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**UNIFIED FORMULATION OF CRYSTALLOGRAPHIC,
ELECTRONIC AND THERMAL PROPERTIES OF CUBIC
STRUCTURED METALS.**

BY

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Dedication

This thesis is dedicated to my parents whose constant prayers illuminated my path.

To my life partner, my lovely wife, I dedicate this my thesis, for her patience, support, and suffering the pain of separation during my study abroad.

To my children (Mohammad and Shahd) my life light, I dedicate my work.

To my brothers and sisters, I dedicate this work, whose their support encouraged me to fulfill this work.

To all my family members and colleagues, I dedicate my thesis.

Statement of originality

This work is an attempt to unify the approach for the determination of crystallographic, thermal and electronic properties of metals with cubic structure.

To the best of the author's knowledge, this unified formulation is an original pedagogical contribution to condensed matter physics. It aims to provide a systematic method to generate systematically the above-mentioned properties of cubic structured metals based only on a minimal set of fundamental characteristics of these materials. In this way, this method offers condensed matter physicists and materials scientists a very useful tool to estimate easily those properties from their most reduced forms without the need to memorize their previous forms.

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GENERAL INTRODUCTION

General Introduction

Solid state physics is the study of physical properties of solids in terms of basic physical laws. It is concerned with the physical properties, which result from the cohesion of atoms, ions or molecules and the distribution of electrons in metals,.

Metals occupy a rather special position in the study of solids, sharing a variety of striking physical properties.

They are excellent conductors of heat and electricity, they are ductile and malleable, and display a striking luster on freshly exposed surfaces.

There are many models which can interpret the physical properties of metals. These properties are interrelated and scattered in solid state physics textbooks. As presently developed in the literature, the formulation of these properties is quite cumbersome and redundant. For this reason, it will be very useful to devise a systematic method to generate these physical properties and establish identities highlighting their interdependence starting from the knowledge on a minimal of basic characteristics of these materials.

Therefore, this work aims at develop a unified algorithmic approach for determining crystallographic characteristics, thermal and electronic properties of cubic structured metals. This study will unify the present formalism in the form of useful “connecting” identities. For this, I will establish the correlations between these physical properties and show that they can be expressed in terms of only a minimal number of the basic characteristics of these metals. The main utility of the present approach consists in generating automatically the whole set of these properties.

In this way, this technique will free potential users (students and practitioners) from the memorization effort to recall the various relevant formulae.

Chapter I starts with free electron model. It is a popular model for its simplicity and its theoretical success in interpreting some electronic properties of metals. In this model, I will show that the mean free path of electron in a metallic sample can be parameterized in terms of known characteristic sample parameters and directly measurable quantities. This parameterization makes the evaluation of mean free path of electron much simpler. I will also establish a systemic method to generate the electronic properties of metals.

Chapter II is devoted mainly to crystal structure, particularly the cubic system. Some basic crystallography concepts and geometric characteristics of cubic lattices are given. The focus here is on the cubic crystal system because many materials including most of the metals crystallize in it.

In Chapter III, I will establish the correlations between the characteristics of cubic lattices and show that they can be expressed in terms of only two independent parameters, namely, the coordination number and the lattice constant.

Also, I will develop a unified formalism for the thermal properties. They can be expressed in terms of the same parameters, and I will find a unified formalism for the electronic properties and show that they can be expressed in terms of only three independent parameters, namely, the coordination number, the lattice constant and the valence of metal.

CHAPTER I

GENERALITES

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Introduction

Metals are of great importance in our daily lives. For example iron is used in automobiles, copper in electrical wiring, silver and gold as jewelry, to give only a few examples. These and other metals have played an exceedingly important role in the growth of our technological, industrial world from early historical times to the present and will continue to do so in the future.

Metals are characterized by common physical properties: great physical strength, high density, good electrical and thermal conductivities, and high optical reflectivity, which is responsible for their characteristic lustrous appearance. The explanation of these properties is important to physicists who are interested in understanding the microscopic structure of materials, and also to the metallurgists and engineers who wish to use metals for practical purposes.

In this chapter, we shall see that these properties are closely related. They can all be explained by assuming that a metal contains a large concentration of essentially free electrons which are able to move throughout the crystal. In the introductory sections, we develop the free electron model.

1-1 Assumptions of free electron model

The most important characteristic of a metal is its high electrical conductivity. The Drude model was developed at the turn of the 20th century by Paul Drude. It came a few years after J.J. Thompson discovered the electron in 1897, people became interested in understanding more about the mechanism of metallic conduction. Drude model predates quantum theory, but still can tell us a lot about electrons in metals. The importance of Drude model is that it can be used to form quick, intuitive pictures for metals. Its basic assumptions are discussed in the following:

- A metal contains free electrons which form an electron gas.
- The electrons have some average thermal energy $\left(\frac{1}{2}mv^2\right)$, but they pursue random motions through the metal so that $v = 0$ even though $v^2 \neq 0$. The random motions result from collisions with the ions.
- Because the ions have a very large mass, they are essentially immovable.
- Independent electron approximation: There is no electron-electron interaction, although the averaged spacing is small.
- Free electron approximation: Ignore electron-phonon interaction.
- Scattering: Somehow, electrons will bump into ion cores, and such scattering events are instantaneous and can abruptly alter the velocity of electrons.
- The probability of an electron undergoing scattering in an infinitesimal time interval of length dt is dt/τ . The time τ is called relaxation time, within this model, is independent of electron's position, energy, momentum, temperature, etc.
- A temperature is used to describe the energy distribution of electrons. The electron velocities before and after a collision bare no relation.

1-2 Electrical conductivity of metals

The law of electrical conduction in metals – ohm's law – is

$$V = R I \quad (1.1)$$

Where I is the current, V the potential difference, and R the electrical resistance of the wire. We want to express this law in a form which is independent of the length and cross section of the wire, since these factors are; after all, irrelevant to the basic physics of conduction. Suppose that L and A are; respectively, the length and the cross section of the wire, then

$$j = \frac{I}{A}, \quad \mathcal{E} = \frac{V}{L} \quad \text{and} \quad R = \frac{L\rho}{A} \quad (1.2)$$

Where j is the current density (current per unit area), \mathcal{E} the electric field, and ρ the electrical resistivity. The inverse of resistivity is called the conductivity, denoted by σ that is:

$$\sigma = \frac{1}{\rho} \quad (1.3)$$

When we substitute (1.2) and (1.3) into (1.1) we arrive at

$$j = \sigma \mathcal{E} \quad (1.4)$$

which is the form of ohm's law which we shall use. Since the dimension of ρ is ohm-m, σ has the dimension ohm⁻¹m⁻¹. Now we want to express σ , in terms of the microscopic properties pertaining to the conduction electrons. The current is due to the motion of the conduction electrons under the influence of electric field. Because these particles are charged, their motion leads to an electrical current, the motion of neutral particles does not lead to an electrical current. We say that it is the conduction electrons which are responsible for the current because the ions are attached to and vibrate about the lattice sites. They have no net translational motion, and hence do not contribute to the current. Let us now treat the motion of the conduction electrons in an electric field.

Consider one typical electron: the electric field exerts on the electron a force $-e\mathcal{E}$. There is also a friction force due to the collision of the electron with the rest of the medium.

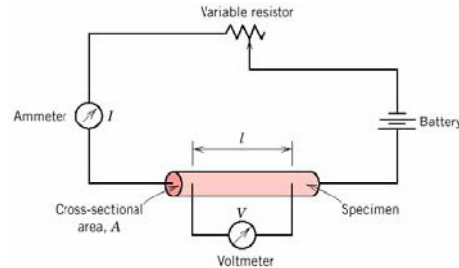


Figure1 :Ohm's law

Let us assume that this friction force has the form $-m v/\tau$ where v is the velocity of the electron and τ is a constant called the collision time. Using Newton's law, we have

$$m \frac{dv}{dt} = -e\mathcal{E} - m \frac{v}{\tau} \quad (1.5)$$

Where m is the mass of the electron. We see that the effect of the collision, as usual in friction or viscous forces, tends to reduce the velocity to zero. We are interested in the steady – state solution, that is, where $\frac{dv}{dt} = 0$. the appropriate solution of (1.5) in this case is:

$$v = \frac{e\tau}{m} \mathcal{E} \quad (1.6)$$

This, is the steady – state velocity of the electron (in discussions of friction it is usually called the terminal velocity). It is opposite to \mathcal{E} because the charge on the electron is negative.

We should make a distinction here between the two different velocities associated with the electron: The velocity appearing in (1.6) is called the drift velocity. This is superimposed on a much higher velocity or speed, known as

the random velocity, due to the random motion of the electron. Just as in an ordinary gas, the electrons have random motion even in the absence of the electric field. This is due to the fact that the electrons move about and occasionally scatter and change direction. The random motion, which contributes zero current, exists also in the presence of a field, but in that case there is an additional net velocity opposite to the field, as given by (1.6), we shall denote the two velocities by v_r and v_d , it will be shown later that $v_d \ll v_r$.

The current density j can be calculated from (1.6). Since there is a charge $(-ne)$ per unit volume, and since each electron has a drift velocity given by (1.6), it follows that the amount of charge crossing a unit area per unit time is,

$$j = (-ne)v_d = (-ne) \left(-\frac{e\tau}{m} \varepsilon \right) = \frac{ne^2\tau}{m} \quad (1.7)$$

The current is parallel to the electric field. Comparing (1.7) with Ohm's law (1.4), one finds the following expression for the conductivity:

$$\sigma = \frac{ne^2\tau}{m} \quad (1.8)$$

1-3 Thermal conductivity of metals

If there is a temperature difference between the two ends of a sample, then some of the electrons move from the hot side to the cold side via thermal diffusion, transporting energy. According to Fourier's law of heat conduction, the heat current j_u resulting from energy transport is proportional to the temperature gradient ∇T :

$$J_u = -K\nabla T \quad (1.9)$$

where K is the thermal (or heat) conductivity of the material. The justification of the choice of the negative sign is that K is then positive, as energy (heat) flows against the direction of the temperature gradient, from the higher temperature part to the lower-temperature one. We can express the thermal conductivity as the thermal conductivity of gases as:

$$K = \frac{1}{3} C_e v l_e \quad (1.10)$$

Where C_e is the specific heat, v is thermal velocity, l_e is the mean free path $l_e = v \tau$, the kinetic energy of a free particle at temperature T is $\frac{3}{2} k_B T$, that is, the mean kinetic energy of electrons satisfies the equipartition theorem $\frac{1}{2} m v^2 = \frac{3}{2} k_B T$. We get

$$v = \left(\frac{3k_B T}{m} \right)^{1/2} \quad (1.11)$$

It is readily seen that the heat capacity per electron is then $C_e = \frac{3}{2} R$

Substituting $l_e = v \tau$ and $C_e = \frac{3}{2} R$ and v from Eq.(1.11) into Eq.(1.10), one finds:

$$K = \frac{3}{2} \left(\frac{n k_B^2 \tau}{m} \right) T \quad (1.12)$$

The thermal conductivity of an electron gas is thus proportional to temperature.

Thermal conductivity can be related to electrical conductivity in a particularly simple way. Making use of the result in (1.8),

$$\frac{K}{\sigma} = \frac{3}{2} \left(\frac{k_B}{e} \right)^2 T \quad (1.13)$$

The ratio of thermal and electrical conductivity is proportional to temperature in the Drude model, and the constant of proportionality is independent of the material properties as it contains only k_B and e . This is in good agreement with an earlier experimental finding, the Weidman–Franz law– which states that the ratio of K and σ , both measured at the same temperature, is independent of material properties, and also with L. V. Lorenz’s observation (1872) that this ratio is proportional to temperature. The constant of proportionality is called the Lorenz number or Lorenz coefficient. In the Drude model its value is

$$L = \frac{3}{2} \left(\frac{k_B}{e} \right)^2 = 1.11 \times 10^{-13} (\text{erg/esu} - K)^2 \quad (1.14)$$

1-4 Ground State of the Electron Gas

In a state of wave number $k = |\mathbf{k}|$, the de Broglie wavelength is $\lambda = 2\pi/k$.

