and \( z \) are the structure factor of the inter layer electron hoping to the N-N sites on the honeycomb lattice [8]. The structure factor, \( x, y \), is given by

\[
y = \sqrt{\frac{3}{4} + \cos(k_x) \cos\left(\frac{\sqrt{3}}{2} k_y\right)} \tag{27}
\]

For small values of \( k_x \), \( k_y \), and \( k_z \), cosine functions of equation (27), using Taylor series expansion, can be expanded as

\[
\cos(k_x) = 1 - \frac{k_x^2}{2},
\cos\left(\frac{1}{2} k_x\right) = 1 - \frac{k_x^2}{8}, \tag{28}
\cos\left(\frac{\sqrt{3}}{2} k_y\right) = 1 - \frac{3k_y^2}{8}.
\]
So, equation (27) becomes
\[
y_{xy}(k) = \sqrt{\frac{9}{4} + \frac{3k_x^2}{8} - \frac{3k_x^2}{8} + \frac{k_x^2 k_y^2}{64}}
\] (29)

For small values of \(k_x\) and \(k_y\), the product of \(k_x^2\) and \(k_y^2\) becomes 0.
\[
y_{xy}(k) = \frac{3}{2} \frac{k_x^2}{8} \frac{k_y^2}{8}
\] (30)

Similarly,
\[
\cos(k_z) = 1 - \frac{k_z^2}{2}.
\] (31)

Substituting equations (32) and (33) into equation (26), we get
\[
E_k = 2t_x \left[ \frac{3}{2} \frac{k_x^2}{8} - \frac{k_y^2}{8} \right] - 2t_z \left[ 1 - \frac{k_z^2}{2} \right].
\] (32)

The tight binding approximation site of the states close to the Fermi level, obtained from ab initio band structure calculation, gives the values of parameters as \([8, 21]\)
\[
t_{xy} = 1.6\text{eV},
\] (33)
and
\[
t_{xyz} = 1.25\text{eV}.
\] (34)

Substituting these values in equation (32), we get
\[
E_k = 2.3 - \frac{2}{5}k_x^2 - \frac{2}{5}k_y^2 + \frac{2}{4}k_z^2.
\] (35)

Hence, equation (35) is an expression for the dispersion relation.

3.3. Electronic Heat Capacity. Near the Fermi level, electrons gain total electronic thermal kinetic energy, \(U_{el}\):
\[
U_{el} = Nk_B \frac{T^2}{T_F}.
\] (36)

From the total electronic thermal kinetic energy, we can calculate the electronic heat capacity as \([22]\)
\[
C_{el} = Nk_B \frac{T}{T_F}.
\] (37)

If \(U\) is the total energy transfer, we can write the \(\Delta U\) as
\[
\Delta U = \int_0^\infty d\varepsilon eD(\varepsilon F)f(\varepsilon) - \int_0^{\varepsilon_F} d\varepsilon eD(\varepsilon F),
\] (38)
where \(f(\varepsilon)\) and \(D(\varepsilon)\) are the Fermi–Dirac function and the number of orbitals per unit energy range, respectively. The total number of electrons, \(N\), inside a sphere of radius, \(k\), is given by \([23]\)
\[
N = \left( \frac{v}{3\pi^2} \right)^{3/2} \left( \frac{v}{3\pi^2} \right)^{3/2} \frac{2m^*e_F^2}{h^2}.
\] (39)
where \(v\) is the volume of the sphere and \(m\) is the mass of the electron. The density of state of electron, \(D(\varepsilon)\), is calculated as \([24]\)
\[
D(\varepsilon F) = \frac{dN}{d\varepsilon F} = \frac{3N}{2\varepsilon F}.
\] (40)

Multiply the identity
\[
N = \int_0^\infty d\varepsilon D(\varepsilon F)f(\varepsilon) = \int_0^{\varepsilon_F} d\varepsilon D(\varepsilon F)f(\varepsilon),
\] (41)
by \(e\) to obtain
\[
\int_0^{\varepsilon_F} d\varepsilon e D(\varepsilon F) + \int_0^\infty d\varepsilon e f(\varepsilon)D(\varepsilon F) = \int_0^{\varepsilon_F} d\varepsilon e fD(\varepsilon F).
\] (42)