In this state the energy of the electron is

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} (k_x^2 + k_y^2 + k_z^2) \quad (1.15)$$

As has been mentioned, the states of a system of N_e particles can be constructed from the known one-particle states by taking the antisymmetrized combination of their products (Slater determinant form). The energy of the state is the sum of the energies of the occupied one-particle states. In the ground state electrons occupy the lowest-lying one-particle states. It follows from (1.15) that the wave vectors associated with the occupied states are inside a sphere in \mathbf{k} -space. The radius k_F of this Fermi sphere is the Fermi wave number, and k_F is the Fermi momentum, even though k_F is often called the Fermi momentum, too. Its value is determined by the requirement that

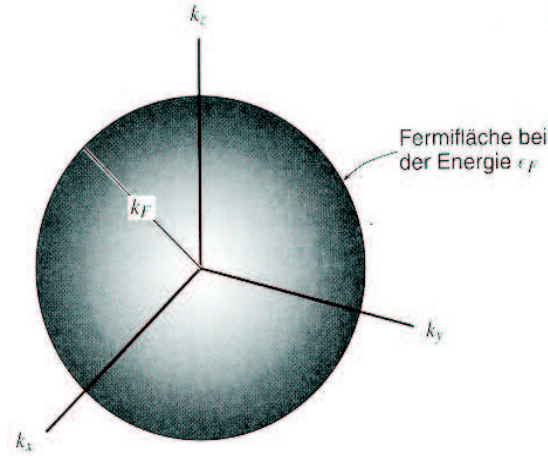


Figure 2: Fermi surface

for N_e electrons the number of allowed \mathbf{k} states inside the Fermi sphere should be $N_e/2$, as two electrons with different spin quantum numbers can have the same quantum number \mathbf{k} . Taking into account the density of \mathbf{k} -space points

$$\frac{N_e}{2} = \frac{4\pi k_F^3}{3} \frac{V}{(2\pi)^3} = \frac{k_F^3}{6\pi^2} V \quad (1.16)$$

That is,

$$n_e = \frac{N_e}{V} = \frac{k_F^3}{3\pi^2} \quad (1.17)$$

Where n_e is the electronic density in the metal.

The set of occupied states inside the Fermi sphere is often referred to as the Fermi sea. The energy of the highest occupied one-particle level in the ground state is the Fermi energy ε_F . It is defined as the energy of the topmost filled level in the ground state of N electrons system. This separates the completely filled states from the completely empty ones in the ground state. For free electrons

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} \quad (1.18)$$

It is the energy of the states on the surface of the Fermi sphere. The velocity associated with such electrons,

$$v_F = \frac{\hbar k_F}{m} \quad (1.19)$$

where v_F is the Fermi velocity. The Fermi energy is related to the electron density by

$$\varepsilon_F = \frac{\hbar^2}{2m} (3\pi^2 n_e)^{2/3} \quad (1.20)$$

Given the ground-state energy E , one can calculate the pressure exerted by the electron gas from the relation $P = -(\partial E / \partial V)_N$. Since $E = \frac{3}{5} N \varepsilon_F$ and ε_F is proportional to k_F^2 , which depends on V only through a factor $(n_e)^{2/3} = (N/V)^{2/3}$, it follows that

$$P = \frac{2}{3} \frac{E}{V} \quad (1.21)$$

1-5 Electronic Properties of metals

1-5-1 The bulk modulus

The bulk modulus K of a substance measures the substance's resistance to uniform compression. Its base unit is the pascal.

One can calculate the compressibility, K , or bulk modulus, $B=1/K$, defined by

$$B = \frac{1}{K} = -V \frac{\partial P}{\partial V} \quad (1.22)$$

where P is pressure, V is volume, and $\partial P/\partial V$ denotes the partial derivative of pressure with respect to volume. The inverse of the bulk modulus gives a substance's compressibility.

Since E is proportional to $V^{-2/3}$, Eq.(1.21) shows that P varies as $V^{-5/3}$, and therefore

$$B = \frac{5}{3}P = \frac{10 E}{9 V} = \frac{2}{3}n_e \varepsilon_F \quad (1.23)$$

1-5-2 Density of states and Magnetic susceptibility of metals

The density of states of a system describes the number of states per interval of energy at each energy level that are available to be occupied. Unlike isolated systems, like atoms or molecules in gas phase, the density distributions are not discrete like a spectral density but continuous. A high density of states at a specific energy level means that there are many states available for occupation. A density of states of zero means that no states can be occupied at that energy level.

The density of states at the Fermi level is given by

$$g(\varepsilon_F) = \frac{3 n_e}{2 \varepsilon_F} \quad (1.24)$$

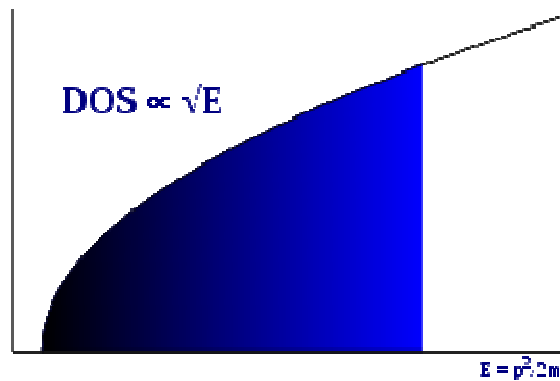


Figure 3: Density of States in 3-dimensional case

The magnetic susceptibility is the degree of magnetization of a material in response to an applied magnetic field¹. It is given by

$$\chi = \mu_B^2 g(\varepsilon_F) \quad (1.25)$$

where μ_B is Bohr magneton.

1-5-3 Electronic Specific Heat

In metals, the conduction electrons are often seen as moving freely through the lattice, and that is responsible for the high thermal and electrical conductivity. In this model, electrons should behave like an ideal gas, and from the equipartition theorem, contribute $\frac{3}{2}R$ per mole of conduction electrons to the total specific heat of the metal. However, the actual specific heat attributed to the conduction electrons is much smaller than what is predicted by classical mechanics; it is only by applying quantum mechanics to the system that one correctly determines the electronic specific heat. In the quantum mechanical picture, all of the conduction electrons must occupy different energy states as expressed by the Pauli Exclusion Principle, and to accommodate all of the conduction electrons, there must be a wide distribution of the energies, up to

¹ N.W. Ashcroft and N.D. Mermin, "Solid State Physics", (Saunders College HRW, 1976) pp.661-662-663.

some maximum energy state. At lower energies, there is zero probability of the electron transitioning to a higher state. It is only electrons at the highest energies that are able to move to higher states, and at some energy, E_F , there is a 50 % probability of transitioning to a higher state, referred to as the Fermi energy. It is the electrons that are able to change energy states that contribute to the specific heat, which from Fermi-Dirac statistics can be expressed by:

$$C_e = \frac{\pi^2}{3} k_B^2 T g(\varepsilon_F) \quad (1.26)$$

1-6 The Hall effect in metals

When a sample in which an electric current is flowing is placed in a magnetic field that is perpendicular to the current flow, electrons are deviated from their rectilinear path by the well-known Lorentz force of classical electrodynamics. Choosing the x -axis along the electric field that drives the current and the z -axis along the magnetic field, an additional electric field is induced in the y -direction, as shown in Fig.4. Consequently, a transverse voltage called the Hall voltage is observed across the sample. Resistivity against a current in the x -direction can be determined from

$$\rho(B) = \frac{E_x}{j_x} \quad (1.27)$$

In principle, this can be different from the value obtained in the absence of a magnetic field, leading to the magnetic-field dependence of resistivity. The change in the electrical resistance of a material upon the application of a magnetic field is called magneto resistance.

The Hall coefficient is defined by:

$$R_H = \frac{E_y}{j_x B} \quad (1.28)$$

To evaluate it, the drift velocity in Eq. (1.7) needs to be specified. In the presence of a magnetic field its value is obtained from a generalization of the equation of motion Eq. (1.15) that takes the Lorentz force into account, too:

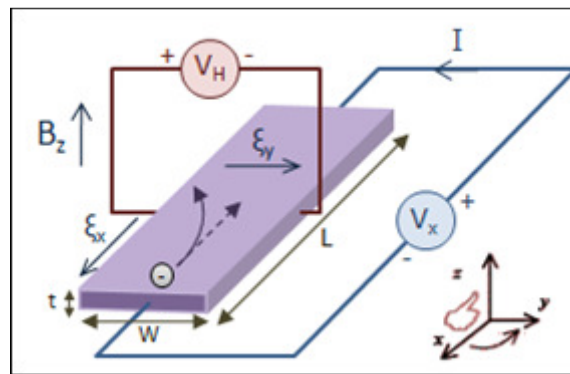


Figure 4: The geometry of the Hall Effect.

$$m \frac{dv}{dt} = -e[E + v \times B] - \frac{mv}{\tau} \quad (1.29)$$

In the stationary state

$$-e[E + v \times B] - \frac{mv}{\tau} = 0 \quad (1.30)$$

Writing out the equation in component form,

$$v_x = -\frac{e\tau}{m} E_x - \frac{eB}{m} \tau v_y \quad (1.31)$$

$$v_y = -\frac{e\tau}{m} E_y - \frac{eB}{m} \tau v_x \quad (1.32)$$

$$v_z = -\frac{e\tau}{m} E_z \quad (1.33)$$

In measurements of the Hall effect current flows only along the x -axis, i.e., $v_y = v_z = 0$. The transverse Hall voltage must precisely compensate for the deflection due to the Lorentz force. From Eq. (1.31),

$$v_x = -\frac{e\tau}{m}E_x \quad (1.34)$$

which is the same as the form obtained in the absence of the magnetic field. The x component of the current and thus the resistivity are independent of the magnetic field applied in the perpendicular direction: $\rho(B) = 1/\sigma$, where σ is the conductivity given in Eq. (1.8). Thus the resistivity does not depend on the magnetic field – i.e., there is no magneto resistance – in the Drude model. However, by eliminating v_x in favor of j_x in Eq.(1.32), and making use of Eq.(1.7),

$$E_y = Bv_x = -B \frac{j_x}{n_e e} \quad (1.35)$$

is obtained. From the definition Eq.(1.28) of the Hall coefficient

$$R_H = \frac{1}{n_e e} \quad (1.36)$$

The negative sign is the consequence of the specific choice of the measurement geometry. When the current flow is along the x -direction, electrons move in the $-x$ -direction. They are then deflected in the $-y$ -direction by the Lorentz force – that is, the current is deflected in the y -direction. This is compensated for by the negative field along the y -axis. In simple, above all monovalent metals a fairly good agreement is found between the Hall coefficients determined theoretically from the number of carriers and measured in experiments: their ratio is close to unity, as can be inferred for the elements in the first column of Fig.5. On the other hand, the fourth column contains some metals for which the agreement is poor: experimental and calculated values differ not only in magnitude but sometimes even in sign, as if carriers were positively charged. This observation

does not lend itself to interpretation in the framework of the Drude model.

<i>element</i>	R_{Hexp}	R_{Hth}	<i>element</i>	R_{Hexp}	R_{Hth}
Li	-1.7	-1.31	Be	2.4	-0.25
Na	-2.1	-2.36	Zn	0.63	-0.46
K	-4.2	-4.46	Cd	0.59	-0.65
Cu	-0.54	-0.74	Pb	0.09	-0.47
Ag	-0.84	-1.04	As	450	-0.50
Au	-0.71	-1.05	Sb	270	-0.43
Al	-0.34	-0.34	Bi	6330	-0.44

Figure 5: Measured and calculated Hall coefficients of some metals in not too strong magnetic fields around room temperature.

1-7 The failures of free electron model

Despite the success achieved by the free electron model in explanation much of metal properties, but it has failed in some sides such as :

- The failure in accommodation between its results and experimental results regarding the specific heat of the conduction electrons , where the specific heat for the electrons according to this model is given by $C_e = \frac{3R}{2}$, whereas in reality the specific heat of electron should include the electrons and phonons to be $C=C_e + C_{ph}$, and in high temperature becomes $c= 3R + \frac{3R}{2} = 4.5 R$, whereas the results and experimental measurements proved that the specific heat at the high temperature equals $3R$.

- The free electron model could not explain the experimental results of Pauli paramagnetism of metals.

The experiments have proved the Pauli paramagnetism of metals almost an independent of the temperature, which the free electron model indicates to the Pauli paramagnetism of metals proportional to the inverse of temperature.

- The free electron model could not explain the long mean free path of electrons in metals where the experiments indicate that the conduction electrons move inside the metal through long atomic distances (at very low temperature 10 cm distances) without collision with each other or with ions exist inside the metal.

All failure sides mentioned above have been solved by using the quantum mechanics whose principles have been applied on the free electron model.

1-8 Thermal properties of lattice

1-8-1 Debye model

The Debye model replaces all the vibrational spectrum with three branches, each with the same linear dispersion relation :

$$\omega = v_s k \quad (1.37)$$

The Debye model is a simplified description of the thermal excitations of a solid because it ignores most of the details of lattice dynamics, but it is very useful for interpreting experiments that measure the average elastic and thermal properties of a solid. Since the (reciprocal) volume per K-point is $(2\pi)^3/V$, the wave vector is given by :

$$k_D = (6\pi^2 n_i)^{1/3} \quad (1.38)$$

Where n_i is the density of ions.

The characteristic vibrational energy of the lattice is given in temperature units by the Debye temperature. Defined as the maximum energy of any sound wave that will propagate in a periodic lattice, this energy is determined by the fact that the wavelength of sound must be greater than the lattice spacing (or lattice constant) a defining the size of the crystallographic unit cell. The characteristic frequency in the Debye model is given in terms of an appropriate average sound velocity v_s and the atomic volume Ω (a sphere of radius $a/2$):

$$\omega_D = \left(\frac{6\pi^2}{\Omega} \right)^{1/3} v_s \quad (1.39)$$

The characteristic Debye temperature is

$$k_B \theta_D = \hbar \omega_D \quad (1.40)$$

where k_B is the Boltzmann constant. The sound velocity is determined by a complicated average over the crystal direction and wave polarization:

$$v_s = \Omega^{1/3} \left(\frac{\beta_{spring}}{A} \right)^{1/2} \quad (1.41)$$

where β_{spring} is an average atomic spring constant and A is the atomic mass. The spring constant tells how much force is required to extend the spring per unit length of extension. The Debye theory predicts that the phonon spectrum has a simple quadratic dependence on frequency up to ω_D and then drops off discontinuously to zero.

1-8-2 Specific heat of lattice

If we make the change of variables $\hbar v_s k / k_B T = x$, the Specific heat can be written in terms of the Debye temperature :

$$c_v = 9n_i k_B \left(\frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x dx}{(e^x - 1)^2} \quad (1.42)$$

This formula expresses the specific heat at all temperature in terms of a single empirical parameter, θ_D . One reasonable way to pick θ_D is by making (1.42) agree with the observed specific heat at low temperatures.

The resulting form for the low-temperature specific heat is

$$c_v = \frac{12\pi^4}{5} n_i k_B \left(\frac{T}{\theta_D} \right)^3 = 234 \left(\frac{T}{\theta_D} \right)^3 n_i k_B \quad (1.43)$$

CHAPTER II

REVIEW OF CRYSTALLOGRAPHY

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Introduction

Solid state physics is largely concerned with crystals and electrons in crystals. The study of state physics began in the early years following the discovery of x-ray diffraction by crystals and the publication of a series of simple calculations and successful predictions of the properties of crystals. In the 18th century, mineralogists discovered that the index numbers of the directions of all faces of a crystal are exact integers.

In 1912 a paper entitled (Interference effects with Rontgen rays) was presented to the Bavarian Academy of Sciences in Munich. In the first part of the paper, Laue developed an elementary theory of the diffraction of x-rays by a periodic array. In the second part, Friedrich and Knipping reported the first experimental observations of x-rays diffraction by crystals.

The work proved decisively that crystals are composed of a periodic array of atoms. With an established atomic model of a crystal, physicists now could think much further. The studies have been extended to include amorphous or non-crystalline solids, glasses, and liquids. The wider field is known as condensed matter physics and it is now the largest and probably the most vigorous area of physics.

2-1 Types of Solids

There are many ways to classify solids, the first classification involves grouping according to the regularity of the atoms/molecules within the solid.

- Crystalline Solids contain atoms or molecules bonded together in a regular pattern. Many important solids are crystalline. A good example of these is quartz crystals SiO_2 where each Si is bonded to four oxygen which in turn are bonded to two silicons in a continuous covalent network extending in three dimensions.
- Amorphous (Non-crystalline) Solid are composed of randomly orientated atoms, ions, or molecules that do not form defined patterns or lattice structures. Amorphous materials have order only within a few atomic or molecular dimensions. Amorphous materials do not have any long-range order, but they have varying degrees of short-range order. Amorphous silicon can be used in solar cells and thin film transistors. Amorphous solids (or glasses) are made up of atoms or molecules with no regular arrangement. Quartz that has been melted into liquid and cooled (moderately) rapidly will form glass. Quartz glass is used for applications like windows on lasers, and fine optics like Zeiss lenses. Examples to amorphous materials include amorphous silicon, plastics, and glasses.

2-2 Basic concepts in crystal structure

In crystallography, crystal structure is a unique arrangement of atoms or molecules in a crystalline liquid or solid. A crystal structure is composed of a pattern, a set of atoms arranged in a particular way, and a lattice exhibiting long-range order and symmetry. Patterns are located upon the points of a lattice, which is an array of points repeating periodically in three dimensions. The points can be thought of as forming identical tiny boxes, called unit cells, that fill the space of the lattice. The lengths of the edges of a unit cell and the angles between them are called the lattice parameters. The symmetry properties of the crystal are embodied in its space group.

A crystal's structure and symmetry play a role in determining many of its physical properties.

2-2-1 Periodic array of atoms

An ideal crystal is constructed by infinite repetition of identical structural units in space. In the simplest crystals the structure unit is a single atom, as in copper, silver, gold, iron, aluminum, and the alkali metals. But the smallest structural unit may comprise many atoms or molecules.

The structure of all crystals can be described in terms of a lattice, with a group of atoms attached to every lattice point. The group of atoms is called the basis; when repeated in space it forms the crystal structure.

2-2-2 Lattice translation vectors

The lattice is defined by three fundamental translation vectors a_1, a_2, a_3 such that the atomic arrangement looks the same in every respect when viewed from the point r as when viewed from the point

$$r' = r + u_1 a_1 + u_2 a_2 + u_3 a_3 \quad (2.1)$$

Where u_1, u_2, u_3 are arbitrary integers. The set of points r' defined by (2.1) for all u_1, u_2, u_3 defines a lattice.

A lattice is a regular periodic array of points in space. A lattice is a mathematical abstraction; the crystal structure is formed when a basis of atoms is attached identically to every lattice point. The logical relation is

$$\text{Lattice} + \text{Basis} = \text{Crystal structure} \quad (2.2)$$

The lattice and the translation vectors a_1, a_2, a_3 are said to be primitive if any two points r, r' from which the atomic arrangement looks the same always satisfy (2.1)

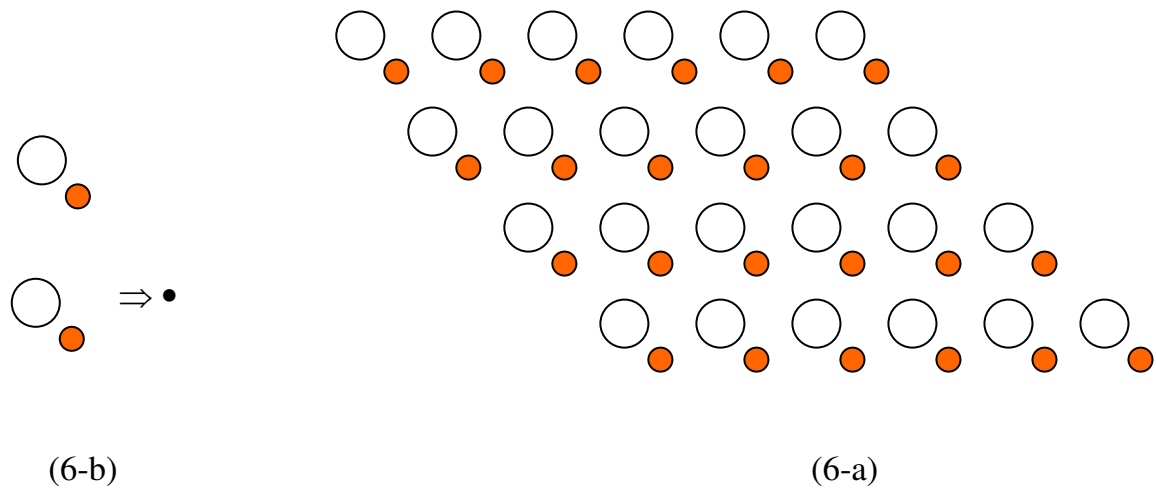


Figure 6:Crystal lattice.

with a suitable choice of the integers u_1, u_2, u_3 . With this definition of the primitive translation vectors, there is no cell of smaller volume that can serve as a building block for the crystal structure.

We often use primitive translation vectors to define the crystal axes. However, nonprimitive crystal axes are often used when they have a simple relation to the symmetry of the structure. The crystal axes a_1, a_2, a_3 form three adjacent edges of a parallelepiped. If there are lattice points only at the corners, then it is a primitive parallelepiped.

A lattice translation operation is defined as the displacement of a crystal by a crystal translation vector

$$T = u_1 a_1 + u_2 a_2 + u_3 a_3 \quad (2.3)$$

Any two lattice points are connected by a vector of this form.

2-2-3 Primitive lattice cell

The parallelepiped defined by primitive axes a_1, a_2, a_3 is called a primitive cell. A primitive cell is a type of cell or unit cell (Figure.7). A cell will fill all space by the repetition of suitable crystal translation operations. A primitive

cell is a minimum-volume cell .There are many ways of choosing the primitive axes and primitive cell for a given lattice .The number of atoms in a primitive cell or primitive basis is always the same for a given crystal structure .There is always one lattice point per primitive cell .If the primitive cell is a parallelepiped with lattice points at each of the eight corners , each lattice point is shared among eight cells , so that the total number of lattice points in the cell is one $\left(8 \times \frac{1}{8} = 1\right)$.

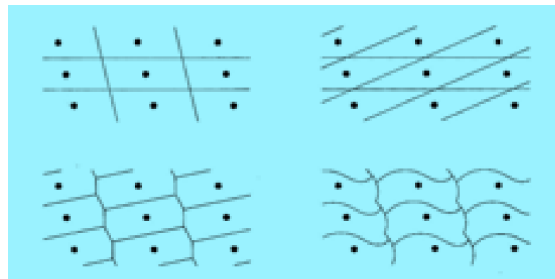


Figure 7:Several Possible choices of primitive cell for a single low-dimensional Bravais lattices

The volume of a parallelepiped with axes a_1, a_2, a_3 is

$$V_c = |a_1 \cdot a_2 \times a_3| , \quad (2.4)$$

By elementary vector analysis .The basis associated with a primitive cell is called a primitive basis .No basis contains fewer atoms than a primitive basis contains .

2-3 Bravais lattice

Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed. Lattice is invariant under a translation. A three-dimensional Bravais lattice consists of all points with position vectors R of the form

$$R = n_1 a_1 + n_2 a_2 + n_3 a_3 \quad (2.5)$$

Where a_1 , a_2 and a_3 are any three vectors not all in the same plane, and n_1 , n_2 , and n_3 range through all integral values. The vectors a_i are called primitive vectors and are said to generate or span the lattice.

There are only seven different shapes of unit cell which can be stacked together to completely fill all space (in 3 dimensions) without overlapping. This gives the seven crystal systems, in which all crystal structures can be classified.

2-3-1 Cubic lattices

Cubic lattices are of interest since a large number of materials have a cubic lattice. There are only three cubic Bravais lattices. Cubic lattices have the highest degree of symmetry of any Bravais lattice. All other cubic crystal structures (for instance the diamond lattice) can be formed by adding an appropriate base at each lattice point to one of those three lattices. The three cubic Bravais lattices are the simple cubic lattice, the body centered cubic lattice and the face centered cubic lattice.