We use equation (42) to rewrite equation (38) as
\[
\Delta U = \int_{\varepsilon_F}^\infty d\varepsilon (\varepsilon - \varepsilon_F)f(\varepsilon)D(\varepsilon F)
\]
\[+ \int_0^{\varepsilon_F} d\varepsilon (\varepsilon_F - \varepsilon)[1 - f(\varepsilon)]D(\varepsilon F).
\] (43)

The first integral on the right hand side of equation (43) gives the energy needed to take electrons from \(\varepsilon_F\) to the orbitals of the energy \(\varepsilon > \varepsilon_F\) and the second integral gives the energy needed to bring the electrons to \(\varepsilon_F\) from orbitals below \(\varepsilon_F\).

In equation (43), the product of the first integral of \(f(\varepsilon)D(\varepsilon_F)\) \(d\varepsilon\) is the number of electrons evaluated to orbitals in the energy range \(d\varepsilon\) at an energy \(\varepsilon\). The factor \([1 - f(\varepsilon)]\) in the second integral is the probability that an electron has been removed from an orbital, \(\varepsilon\).

The heat capacity of electron gas is calculated as
\[
C_{el} = \frac{dU}{dT} = \int_0^\varepsilon d\varepsilon (\varepsilon - \varepsilon_F) \frac{df(\varepsilon)}{dT} D(\varepsilon F).
\] (44)

For \(kBT \ll e\), we ignore the temperature dependency of the chemical potential, \(m\), in the Fermi–Dirac function and replace \(m\) by the constant \(\varepsilon_F\). Let \(kBT = \tau\), and consider the Fermi–Dirac distribution function \([25, 26]\).
\[
\frac{df(\varepsilon)}{d\tau} = \frac{\varepsilon - \varepsilon_F}{\tau^2} \exp\left[\frac{\varepsilon - \varepsilon_F/\tau}{\tau} + 1\right].
\] (45)

Let \(x = \varepsilon - \varepsilon_F/\tau\), and from equation (44) and (45), we get
\[
C_{el} = k_B^2 TD(\varepsilon F) \int_0^\infty \frac{\varepsilon x^2 e^x}{[e^{x} + 1]^2} dx.
\] (46)

We can replace the lower limit by \(-\infty\). Because the factor \(e^x\) in the integrand is already negligible at \(-\varepsilon F/\tau\) for low
temperatures such that \(-\varepsilon F / \tau \sim \infty\), the integral in equation (46) becomes
\[
\int_{-\infty}^{\infty} x^2 \frac{e^x}{[e^x + 1]^2} \, dx = \frac{\pi^2}{3}.
\] (47)

Thus, the heat capacity of an electron gas is given by
\[
\text{Cel} = \frac{1}{3} \pi^2 D (eF) k_B^2 T.
\] (48)

Substituting equation (40) into equation (48) gives
\[
\text{Cel} = \frac{\pi^2 N k_B^2 T}{2 e_F} = \frac{1}{2} \pi^2 N k_F \left( k_B T \varepsilon F \right).
\] (49)

This is the heat capacity of free electron Fermi gas in the temperature region where \(k_BT \ll eF\). For free electron gas approximation at the Fermi level, we have
\[
\frac{3}{2} k_B T_F \equiv eF \equiv \frac{1}{2} m v_F^2.
\] (50)

Substituting (50) into (49) gives the heat capacity of electron gas at the Fermi level in terms of the total number of electrons \(N\), mass of electron gas \(m\), velocity \(v\), and temperature \(T\) at the Fermi level as
\[
\text{Cel} = \frac{\pi^2 N k_B^2 T}{2 e_F} + \frac{1}{3} \frac{33 \pi^2 N k_B^2 T}{20 m v_F^2}.
\] (51)

Consider
\[
E_k = 2.3 - \frac{2}{5} k^2_x - \frac{2}{5} k^2_y + \frac{5}{4} k^2_z,
\] (52)

\[
\Rightarrow E_k = 2.3 - \frac{2}{5} k^2 + \frac{33}{20} k^2_z.
\] (53)

Let \(x = \varepsilon - \varepsilon_F / k_B T\).
\[
\Rightarrow dx = k_B T \, dx
\] (54)