➤ Simple cubic lattice

The simple cubic lattice consists of the lattice points identified by the corners of closely packed cubes.

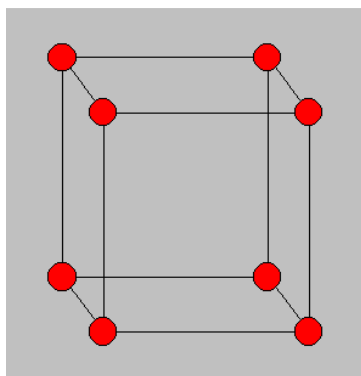


Figure 8: Simple Cubic lattice.

The simple cubic lattice contains 1 lattice point per unit cell. The unit cell is the cube connecting the individual lattice points. The atoms in the picture are shown as an example and to indicate the location of the lattice points. The

maximum packing density occurs when the atoms have a radius which equals half of the side of the unit cell. The corresponding maximum packing density is 52 %.

➤ **Body centered cubic lattice**

The body centered lattice equals the simple cubic lattice with the addition of a lattice point in the center of each

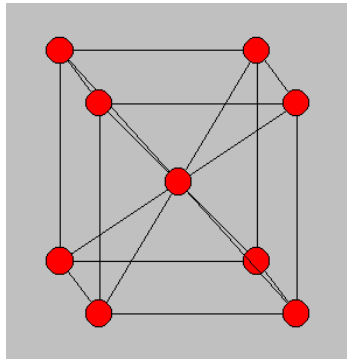


Figure 9: body centered cubic lattice

The body centered cubic lattice contains 2 lattice points per unit cell. The maximum packing density occurs when the atoms have a radius which equals one quarter of the body diagonal of the unit cell. The corresponding maximum packing density is 68%.

➤ **Face centered cubic lattice**

The face centered lattice equals the simple cubic lattice with the addition of a lattice point in the center of each of the six faces of each cube

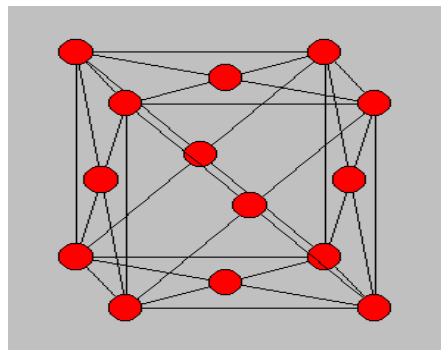


Figure10: face centered lattice

The face centered cubic lattice contains 4 lattice point per unit cell. The maximum packing density occurs when the atoms have a radius which equals one quarter of the diagonal of one face of the unit cell. The corresponding maximum packing density is 74 %. This is the highest possible packing density of any crystal structure as calculated using the assumption that atoms can be treated as rigid spheres.

➤ **Diamond lattice**

The diamond lattice consists of a face centered cubic Bravais point lattice which contains two identical atoms per lattice point. The distance between the two atoms equals one quarter of the body diagonal of the cube. The diamond lattice represents the crystal structure of diamond, germanium and silicon.

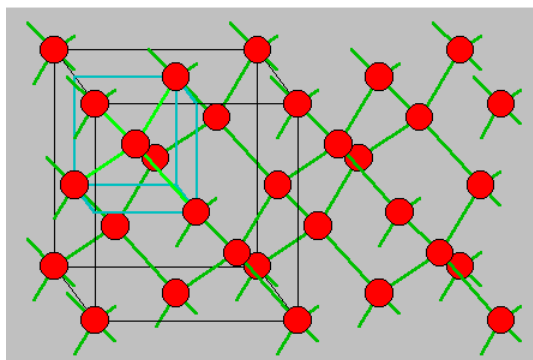


Figure11: diamond lattice

The diamond lattice contains also 4 lattice point per unit cell but contains 8 atoms per unit cell. The maximum packing density occurs when the atoms have a radius which equals one eighth of the body diagonal of the unit cell. The corresponding maximum packing density is 34 %.

➤ **Zincblende lattice**

The zincblende lattice consists of a face centered cubic Bravais point lattice which contains two different atoms per lattice point. The distance between the two atoms equals one quarter of the body diagonal of the cube. The diamond lattice represents the crystal structure of zincblende (ZnS), gallium arsenide, indium phosphate, cubic silicon carbide and cubic gallium nitride.

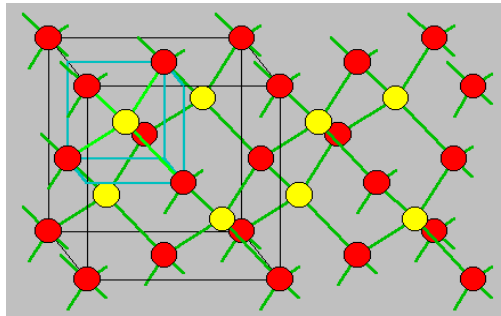


Figure12: zincblende lattice

2-4 Geometric properties of the cubic lattice systems

2-4-1 Coordination number

The points in a Bravais lattice that are closest to a given point are called its nearest neighbors. Because of the periodic nature of a Bravais lattice, each point has the same number of nearest neighbors. This number is thus a property of the lattice, and is referred to as the coordination number of the lattice. The coordination number is different from system to another. A simple cubic lattice has a coordination number of 6; a body-centered cubic lattice, 8; and a face-centered cubic lattice, 12. The notion of a coordination number can be extended in the obvious way to some simple arrays of points that are not Bravais lattices, provided that each point in the array has the same number of nearest neighbors.

2-4-2 The number of points in a unit cell for cubic systems:

➤ Simple cubic structure:

In a simple cubic unit cell, there would be an atom on each of the eight corners of the cell. Because only one-eighth of these atoms can be assigned to a given unit cell, each unit cell in a simple cubic structure would have one net atom.

$$8 \text{ corners} \times \frac{1}{8} = 1 \text{ atom}$$

➤ **Body-centered cubic structure**

In a body-centered cubic structure, there would be two atoms per unit cell, because the 1 atom in the center of the body would not be shared with any other unit cells.

$$(8 \text{ corners} \times 1/8) + 1 \text{ body} = 2 \text{ atoms}$$

➤ **Face-centered cubic structure**

In a face-centered cubic structure, the six atoms on the faces of the unit cell would contribute three net atoms, for a total of four atoms per unit cell.

$$(8 \text{ corners} \times 1/8) + (6 \text{ faces} \times 1/2) = 4 \text{ atoms}$$

2-4-3 Packing fraction

There are a number of factors that dictate which crystal structure will be realized for a given compound. As we indicated earlier, the tetrahedral covalent bond favors the diamond (or zinc blende) structure. In the case where the forces that hold the crystal together are not directional, as in the case of the covalent bond, packing considerations are often important. A convenient measure of the packing efficiency of a given structure is the packing fraction. It is the fraction of volume in a crystal structure that is occupied by atoms. It is dimensionless and always less than unity. For practical purposes, the APF of a crystal structure is determined by assuming that atoms are rigid spheres. The radius of the spheres is taken to be the maximal value such that the atoms do not overlap. For one-component crystals (those that contain only one type of atom), the APF is represented mathematically by

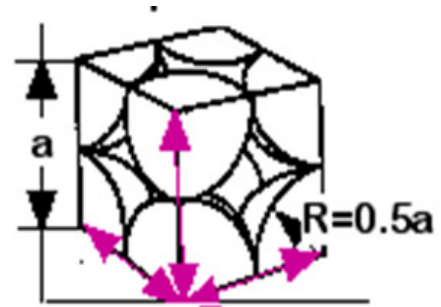
$$APF = \frac{N_U V_{at}}{V_U} \quad (2.6)$$

where N_U is the number of atoms in the unit cell, V_{at} is the volume of an atom, and V_U is the volume occupied by the unit cell.

➤ **simple cubic**

Simple cubic has one lattice point so its primitive cell. In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) belongs to that cell. The rest of the atom belongs to neighboring cells. From fig.13, we have, $a = 2R$, we can calculate APF as :

$$APF = \frac{1 \left(\frac{4}{3} \pi R^3 \right)}{(2R)^3} = \frac{\pi}{6} = 0.52$$

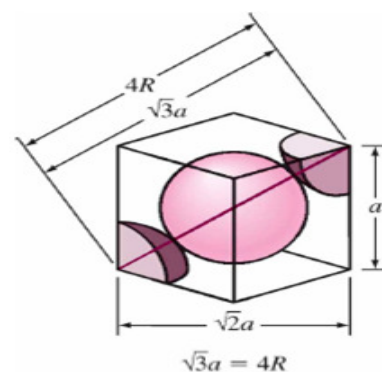


➤ **body-centered cubic**

fraction of Simple cubic lattice

The body-centered cubic has two lattice points, so it is a non-primitive cell. And it has eight nearest neighbors. Each atom is in contact with its neighbors only along the body-diagonal directions. Many metals (Fe, Li, Na.etc), including the alkali and several transition elements crystalline in the BCC structure. A line that is drawn from one corner of the cube through the center and to the other corner passes through $4R$, where R is the radius of an atom. By geometry, the length of the diagonal is $a\sqrt{3}$. Therefore, the length of each side of the BCC structure can be related to the radius of the atom by $a = \frac{4R}{\sqrt{3}}$. Knowing this and the formula for the volume of a sphere $\frac{4}{3}\pi R^3$, it becomes possible to calculate the APF as follows

$$APF = \frac{2 \left(\frac{4}{3} \pi R^3 \right)}{\left(\frac{4R}{\sqrt{3}} \right)^3} = \frac{\sqrt{3}\pi}{8} = 0.6$$



packing of fraction body-centered cubic

➤ **Face-centered cubic**

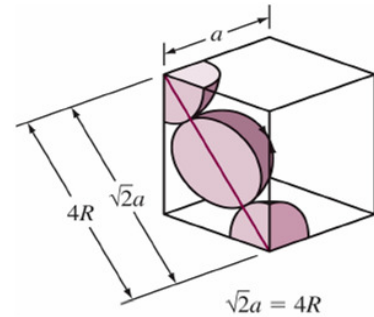
There are atoms at the corners of the unit cell and at the centre of each face.

Face entered cubic has 4 atoms so its non primitive cell. Many of common

metals (Cu, Ni, Pb..etc) crystallize in FCC. From (fig.15), we have $= \frac{4R}{\sqrt{2}}$, one

find

$$APF = \frac{4 \left(\frac{4}{3} \pi R^3 \right)}{\left(\frac{4R}{\sqrt{2}} \right)^3} = \frac{\sqrt{2} \pi}{6} = 0.74$$



**f fraction of face-centered
ibic**

Geomtry properties	crystal⇒ property↓	SC	BCC	FCC
Coordination Number	Z	6	8	12
Number of points	N	1	2	4
Volume of unit cell	V	a^3	a^3	a^3
Radius of atom	R	$\frac{a}{2}$	$\frac{a\sqrt{3}}{4}$	$\frac{a\sqrt{2}}{4}$
$\lambda = \frac{R}{a}$	λ	$\frac{1}{2}$	$\frac{\sqrt{3}}{4}$	$\frac{\sqrt{2}}{4}$
Packing fraction	APF	$\frac{\pi}{6}$	$\frac{\pi\sqrt{3}}{8}$	$\frac{\pi\sqrt{2}}{8}$

Figure 16: Geometric properties of the cubic lattice systems.

CHAPTER III

UNIFIED FORMULATION OF ELECTRONIC PROPERTIES OF METALS

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Introduction

After we have explained the electronic properties in chapter I according the free electron model, in this chapter I will develop a unified formulation approach for determining the electronic properties of metals. I will establish the correlations between electronic properties of metals, and show that they can be expressed in terms of only three independent parameters, namely, the atomic mass, the mass density and the valence of element.

Also, I will deduce a chart that shows most of the electronic properties of a metal in a specific order that is expected to enable scholars to get these electronic properties by knowing only the basic characteristic of a metal.

3-1 Some essential formulae of electronic properties of metals

We can do the process of reduction and integration of some particular relations of electronic properties of metals, to the end of exploring more simple and important formulas, so that researchers in the materials science, chemical and physics can make use of these formulae.

Let's start from the specific heat of a metal that is given by Eq. (1.26). Recall, the Bulk modulus B of metal which is given by Eq. (1.23) , also, the density of levels at the Fermi energy is given by Eq. (1.24).

Substituting ε_F from Eq. (1.23) into Eq. (1.24) and substituting the result into Eq.(1.26),one gets:

$$BC_e = LT(ne)^2 \quad (3.1)$$

where L is the Lorenz number $L = \frac{\pi^2}{3} \left(\frac{k_B}{e}\right)^2$.

The Eq. (3.1) is relating some electronic properties of metal.

By using the Hall constant which is given by Eq. (1.36),we can rewrite Eq. (3.1) as follows:

$$R_H^2 BC_e = LT \quad (3.2)$$

By using the Weidman-Franz law $L = \frac{K}{\sigma T}$,we rewrite Eq. (3.2) as following:

$$\frac{\sigma R_H^2 C_V B}{K} = 1 \quad (3.3)$$

As noticed in Eq.(3.3) ,it includes several electronic properties of a metal are encompassed in a single formula. Also, using The Pauli paramagnetic susceptibility that is given by Eq. (1.25). using Eq. (1.36), Eq. (1.23), Eq. (1.24) and Eq. (1.25), one finds:

$$R_H^2 \chi B = \left(\frac{\hbar}{2m}\right)^2 \quad (3.4)$$

Eq. (3.4) relates three electronic properties of a metal and the right side of it represent a constant.

3-2 Mean free path of electron

The mean free path is a common concept to various physical systems such as a molecular gas and a metal. For example, in a molecular gas, the mean free path of a molecule is the average distance such a molecule goes between collisions. It is a key parameter in the mathematical formulation of diffusion and transport processes in those physical systems. The electron mean free path, usually denoted by l_e , is the average distance travelled by electrons between successive collisions in a metal. l_e plays a central role in providing a physical picture for the scattering mechanism governing the electron diffusion process in a metal. It also appears in electron transport properties of metals such as the electrical and thermal conductivity. This is the main reason why l_e is usually introduced quite early in introductory solid state physics textbooks. Therefore, due to the importance of this physical parameter, it is obviously very useful to parameterize it using compact formulae which involve a minimum number of independent and directly measurable quantities to make its evaluation easier. The purpose of the present work is twofold. Firstly, it aims to meet the need of physics teachers in having at their disposal a practical tool for quick estimates of the electron mean free path in metallic samples. Secondly, its goal is to apply the measurement of the electron mean free path in a metallic sample to get a qualitative indication of the sample purity. The interest in getting an indicator of the sample purity is basically due to the fact that most of the physical properties of the sample are very sensitive to its purity.

3-2-1 Basics of the electron mean free path

The simplest classical picture of the trajectory of a conduction electron in a metal is that of a random walk as shown in (Figure 17). The solid dots at points of direction change in Figure 17 represent scattering events that conduction electrons are subject to when colliding with the impurities or lattice imperfections in the metal. The average distance between dots is the electron mean free path l_e . It follows from this description that an electron picked at

random at a given position in the sample will, on average, travel a distance l_e before its next collision, and will, on average, have been traveling a distance l_e since its last collision.

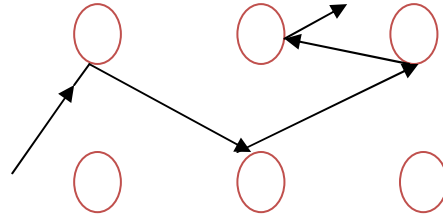


Figure 17: Pictorial view of the path of an electron in a metal.

3-2-2 Derivation of the formulae

Our starting point is the Drude model for the electron conduction in a metal. The main result of this model is the Drude formula for the electrical conductivity in a metallic sample, denoted by σ , which is given by Eq.(1.8).

Recall the electron mean free path l_e that is given by:

$$l_e = v_F \tau \quad (3.5)$$

Where v_F is the Fermi velocity of the free electron gas in the sample.

Substituting τ from Eq. (1.8) into Eq. (3.5) and using the expression of the Fermi momentum $p_F = mv_F = \hbar k_F$ where \hbar is the Planck's constant, l_e can be expressed as:

$$l_e = \frac{\hbar k_F}{e^2 n} \sigma \quad (3.6)$$

Recall that the Fermi wave vector k_F is given in terms of the electron density n in the free electron model by Eq. (1.17), Substituting k_F from Eq. (1.17) into Eq. (3.6), one finds:

$$l_e = (3\pi^2)^{1/3} \frac{\hbar}{e^2} \frac{1}{n^{2/3}} \sigma \quad (3.7)$$

The electrical conductivity σ can be derived from Ohm's law expressed in its standard form Eq.(1.1).

which R is the electrical resistance of the sample depending on its geometric dimensions. Using the inverse of R , $G = \frac{1}{R}$, known as the electrical conductance of the sample which is defined as :

$$G = \sigma \frac{S}{L} = \frac{I}{V} \quad (3.8)$$

where L is the sample length and S its cross-sectional area.

Substituting σ from Eq. (3.8) into Eq. (3.7) yields the following formula for l_e :

$$l_e = (3\pi^2)^{1/3} \frac{\hbar}{e^2} \frac{1}{n^{2/3}} \frac{I L}{V S} \quad (3.9)$$

Eq.(3.9)explicitly shows that the electron mean free path l_e can be simply evaluated by directly measuring two electric quantities; the electric current I and the voltage V and two geometric dimensions of the sample; L and S provided that one knows the electron density n in the sample.

If the sample in use is identified, particularly if one knows the following sample characteristics: its mass density, ρ_m , its atomic mass A and its number of valence electrons per atom z , then one can easily evaluate the electron density n in it as follows: since each atom in the sample contributes z valence electrons, then the number of electrons per unit volume i.e. n is given by:

$$n = \frac{zN_{at}}{V_s} \quad (3.10)$$

where N_{at} is the number of atoms in the sample with a volume V_s . By definition

$\rho_m = \frac{M}{V_s}$ where M is the mass of the sample, therefore Eq.(3.10) becomes :

$$n = \frac{zN_{at}}{M} \rho_m \quad (3.11)$$

Recognizing straightforwardly that $\frac{M}{N_{at}}$ is just the mass of a single atom in the sample which is equal by definition to $\frac{A}{N_A}$ where N_A is the Avogadro's number. Therefore, n is given by:

$$n = z \frac{\rho_m}{A} N_A \quad (3.12)$$

Eq.(3.12) explicitly shows that n depends only on the sample characteristics: z , ρ_m and A therefore n is a physical property of the sample. Consequently, Eq.(3.7) shows that the electron mean free path l_e is also a physical property since itself depends only on two physical properties of the sample namely n and σ .

Substituting n from Eq.(3.12) into Eq.(3.9), one gets:

$$l_e = K \left[\frac{1}{z} \frac{A}{\rho_m} \right]^{2/3} \frac{I}{V} \frac{L}{S} \quad (3.13)$$

where K is the universal constant $\left(\frac{3\pi^2}{N_A^2} \right)^{1/3} \frac{\hbar}{e^2}$ which is numerically equal to $1.8 \times 10^{-12} \Omega \cdot mol^{2/3}$.

Eq.(3.13) simply parameterizes the electron mean free path l_e in a known metallic sample in terms of seven parameters : three sample characteristics: z , A , ρ_m and four directly measurable quantities; two electric ones: I , V and two geometric ones: L , S . As expressed, Eq.(3.13) represents the most reducible formula for l_e in a metallic sample.

Using practical units by taking A in $g/mol.$, ρ_m in g/cm^3 and measuring I in A , V in $volt$, L in cm and S in mm^2 , l_e is given in \AA by :

$$l_e [A^\circ] = 1.8 \times 10^{-2} \left[\frac{1}{z} \frac{A}{\rho_m} \right]^{2/3} \frac{I}{V} \frac{L}{S} \quad (3.14)$$

If, in addition, the metallic sample in use has a crystalline structure and particularly a cubic one, one can deduce its lattice parameter a as follows: if n_a is the number of atoms per unit cell (which is equal to 2 for the body-centered cubic lattice and 4 for the face-centered one) then one can microscopically

define ρ_m as $\rho_m = \frac{n_a A / N_A}{a^3}$, therefore a is given by:

$$a = \left[\frac{n_a A}{N_A \rho_m} \right]^{1/3} \quad (3.15)$$

Combining Eq.(3.13) and Eq.(3.15), one gets the dimensionless ratio α of l_e to a :

$$\alpha = \frac{l_e}{a} = P \left[\frac{1}{n_a z^2} \frac{A}{\rho_m} \right]^{1/3} \frac{I L}{V S} \quad (3.16)$$

where P is the universal constant $\left(\frac{3\pi^2}{N_A} \right)^{1/3} \frac{\hbar}{e^2}$ which is numerically equal to $1.5 \times 10^{-4} \Omega \cdot mol^{1/3}$.

Using the same units for A , ρ_m , I , V , L and S as above, α is given by :

$$\alpha = 1.5 \times 10^{-2} \left[\frac{1}{n_a z^2} \frac{A}{\rho_m} \right]^{1/3} \frac{I L}{V S} \quad (3.17)$$

But in the case where the metallic sample in use is unidentified, its electron density n is unknown. To get l_e through Eq.(3.9), one must previously evaluate n . One of the most commonly used technique to determine n in metallic sample is the Hall Effect. The latter takes place whenever an electric field and a magnetic field applied at right angles to a sample producing an electric field E_H in the third direction, called the Hall field, in order to produce zero current in that direction. In the Hall effect experiment, the current I and the Hall voltage V_H are measured. Usually, we define the Hall coefficient R_H as:

$$E_H = R_H J_x B \quad (3.18)$$

where J_x is the electric current density and B the magnetic field. Assuming that the free electron model holds in the sample in use then one can readily use the free electron result for $R_H = \frac{1}{ne}$ and by expressing E_H and J_x in terms of V_H , I and the sample geometric dimensions: its width l and its thickness d i.e.

$$E_H = \frac{V_H}{l}; \quad J_x = \frac{I}{ld}, \quad R_H \text{ reads:}$$

$$R_H = \frac{1}{n} = \frac{V_H d}{I B} \quad (3.19)$$

Then, one gets for n :

$$n = \frac{I B}{e V_H d} \quad (3.20)$$

Thus, the measurement of the Hall coefficient R_H gives a direct measurement of the electron density n .

Expressing n in cm^{-3} and using the same units for I , V , L and S as specified above, l_e is given in \AA by:

$$l_e [A^\circ] = 1.3 \times 10^{14} \frac{1}{n^{2/3}} \frac{I L}{V S} \quad (3.21)$$

3-2-3 A qualitative indicator of the sample purity

Recall that the sample purity is an important characteristic of a given sample since it affects most of its physical properties. As a typical example of the latter, the electrical resistivity of a metallic sample is very sensitive to the concentration of impurity atoms in that sample. Hence the importance of the definition of indicators of sample purity in order to quantify its effects on the physical properties of the sample. One convenient indicator of sample purity is defined as the resistivity ratio of the sample which is defined as the ratio of its

resistivity at room temperatures to its residual resistivity which is the extrapolated resistivity at 0 K. Though this indicator of sample purity is quite simple but its determination needs careful resistivity measurements at room and low temperatures. An alternate indicator of sample purity which will be more accessible to college science students is highly recommended. For this, it turns out that the measured value of l_e via Eqs(3.14, 3.21) in a given sample can be used as a qualitative indicator of its purity as follows: since the frequency of collisions in the sample is proportional to the concentration of impurities in the sample, the electron mean free path will vary in length. The shorter the electron mean free path, the higher this concentration, and vice versa i.e. the longer the electron mean free path, the lower that concentration. Therefore, l_e offers a microscopic measure of the sample purity. In the case of a crystalline sample, one can use the measured dimensionless parameter α given by Eq.(3.17) as an approximate indicator of the sample purity. The limit $\alpha \gg 1$ or equivalently $l_e \gg a$ simply implies the dilute case of the impurity concentration whereas the limit $\alpha \sim 1$ or equivalently $l_e \sim a$ means its dense case.