Substituting equation (58) into equation (57) gives
\[
\text{Cs} = 2D (eF) k_B \int_{\varepsilon_F}^{\infty} dx \left( \frac{\varepsilon - \varepsilon_F}{k_B T} \right)^2 \exp \left( -\frac{\varepsilon - \varepsilon_F}{k_B T} \right).
\] (55)

3.4. Thermal Conductivity. Thermal conductivity of ErNi_2B_2C is related to the thermal heat current density as
\[
J_Q = -\nabla T.
\] (60)

From equations (25) and (60), the expression for electronic thermal conductivity of ErNi_2B_2C in its normal state is given as
\[
K_n = \frac{1}{\Omega T} \sum_l l_v (E_k - EF) \frac{\partial f^O_k}{\partial E}.
\] (61)

Rearranging equation (9) gives
\[
\frac{\partial f^O_k}{\partial E} = -\frac{1}{E_k - EF} \frac{\partial f^O_k}{\partial T}.
\] (62)

From equations (61) and (62), we get
\[
Kn = \frac{1}{\Omega} \sum l_k v_k (E_k - E_F) \frac{\partial f_k^O}{\partial T}.
\]  
(63)

Changing the summation to integration over the allowed \( k \)-space and using the relation for any function \( F(k) \) gives

\[
\sum F = \frac{2\Omega}{(2\pi)^3} \int F(k) dE \frac{dS_k}{\hbar v_k}.
\]  
(64)

where \( dS_k \) is the area element in \( k \)-space of constant energy and \( \hbar \) is the electronic thermal conductivity of \( \Delta \) becoming given by equation (70) holds true also as in a heat capacity.

\[
Kn = \frac{1}{4\pi} \int_0^\infty l_k u_k \frac{dS_k}{\hbar v_k} \int_0^{\infty} \left( E_k - E_F \right) \frac{\partial f_k^O}{\partial T} dE.
\]  
(65)

The Fermi–Dirac distribution function at equilibrium condition, \( f_k(0) \), is described in equation (7). Let \( x = E_k - E_F / k_B T \). Using these expressions in equation (65), we get

\[
Kn = \frac{k^2_B T}{4\pi} \int_0^\infty l_k u_k \frac{dS_k}{\hbar v_k} \int_0^{\infty} \left( x^2 e^x \right) dE.
\]  
(66)

From the relation of mean free path to the electron velocity, we have \( l_k = rv_k \), where \( r \) is the average time between collisions of electrons and \( l_k \) is the vector displacement of the electron. Moreover, the momentum in \( k \)-space can be found from the kinetic term of the electron \( k = 1/2 \sqrt{m \hbar^2 k^2} \) as

\[
h\hbar = m v_k \Rightarrow \hbar = \frac{m v_k}{k}.
\]  
(67)

Substituting these expressions into equation (66) gives

\[
K_n = \frac{\pi^2 k_B^2 \tau}{3m} T.
\]  
(69)

If \( N \) is the total number of conduction electrons involved in a metal, then the electronic thermal conductivity of ErNi\(_2\)B\(_2\)C in its normal state becomes

\[
K_n = \frac{N \pi^2 k_B^2 \tau}{3m} T.
\]  
(70)

If the energy varies with \( k^2 \), i.e., from the kinetic energy \( E_k = \hbar^2 k^2 / 2m \), then the expression of thermal conductivity given by equation (70) holds true also as in a heat capacity.

Thus, applying similar analogy as equation (53), the thermal conductivity becomes

\[
K_n = \frac{1}{3} \frac{N \pi^2 k_B^2 \tau}{m} T + \frac{1}{3} \frac{x - 1}{3} \frac{33 N \pi^2 k_B^2 \tau}{20 m} T,
\]  
(71)

Since \( N \pi^2 k_B^2 \tau / 2m \) is constant, the electronic thermal conductivity of ErNi\(_2\)B\(_2\)C in its normal state is directly proportional to temperature.

In a superconducting state, the superconductor is characterized by a weak coupling energy gap parameter, \( \Delta \), where the relation is given by

\[
\tilde{E}_k^2 = E_k^2 + \Delta^2.
\]  
(72)

where \( E_k \) is the excitation energy measured relative to \( E_F - \mu \) and we use the symbol \( \tilde{E}_k = E_k - \mu \) where \( \mu \) is the chemical potential which is equivalent to the Fermi energy \( E_F \).