3-3 Reduction of electronic properties of metals

The free electron move inside the crystal randomly and during movement, they collide with crystal lattice generating changing in their velocity whether in the amount or direction or even both.

The change in the electron velocity leads to changing in its dynamic energy, and according to the thermal equanimity condition, the electronic gas temperature should be equal to the temperature of lattice ions. This means non-availability of thermal exchange between the electrons and the lattice, but if the electronic gas temperature has changed then , the lattice temperature should be changed as well as a result of energy exchange between electrons and ions , and this seems to be useful result in explaining the conduction in metals and semiconductor .

The free electron theory attributes the change in velocity to the alternate instantaneous affection between the electron and crystal lattice , namely it assumes that the alternate affection between the electron and crystal lattice is similar to the collision in mechanics , and amongst each two collision , the electrons move as a free system , non affecting of the lattice field or other electron field , and to the end of assimilating the electrons movement , the concept of the time collision of electrons has been involved , and that is the time spend by the free electron between two successive collisions .

From Eq.(3.1) and Eq.(3.12) and using the expression of the Fermi momentum $p_F = mv_F = \hbar k_F$ where \hbar is the Planck's constant, we find the time collision τ_F as following:

$$\tau_F = 5.9 \times 10^{-14} \left(\frac{A}{z\rho_m} \right) \frac{I}{V} \frac{L}{S} \quad (3.22)$$

By following the same approach, we can find directly several electronic properties of metal in terms of the basic characteristics of metal, as functions of A, z, ρ_m :

Using Eq.(1.17) and Eq.(3.12) the Fermi wave vector k_F is given in terms of A, z, ρ_m by:

$$k_F = 2.6 \times 10^8 \left(\frac{z\rho_m}{A} \right)^{1/3} \quad (3.23)$$

By using the expression of the Fermi momentum $p_F = mv_F = \hbar k_F$ we find the Fermi velocity as:

$$v_F = 3 \times 10^8 \left(\frac{z\rho_m}{A} \right)^{1/3} \quad (3.24)$$

By using the Fermi energy is given by Eq.(1.18), Substituting k_F from Eq.(3.23) into Eq.(1.18) one finds:

$$\varepsilon_F = 0.4 \times 10^{-10} \left(\frac{z\rho_m}{A} \right)^{2/3} \quad (3.25)$$

Substituting n from Eq.(4.12), and ε_F from Eq.(3.25) into (1.24), one gets:

$$g(\varepsilon_F) = 2.2 \times 10^{34} \left(\frac{z\rho_m}{A} \right)^{1/3} \quad (3.26)$$

Also, by using the Fermi temperature which is given as:

$$T_F = \frac{\varepsilon_F}{k_B} \quad (3.27)$$

We put Eq.(3.26) into Eq.(3.27), one finds:

$$T_F = 0.28 \times 10^6 \left(\frac{z\rho_m}{A} \right)^{2/3} \quad (3.28)$$

Substituting n from Eq.(3.12), and ε_F from Eq.(3.25) into Eq. (1.23), one gets:

$$B = 0.16 \times 10^{14} \left(\frac{z\rho_m}{A} \right)^{5/3} \quad (3.29)$$

Substituting $g(\varepsilon_F)$ from Eq.(3.26) into Eq.(1.25),one gets:

$$\chi=1.89 \times 10^{-6} \left(\frac{z\rho_m}{A} \right)^{1/3} \quad (3.30)$$

Finally we can find the Hall coefficient by Substituting n from Eq. (3.12) into Eq. Eq.(1.36),one finds:

$$R_H=1.04 \times 10^{-5} \left(\frac{A}{z\rho_m} \right) \quad (3.31)$$

3-4 The chart of electronic properties of metals

The theory of free electron or what is known as the Classic Theory though being simple, is able to explain many of the metals properties like electric conductivity, thermal conductivity, etc. This theory proved to be successful in many important areas and fields. This makes it one of necessary needs of researchers.

However, one of the problems that faces the researchers using the relations of the free electron theory is that these relations are scattered in different references. This adds a lot of burden on those researchers. Consequently, it might be a great help for researchers to collect these relations and put them together in one reference; and to establish a kind of relations among these formulae with the help of which it becomes easy to recognize most of the electronic properties of any metal.

Here, I have tried to tackle this problem. I try to draw a chart that shows most of the relations of the Free Electron theory in a specific order that is expected to enable scholars to get the results of these relations by knowing only the basic properties of a metal. Getting the results of these relations means knowing most of the electronic properties of a metal.

In this part, we introduce this chart that explains how to generate these properties and how effective it is in helping researchers to know the electronic properties of any metal.

3-4-1 The Flow Chart

It is well known that the recognition of most of the electronic properties of metal is based on the calculation of its electronic density n (electron concentration). That is to say, for recognizing the electronic properties of any metal, we should first know its electronic density n . That is because most of the relations of the Free Electron Theory that help us to know the electronic properties of metals, directly or indirectly, contain n as one of the variables. In most of these relations the rest of variables are constants. To make it clearer, I have devised the chart given below. This chart represents a systematic method to generate the results of the relations of the Free Electron Theory. (See Figure 18).

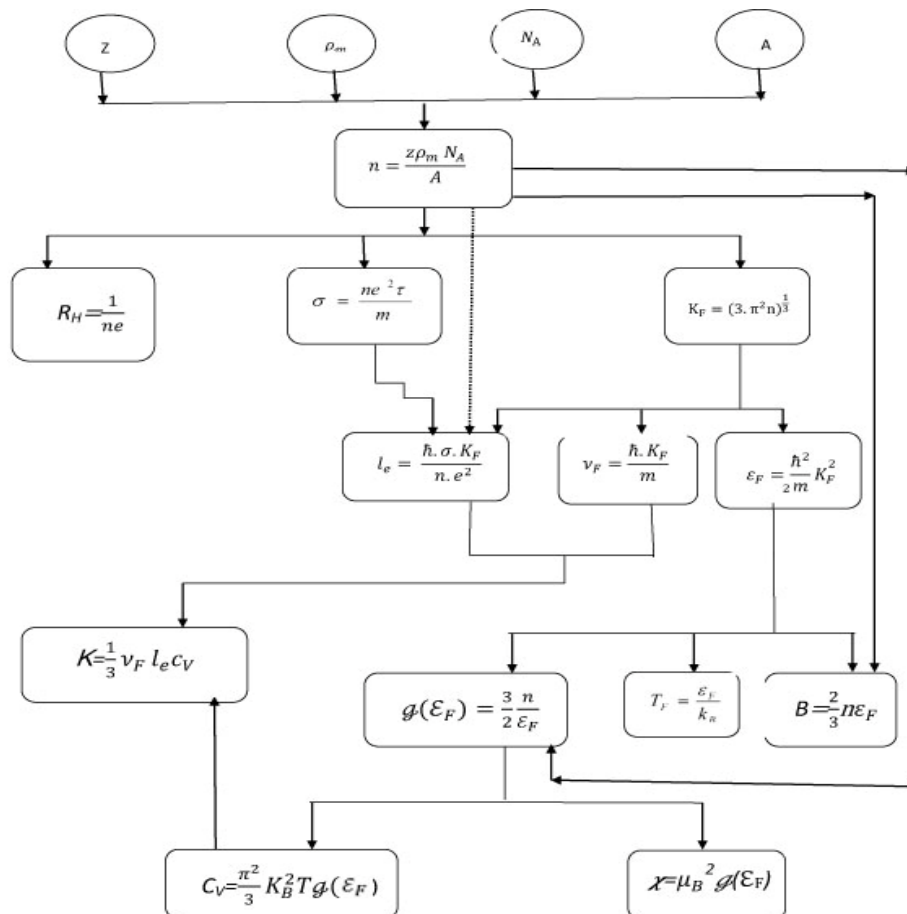


Figure 18: The Interrelation of the Electronic Properties of Metals .

CHAPTER IV

A UNIFIED FORMALISM OF CRYSTALLOGRAPHY OF METALS WITH CUBIC LATTICES

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Introduction

Crystallography is a fundamental cross-disciplinary scientific field. It encompasses a wide range of scientific disciplines including condensed matter physics, solid chemistry, metallurgy and materials science. The teaching of crystallography is usually introduced early in any general textbook of the above-mentioned disciplines due to the fact that many physical properties of certain materials are directly linked to their crystalline structure. Because of the importance of crystallography in those disciplines, its teaching must be made as simple and manageable as possible. This is particularly so since, in the practice of crystallography, many physics and chemistry textbooks frequently assign exercises and problems to determine the geometrical characteristics of crystal structures separately i.e. ignoring correlations between them. This will result in a fragmentary approach involving a lot of computational redundancy. Therefore, it is pedagogically very desirable to avoid this by reducing the calculations involved in obtaining these characteristics. To contribute to this goal, in this chapter I will develop an algorithmic approach to determine the characteristics of cubic lattices in a unified and systematic way. And I will establish here the correlations between these characteristics and show that they can be expressed in terms of only two independent parameters, namely, the coordination number and the lattice constant. The main utility of the present approach consists in generating automatically the whole set of the characteristics of cubic lattices.

The focus here is on the cubic crystal system because many solid materials including most of the metals crystallize in it.

4-1 Derivation of the formulae

From chapter tow, one can easily check that the number of lattice points per unit cell N_u in the three cubic lattices is simply correlated to the coordination number Z as $Z - 2N_u = 4$. Therefore, the generating function of N_u in cubic lattices is given by:

$$N_U(Z) = \frac{Z - 4}{2} \quad (4.1)$$

By establishing Eq.(4.1), one aims to establish further analytical functions relating other characteristics of cubic lattices to the coordination number Z . For this, from the table of (Fig.16), one first rewrites the ratio λ of the atomic radius r to the lattice constant a i.e. $\lambda = r/a$ such that the parameter $\lambda_2 = (4 \lambda)^2$ takes the values 4, 3 and 2 for the SC, BCC and FCC lattices respectively. Similarly, one can establish here that the coordination number Z in the three cubic lattices is correlated to the parameter λ_2 as $Z\lambda_2 = 24$ or equivalently $Z\lambda^2 = \frac{3}{2}$. The generating function of λ in cubic lattices is then given by:

$$\lambda(Z) = \sqrt{\frac{3}{2Z}} \quad (4.2)$$

Replacing v and V_u by their above expressions in Eq.(2.6), the packing fraction P becomes in terms of N_u and λ as:

$$P = \frac{4}{3} \pi N_U \lambda^3 \quad (4.3)$$

By using Eq. (4.1) and Eq. (4.2), P can be expressed in terms of Z as:

$$P(Z) = \sqrt{\frac{3}{2}} \pi \frac{(Z - 4)}{Z^{3/2}} \quad (4.4)$$

One can also check here that the four characteristics Z , N_U , λ and P , in the three cubic lattices, obey the following relation:

$$PZ = 2\pi N_U \lambda \quad (4.5)$$

being mathematically analogous to the well-known state equation $PV = R n T$ characteristic of an ideal gas . This mathematical analogy will help in remembering the form of Eq.(4.5).

Now, from Eq.(4.2), one can deduce the atomic radius r in terms of Z and a as:

$$R(Z, a) = \sqrt{\frac{3}{2Z}} a \quad (4.6)$$

A frequently calculated physical characteristic of crystalline materials is their atomic number density. It is defined as the number of atoms or formula units per unit volume of the material. Crystallographically, it is given by:

$$n_a = \frac{N_U}{V_U} \quad (4.7)$$

Using Eq.(4.1) and replacing V_U by its above expression in Eq.(4.7), the atomic number density n in a cubic lattice can be expressed in terms of Z and a as:

$$n_a(Z, a) = \frac{Z - 4}{2a^3} \quad (4.8)$$

Another frequently calculated physical characteristic of crystalline materials is their mass density, usually denoted by ρ , which can be defined at the atomic scale as:

$$\rho_m = \frac{N_U m_a}{V_U} \quad (4.9)$$

where m_a is the mass of a single atom of the material. By definition, m_a is equal $\frac{A}{N_A}$

where A is the atomic mass and N_A Avogadro's number. Therefore, Eq.(4.9) becomes:

$$\rho_m = \frac{N_U}{V_U} \frac{A}{N_A} \quad (4.10)$$

Using Eq.(4.7), ρ_m will relate to n as :

$$\rho_m = n_a \frac{A}{N_A} \quad (4.11)$$

Using the expression of n given by Eq.(4.8), the mass density ρ of a cubic lattice can be expressed in terms of Z and a as:

$$\rho_m(Z, a) = \frac{Z - 4}{2a^3} \frac{A}{N_A} \quad (4.12)$$

Another variant of Eq.(4.12) written in the following form :

$$Z = 4 + 2 \frac{N_A \rho_m a^3}{A} \quad (4.13)$$

will help in determining experimentally the coordination number Z to identify the type of the cubic lattice of the considered crystalline material whose ρ_m in Eq.(4.13) is now its measured mass density by any standard experimental method.

For an automatic generation of the characteristics of cubic lattices defined here, one can write a short program using one's preferred programming language. A typical Mathematica procedure for that purpose is shown in Figure (19). The output of this procedure is displayed as a table given by Figure 20.

```

CN[Z_] := Z
NU[Z_] := (CN[Z] - 4) / 2

λ[Z_] := Sqrt[3 / (2 CN[Z])]

P[Z_] := (4 π / 3) NU[Z] λ[Z]^3
r[Z_, a_] := λ[Z] * a
n[Z_, a_] := NU[Z] / a^3
ρ[Z_, a_] := n[Z, a] * (A / NA)

TableForm[
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   "SC_Value", "BCC_Value", "FCC_Value"}}]
(*N.B.: a is the_lattice_constant, A the_Atomic_Mass and NA Avogadro_Number*)

```

Figure 19: A Mathematica procedure for generating the characteristics of cubic lattices.

	Characteristic's_Name	Generating_Function	SC_Value	BCC_Value	FCC_V
1	Coordination_Number	Z	6	8	12
2	Number_of_Lattice_Points_per_Unit_Cell	$\frac{Z-4}{2}$	1	2	4
3	Ratio_of_Atomic_Radius_to_Lattice_Constant	$\sqrt{\frac{3}{2}} \sqrt{\frac{1}{Z}}$	$\frac{1}{2}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{2\sqrt{2}}$
4	Packing_Fraction	$\sqrt{\frac{3}{2}} \pi (Z-4) \left(\frac{1}{Z}\right)^{3/2}$	$\frac{\pi}{6}$	$\frac{\sqrt{3}\pi}{8}$	$\frac{\pi}{3\sqrt{2}}$
5	Atomic_Radius	$\sqrt{\frac{3}{2}} a \sqrt{\frac{1}{Z}}$	$\frac{a}{2}$	$\frac{\sqrt{3}a}{4}$	$\frac{a}{2\sqrt{2}}$
6	Number_Density	$\frac{Z-4}{2a^3}$	$\frac{1}{a^3}$	$\frac{2}{a^3}$	$\frac{4}{a^3}$
7	Mass_Density	$\frac{A(Z-4)}{2a^3 N_A}$	$\frac{A}{a^3 N_A}$	$\frac{2A}{a^3 N_A}$	$\frac{4A}{a^3 N_A}$

Figure 20: Characteristics of cubic lattices generated by the Mathematica procedure shown in figure(19).

CHAPTER V

A UNIFIED FORMALISM OF ELECTRONIC AND THERMAL PROPERTIES OF METALS WITH CUBIC LATTICES

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Introduction

In this chapter, I will develop an algorithmic approach to determine the electronic properties of metals with cubic lattice in a unified and systematic way. And I will establish here the correlations between these electronic properties and show that they can be expressed in terms of only three independent parameters, namely, the coordination number, the lattice constant and the valence of element. The main utility of the present approach consists in generating automatically the whole set of electronic properties of cubic lattices.

Also, I will establish correlations between the thermal properties of metals with cubic lattice, and show that they can be expressed in terms of only two independent parameters, namely, the coordination number and the lattice constant.

The advantage of this approach is that researchers need only to memorize the relevant generating functions of these electronic and thermal properties and to determine correctly the coordination numbers of cubic lattices in order to get the desired results.

5-1 Electronic properties of metals with cubic structure

The number of electrons per cubic centimeter (electronic density n) is given by :

$$n_e = zn_a \quad (5.1)$$

By using Eq.(4.8) ,one can rewrite Eq.(5.1) in terms of z (electron valence) , Z (coordination number) , a (constant lattice) as follows:

$$n_e = \frac{z(Z - 4)}{2a^3} \quad (5.2)$$

Now, using Eq. (5.2), we can write the electronic proprieties of a metal with cubic structure as function of Z , z , a .

Substituting Eq.(5.2) into Eq.(1.26),one finds The Fermi vector k_F as:

$$k_F = \pi^{2/3} \left[\frac{3z(Z - 4)}{2a^3} \right]^{1/3} \quad (5.3)$$

Also, using Eq.(5.2), we can rewrite Hall constant as:

$$R_H = \frac{2a^3}{ze(Z - 4)} \quad (5.4)$$

Substituting k_F from Eq. (5.3) into the expression of the Fermi momentum $p_F = mv_F = \hbar k_F$ we find the Fermi velocity as:

$$v_F = \frac{\pi^{2/3} \hbar}{m} \left[\frac{3z(Z - 4)}{2a^3} \right]^{1/3} \quad (5.5)$$

where m is the mass of electron \hbar is the Planck's constant.

Substituting Eq. (5.3) into Eq.(1.18),one finds The Fermi energy as following:

$$\varepsilon_F = \frac{\pi^{4/3} \hbar^2}{2m} \left[\frac{3z(Z - 4)}{2a^3} \right]^{2/3} \quad (5.6)$$

Substituting Eq.(5.2) and Eq.(5.6) into Eq.(1.24),one gets the density of levels at the Fermi energy as

$$g(\varepsilon_F) = \frac{\pi^{-4/3}m}{\hbar^2} \left[\frac{3z(Z-4)}{2a^3} \right]^{1/3} \quad (5.7)$$

Substituting Eq. (5.6) into Eq.(3.27) ,one gets The Fermi temperature as:

$$T_F = \frac{\pi^{4/3}\hbar^2}{2mk_B} \left[\frac{3z(Z-4)}{2a^3} \right]^{2/3} \quad (5.8)$$

And Substituting Eq.(5.2) and Eq.(5.6) into Eq.(1.23),one gets the Bulk modulus B as:

$$B = \frac{2\pi^{4/3}\hbar^2}{9mk_B} \left[\frac{3z(Z-4)}{2a^3} \right]^{5/3} \quad (5.9)$$

We can find the Pauli paramagnetic susceptibility by substituting Eq.(5.2) into Eq.(1.25) as:

$$\chi = \frac{\pi^{-4/3}m\mu_B^2}{\hbar^2} \left[\frac{3z(Z-4)}{2a^3} \right]^{5/3} \quad (5.10)$$

Also, one gets to the specific heat of a metal in terms of z(electron valence) ,Z(coordination number) ,a(constant lattice) ,by Substituting Eq.(5.2) into Eq.(1.26) :

$$C_e = \frac{\pi^{2/3}mk_B^2T}{3\hbar^2} \left[\frac{3z(Z-4)}{2a^3} \right]^{5/3} \quad (5.11)$$

one can write a program using Mathematica program language to generate electronic properties of metals as follows:

$$\text{CN}[Z_] := Z$$

$$\text{NU}[Z_] := \frac{\text{CN}[Z] - 4}{2}$$

$$n_a[Z_ , a_] := \frac{\text{NU}[Z]}{a^3}$$

$$n_e[Z_ , a_ , z_] := \frac{z * \text{NU}[Z]}{a^3}$$

$$K_F[Z_ , a_ , z_] := \pi^{2/3} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{1/3}$$

$$v_F[Z_ , a_ , z_] := \frac{\hbar * \pi^{2/3}}{m} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{1/3}$$

$$\mathcal{E}_F[Z_ , a_ , z_] := \frac{\hbar^2 * \pi^{4/3}}{2 * m} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{2/3}$$

$$D_F[Z_ , a_ , z_] := \frac{3 * m * \pi^{-4/3}}{\hbar^2} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{1/3}$$

$$T_F[Z_ , a_ , z_] := \frac{\hbar^2 * \pi^{4/3}}{2 * m * k_B} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{2/3}$$

$$B[Z_ , a_ , z_] := \frac{2 * \hbar^2 * \pi^{4/3}}{9 * m * k_B} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{5/3}$$

$$c_v[Z_ , a_ , z_] := \frac{m * k_B^2 * \pi^{2/3} T}{\hbar^2} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{5/3}$$

$$\chi[Z_ , a_ , z_] := \frac{m * \mu_B^2 * \pi^{-4/3}}{3 * \hbar^2} * \left(\frac{3 * z}{a^3} * \text{NU}[Z] \right)^{5/3}$$

$$R_H[Z_ , a_ , z_] := \frac{a^3}{e * z * \text{NU}[Z]}$$

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2 | *electronic properties.nb*