Thus, we have

\[
\tilde{E}_k^2 = E_k^2 \left( 1 + \frac{\Delta^2}{2E_k^2} \right).
\]  
(73)

For small \( \Delta \), using the Taylor series, we have

\[
\tilde{E}_k = E_k + \frac{\Delta^2}{4E_k^2}.
\]  
(74)

From equation (63), we have

\[
K_s = \frac{1}{\Omega} \sum l_k u_k (E_k - E_F) \frac{\partial f_k^O}{\partial E}.
\]  
(75)

Hence,

\[
(\tilde{E}_k - E_F)^2 = (E_k - E_F)^2 + \Delta^2 \frac{2 \Delta^2}{2E_k^2} (E_k - E_F) + \Delta^4 + \ldots
\]  
(76)

Ignoring higher-order terms of the gap parameter gives

\[
(\tilde{E}_k - E_F)^2 = (E_k - E_F)^2 + \Delta^2 \frac{2 \Delta^2}{2E_k^2} (E_k - E_F).
\]  
(77)

Substituting equation (77) into equation (75) gives

\[
K_s = \frac{1}{\Omega} \sum l_k u_k (E_k - E_F) \frac{\partial f_k^O}{\partial E} + \frac{1}{\Omega} \sum l_k u_k \frac{2 \Delta^2}{2E_k^2} (E_k - E_F) \frac{\partial f_k^O}{\partial E}.
\]  
(78)

Substituting equation (80) into the first term of equation (78) gives

\[
K_s = \frac{1}{3} \frac{n N \pi^2 k_B^2 \tau}{m} T - \frac{1}{\Omega} \sum l_k u_k \frac{2 \Delta^2}{2E_k} (E_k - E_F) \frac{\partial f_k^O}{\partial E}.
\]  
(79)

Using equation (64) in the second term of equation (79) gives

\[
K_s = \frac{1}{3} \frac{n N \pi^2 k_B^2 \tau}{m} T + \frac{2 \Delta^2}{(2\pi)^3} T \int l_k u_k \frac{dS_k}{\hbar v_k} \frac{\partial f_k^O}{\partial E} dE,
\]  
(80)
But the last integral contributes only if \( E_k = E_F \); otherwise, it becomes zero. Since \( E_k \neq E_F \), we neglect the last integral.

Furthermore, we have the following relations:

\[
\int l_k v_k \frac{dS_k}{\hbar v_k} = \frac{\tau}{m} \int k dS_k = \frac{4\pi^2}{m} r^2 \text{ and } \frac{df_k}{dE} = 1. \tag{81}
\]

Thus, using the above expressions in equation (80) gives

\[
K_s = \frac{1}{3} \frac{N\pi^2 k_B^2 r^2}{m} T + \frac{\Delta^2 \tau}{m} \frac{1}{T}. \tag{82}
\]

\[
K_s \Rightarrow K_s = aT + \frac{\Delta^2 \beta}{T}. \tag{82}
\]

Equation (82) gives the general expression for electronic thermal conductivity of ErNi\(_2\)B\(_2\)C in its superconducting state.

### 3.5. Electrical Conductivity and Wiedemann–Franz Law

The electrical conductivity, \( \delta \), is determined for any metallic material as

\[
\delta = -\frac{e^2}{\Omega} \sum l_k v_k \frac{\partial f_k^0}{\partial E}. \tag{83}
\]

Applying similar steps as we did for thermal conductivity, one can arrive at

\[
\delta = -\frac{e^2}{4\pi^2} \int l_k v_k \frac{dS_k}{\hbar v_k} (E - E_F)^2 \frac{\partial f_k^0}{\partial E}. \tag{84}
\]

Evaluating the second integral yields

\[
\int_{-\infty}^{\infty} (E - E_F)^2 \frac{\partial f_k^0}{\partial E} = \frac{(\pi k_B T)^2}{3}. \tag{85}
\]

Similarly, interchanging the thermal conductivity (\( K_n \)) by electrical conductivity (\( \sigma \)) gives

\[
\sigma = -\frac{e^2}{4\pi^2} \sum l_k v_k \frac{dS_k}{\hbar v_k}, \tag{86}
\]

and

\[
K_n = \frac{-1}{4\pi^2 T} \times \frac{(\pi k_B T)}{3} \int l_k v_k \frac{dS_k}{\hbar v_k}. \tag{87}
\]

Taking the ratio of the thermal conductivity to the electrical conductivity gives

\[
K_n = \sigma \left\{ \frac{\pi^2 k_B^2}{3e^2} \right\} T. \tag{88}
\]

Equation (88) relates thermal conductivity to the electrical conductivity.