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 RH[6, a, z], RH[8, a, z], RH[12, a, z]]},
TableHeadings -> {Automatic,
 {"Electronic_Property's_Name", "Generating_Function",
 "SC_Value", "BCC_Value"}]}

```

	Electronic_Property's_Name	Generating_Function	SC_Value	BCC_Value
1	Coordination_Number	Z	6	8
2	Number_of_Lattice_Points_per_Unit_Cell	$\frac{Z-4}{2}$	1	2
3	Atomic_Density	$\frac{Z-4}{2 a^3}$	$\frac{1}{a^3}$	$\frac{2}{a^3}$
4	Electronic_density	$\frac{z (Z-4)}{2 a^3}$	$\frac{z}{a^3}$	$\frac{2 z}{a^3}$
5	Fermi_Vector	$\sqrt{\frac{3}{2}} \pi^{2/3} \sqrt{\frac{z (Z-4)}{a^3}}$	$3^{1/3} \pi^{2/3} \left(\frac{z}{a^3}\right)^{1/3}$	$6^{1/3} \pi^{2/3} \left(\frac{z}{a^3}\right)^{1/3}$
6	Fermi_Velocity	$\frac{\sqrt{\frac{3}{2}} \pi^{2/3} \sqrt{\frac{z (Z-4)}{a^3}} \hbar}{m}$	$\frac{3^{1/3} \pi^{2/3} \left(\frac{z}{a^3}\right)^{1/3} \hbar}{m}$	$\frac{6^{1/3} \pi^{2/3} \left(\frac{z}{a^3}\right)^{1/3} \hbar}{m}$
7	Fermi_Energy	$\frac{\left(\frac{3}{2}\right)^{2/3} \pi^{4/3} \left(\frac{z (Z-4)}{a^3}\right)^{2/3} \hbar^2}{2 m}$	$\frac{3^{2/3} \pi^{4/3} \left(\frac{z}{a^3}\right)^{2/3} \hbar^2}{2 m}$	$\frac{3^{2/3} \pi^{4/3} \left(\frac{z}{a^3}\right)^{2/3} \hbar^2}{2^{1/2} m}$
8	Density_of_Energy	$\frac{3 \sqrt{\frac{3}{2}} \pi m \sqrt{\frac{z (Z-4)}{a^3}}}{\pi^{4/3} \hbar^2}$	$\frac{3 \cdot 3^{1/3} m \left(\frac{z}{a^3}\right)^{1/3}}{\pi^{4/3} \hbar^2}$	$\frac{3 \cdot 6^{1/3} m \left(\frac{z}{a^3}\right)^{1/3}}{\pi^{4/3} \hbar^2}$
9	Fermi_temperature	$\frac{\left(\frac{3}{2}\right)^{2/3} \pi^{4/3} \left(\frac{z (Z-4)}{a^3}\right)^{2/3} \hbar^2}{2 m k_B}$	$\frac{3^{2/3} \pi^{4/3} \left(\frac{z}{a^3}\right)^{2/3} \hbar^2}{2 m k_B}$	$\frac{3^{2/3} \pi^{4/3} \left(\frac{z}{a^3}\right)^{2/3} \hbar^2}{2^{1/2} m k_B}$
10	Bulk_modulus	$\frac{\pi^{4/3} \left(\frac{z (Z-4)}{a^3}\right)^{5/3} \hbar^2}{2^{2/3} \sqrt{3} m k_B}$	$\frac{2 \pi^{4/3} \left(\frac{z}{a^3}\right)^{5/3} \hbar^2}{3^{2/3} m k_B}$	$\frac{4 \cdot 2^{2/3} \pi^{4/3} \left(\frac{z}{a^3}\right)^{5/3} \hbar^2}{3^{2/3} m k_B}$
11	Specific_Heat	$\frac{3 m \left(\frac{3 \pi}{2}\right)^{2/3} T \left(\frac{z (Z-4)}{a^3}\right)^{5/3} k_B^5}{2 \hbar^2}$	$\frac{3 m (3 \pi)^{2/3} T \left(\frac{z}{a^3}\right)^{5/3} k_B^5}{\hbar^2}$	$\frac{4 \cdot 2^{2/3} \pi^{4/3} m \left(\frac{z}{a^3}\right)^{5/3} k_B^5}{3^{1/2} m k_B}$
12	Pauli_Paramagnetic_suscpitibility	$\frac{\left(\frac{3}{2}\right)^{2/3} \pi m \left(\frac{z (Z-4)}{a^3}\right)^{5/3} \mu_B^2}{2 \pi^{4/3} \hbar^2}$	$\frac{3^{2/3} m \left(\frac{z}{a^3}\right)^{5/3} \mu_B^2}{\pi^{4/3} \hbar^2}$	$\frac{2 \cdot 6^{2/3} m \left(\frac{z}{a^3}\right)^{5/3} \mu_B^2}{\pi^{4/3} \hbar^2}$
13	Hall_Constant	$\frac{2 a^3}{z (Z-4)}$	$\frac{a^3}{z}$	$\frac{a^3}{2 z}$

5-2 Thermal properties of metals with cubic structure

Also, we write thermal properties of metals with cubic structure in terms of Z, a .

Recall the density of ions that is given by Eq.(1.38),

And, we have a relation relating between n_i (ionic density) and n_e (electronic density), it is given by:

$$n_e = zn_i \quad (5.12)$$

where z is the valence of the metal.

Substituting n_e from Eq.(3.5), and Eq.(1.38) into Eq.(5.12), one gets the relation between k_F, k_D as:

$$k_D = \left(\frac{2}{Z}\right)^{1/3} k_F \quad (5.13)$$

Substituting Eq.(5.3) into Eq.(5.13), one finds k_D in terms of Z, a as:

$$k_D = \pi^{2/3} \left[\frac{3(Z-4)}{a^3} \right]^{1/3} \quad (5.14)$$

Recall the Debye frequency that is given by Eq.(1.37).

Substituting Eq.(5.14) into Eq.(1.37), it becomes as following:

$$\omega_D = \pi^{2/3} v_s \left[\frac{3(Z-4)}{a^3} \right]^{1/3} \quad (5.15)$$

Also, we have the Debye temperature that is given by Eq.(1.40)

Substituting Eq.(5.15) into Eq.(1.40), one gets

$$T_D = \pi^{2/3} v_s \frac{\hbar}{k_B} \left[\frac{3(Z-4)}{a^3} \right]^{1/3} \quad (5.16)$$

The saturation magnetization of ferromagnetic of metals with cubic structure is given by:

$$M_s = \mu_B n_B n_a \quad (5.17)$$

Where μ_B is the Bohr magnetron, n_B is the Bohr number, n_a is the atomic density. We can write the saturation magnetization of ferromagnetic of metals with cubic structure in terms of Z (coordination number) and, a (constant lattice) as follows:

Substituting Eq.(4.8) into Eq.(5.17), one gets

$$M_s = \mu_B n_B \left(\frac{Z-4}{2a^3} \right) \quad (5.18)$$

one can write a program using Mathematica program language to generate thermal properties of metals as follows:

```

(*This is an algorithmic thermal properties of cubic lattices *)
CN[Z_] := Z
NU[Z_] := (CN[Z] - 4) / 2
KD[Z_, a_] := π2/3 * (6 * NU[Z])1/3
WD[Z_, a_] := C * KD[Z, a]
TD[Z_, a_] := (ħ * WD[Z, a]) / KB
TableForm[
{
{"Coordination_Number", TraditionalForm[CN[Z]], CN[6], CN[8], CN[12]},
{"Number_of_Lattice_Points_per_Unit_Cell",
TraditionalForm[NU[Z]], NU[6], NU[8], NU[12]},
{"Debye_Vector", TraditionalForm[KD[Z, a]], KD[6, a], KD[8, a], KD[12, a]},
{"Debye_Frequency", TraditionalForm[WD[Z, a]], WD[6, a], WD[8, a], WD[12, a]},
{"Debye_temperature", TraditionalForm[TD[Z, a]], TD[6, a], TD[8, a], TD[12, a]}},
TableHeadings -> {Automatic, {"Properties's_Name", "Generating_Function",
"SC_Value", "BCC_Value", "FCC_Value"}}]
(*N.B.: a is the_lattice_constant, A the_Atomic_Mass and NA Avogadro_Number*)

```

	Properties's_Name	Generating_Function	SC_Value	BCC_Value	FCC_Va
1	Coordination_Number	Z	6	8	12
2	Number_of_Lattice_Points_per_Unit_Cell	$\frac{Z-4}{2}$	1	2	4
3	Debye_Vector	$\sqrt{3} \pi^{2/3} \sqrt{Z-4}$	$6^{1/3} \pi^{2/3}$	$3^{1/3} (2\pi)^{2/3}$	$2 \cdot 3^{1/3} \pi$
4	Debye_Frequency	$\sqrt{3} C \pi^{2/3} \sqrt{Z-4}$	$6^{1/3} C \pi^{2/3}$	$3^{1/3} C (2\pi)^{2/3}$	$2 \cdot 3^{1/3} C$
5	Debye_temperature	$\frac{\sqrt{3} C \pi^{2/3} \sqrt{Z-4} \hbar}{k_B}$	$\frac{6^{1/3} C \pi^{2/3} \hbar}{k_B}$	$\frac{3^{1/3} C (2\pi)^{2/3} \hbar}{k_B}$	$\frac{2 \cdot 3^{1/3} C \hbar}{k_B}$

CONCLUSION

Conclusion

In this thesis, I have developed a unified formulation approach for determining the electronic properties of metals. And I have established the correlations between electronic properties of metals, and show that they can be expressed in terms of only three independent parameters, namely, the atomic mass, the mass density and the valence of element.

And, I have established a chart that shows most of the electronic properties of a metal in a specific order that is expected to enable scholars to get these electronic properties by knowing only the basic characteristic of a metal.

Also, I have shown that the electron mean free path l_e in a metallic sample can be parameterized in terms of known characteristic sample parameters and directly measurable quantities. This parameterization makes the evaluation of l_e much simpler. Also, by proposing the present method of the measurement of l_e in a metallic sample, I am not seeking the precise determination of the sample purity but mainly focusing on the pedagogical aspect of the method illustrating how a characteristic microscopic length in the sample namely l_e can be used to get an approximate indicator of a macroscopic characteristic i.e. the sample purity.

I have developed a unified algorithmic approach for determining the characteristics of cubic lattices. And I have established the correlations between these characteristics and show that they can be expressed in terms of only two independent parameters, namely, the coordination number and the lattice constant. The main utility of the present approach consists in generating automatically the whole set of the characteristics of cubic lattices.

And I have established the correlations between electronic properties of metals, and show that they can be expressed in terms of only three independent parameters, namely, the coordination number, the lattice constant and the valence of element.

REFERENCES

References

- [1] J.S.Blakemore,"*Solid State Physics*", Cambridge University press, 1987.
- [2] H.P.Myers,"*Solid State Physics*», (Taylor & Francis, London), 1997.
- [3] H.M.Omar,"*Elementary Solid State Physics*", Adison Wesley, 1993.
- [4] H.M.Rosenbery,"*The Solid State*», Oxford University Press,1997.
- [5] P.M.Chaikin and T.C.Lubensky,"*Principle of Condensed Matter Physics*", Combridge University Press, 1995.
- [6] W.A.Harrison,"*Solid State Theory*", Dover, 1980.
- [7] H.Ibach and H.Lüith,"*Solid State Physics*", Springer-Veriag, 1990.
- [8] A.Ishara," *Condensed Matter Physics*", Oxford University Press, 1991.
- [9] N.W. Ashcroft and N.D. Mermin, "*Solid State Physics*", (Saunders College HRW, 1976)
- [10] C. Kittle, "*Introduction to Solid State Physics*", (J. Wiley & Sons, Inc., 1976), 5th edition.
- [11] The electron diffusion in a metal is satisfactorily explained by the random walk model which is treated in detail in any self-contained statistical mechanics textbook. See e.g. L.E. Reichl, *A Modern Course in Statistical Mechanics* (Wiley-Interscience, 1998), 2nd Edition.
- [12] For a clear development of the Drude model for the electron conduction in metals, one can consult Chapter 1 from the excellent Ref. [9]
- [13] M.P. Marder, *Condensed Matter Physics* (J. Wiley & Sons, Inc., 2000), pp. 141--142

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- [14] W. Benenson, J.W. Harris, H. Stocker and H. Lutz, *Handbook of Physics* (Springer-Verlag, New York, Inc., 2002) p. 1004
- [15] Ref. [10] pp. 171—172
- [16] W. A. Harrison, "*Electronic Structure and the Properties of Solids*", Dover Publications, 1989.
- [17] J. S. Dugdale, "*The Electrical Properties of Metals and Alloys*", Edward Arnold, London, 1977.
- [18] F. J. Blatt, "*Physics of Electronic Conduction in Solids*", McGraw-Hill Book Company, New York, 1968.
- [19] H. T. Stokes, "*Solid State Physics*", Provo, Utah: Brigham Young University, 3rd edn. 2000.
- [20] T. H. K. Barron and G. K. White, "*Heat Capacity and Thermal Expansion at Low Temperatures*", New York: Kluwer Academic/Plenum Publishers, 1999.
- [21] E. S. R. Gopal, "*Specific Heats at Low Temperatures*", New York: Plenum Press, 1966.
- [22] M.C.Lovell, A.J.Avery, M.W.Vernon, "*Physical Properties of Materials*", Van Nostrand Reinhold, 1983.
- [23] J.Sólyom, "*Fundamentals of the Physics of Solids*", Springer-Verlag, 2003.
- [24] A.C.Lawson, B.Martinez, J.A.Roberts, J.W.Richardson, Jr., and B.I .Bennett, "*Atomic Vibrations and Melting in Plutonium*", Los Alamos Science, 26, 2000, pp(193).
- [25] J. D. Patterson and B. C. Bailey "*Solid State Physics*", Springer-Verlag Berlin Heidelberg, 2007.
- [26] E. A. Irene "*Electronic Materials Science*", John Wiley & Sons, Inc., Hoboken, New Jersey, 2005.
- [27] A.P.Cracknell, "*Crystals and Their structures*", Oxford Pergamon Press, 1969.

- [28] W.R.Beam," *Electronic of Solids* ", New York Mc Graw Hill, 1965.
- [29] N.F.Mott and H.Jones," *The Theory of the Properties of Metals and Alloys* ", New York, Dover Publications Inc, 1958.
- [30] C.A.Wert and R.M.Thomson," *Physics of Solids* ", New York, Mc Graw Hill, 1964.
- [31] I.M.Lifshits, M.Ya.Azbel and M.I.Kaganov," *Electron Theory of Metals*", Consultants Bureau, 1973.
- [32] A.A.Abrikosov, "*Fundamentals of The Theory of Metals* ",North-Holland, 1988.
- [33] D.Shoenberg, "*Electrons at The Fermi Surface*", Combrige University Press, 1980.