At a given temperature, thermal and electrical conductivities of metals are proportional but raising the temperature increases the thermal conductivity while decreasing the electrical conductivity. This relation is known as Wiedemann–Franz law.

Hence,

\[
\frac{K_n}{\sigma T} = \frac{1}{3} \left( \frac{\pi k_B^2}{e^2} \right)^2 = 2.44 \times 10^{-8} V^2 K^2. \tag{89}
\]

### 4. Results

Using Boltzmann Transport Equations (BTE), appropriate energy dispersion relation and tight binding approximation were applied to calculate the electronic thermal conductivity and heat capacity of ErNi\(_2\)B\(_2\)C in both the normal and superconducting states.

The tight binding approximation is given as

\[
E_k = 2.3 - \frac{2}{5} K_x + \frac{33}{20} K_x^2. \tag{90}
\]

Using this approximation, the calculated electronic heat capacity of ErNi\(_2\)B\(_2\)C in its normal state is

\[
C_n \approx \frac{3}{2} \frac{N\pi^2 k_B^2}{m v_F^2} T. \tag{91}
\]

\[
\Rightarrow C_n \approx T. \tag{91}
\]

The expression for electronic heat capacity of ErNi\(_2\)B\(_2\)C in its superconducting state is also determined as

\[
C_s = \frac{2N}{\frac{1}{K_B} (\frac{\Delta}{T})^2} \exp \left( -\frac{\Delta}{K_B T} \right). \tag{92}
\]

In the superconducting state, the heat capacity falls exponentially as the temperature decreases:

\[
C_s \propto \exp \left( -\frac{\Delta}{k_B T} \right). \tag{93}
\]

Similarly, in its normal state, the electronic thermal conductivity is calculated as

\[
K_n = \propto T. \tag{94}
\]

where

\[
\alpha = \frac{1}{2} \frac{N\pi^2 k_B^2}{m}. \tag{95}
\]

The electronic thermal conductivity in its normal state varies linearly with temperature (Figure 2).

The electronic thermal conductivity of ErNi\(_2\)B\(_2\)C in its superconducting state is determined as

\[
K_s = \propto T + \frac{\Delta^2 \beta}{T}. \tag{96}
\]

where

\[
\alpha = \frac{1}{3} \frac{N\pi^2 k_B^2}{m}. \tag{97}
\]

and \( \beta = \tau/m \) are constants. Figure 2 shows the graph of electronic thermal conductivity of ErNi\(_2\)B\(_2\)C in its superconducting state.
As can be seen from Figure 3, the electronic thermal conductivity of ErNi$_2$B$_2$C has a shoulder (kink) above the superconducting transition temperature.

In a superconductor, the thermal conductivity below $T_c$ rises sharply and reaches the superconducting transition temperature, $T_c$, near $T = 10$ K. After it reaches its maxima value, the kink, then begin to decrease.

The drop in the thermal conductivity beyond its peak value, kink, is due to the formation of energy gap and the absence of Cooper pairs [4]. Figure 3 shows the electronic thermal conductivity of ErNi$_2$B$_2$C in its superconducting state.

5. Conclusion

In this paper, the total electronic energy, the electronic thermal conductivity, and the heat capacity of erbium nickel borocarbide, ErNi$_2$B$_2$C, in its normal and superconducting states are calculated using the energy dispersion relation and Boltzmann transport equations. From the result, we concluded that the electronic thermal conductivity, at low temperature, of ErNi$_2$B$_2$C is directly proportional to the temperature in its normal state and obeyed the Wiedemann–Franz law as in most metals but at the transition temperature, $T_c$, near 10 K, a kink is formed below which the state is superconducting.

Above the superconducting transition temperature, increasing the temperature further decreases the thermal conductivity. The drop in the thermal conductivity beyond its peak value, kink, is due to the formation of energy gap and the absence of Cooper pairs, and erbium nickel borocarbide, ErNi$_2$B$_2$C, becomes normal conductor.

Data Availability

No data were used to support this study.

Conflicts of Interest

The author declares that there are no conflicts of interest.

References


