Intro to Condensed Matter Physics

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Abstract

This document is a comprehensive summary of the physics textbook Solid State Physics by Ashcroft and Mermin. This midterm report covers the first 4 chapters and concepts presented in the textbook, providing a concise and clear overview.

Table of contents

${\bf Contents}$

1	Cha	apter 1: Drude Theory of metals	2
	1.1	Assumptions	2
		1.1.1 Basic Assumptions	2
	1.2	Electrical Predictions	3
		1.2.1 DC Electrical Conductivity	3
		1.2.2 Hall Effect and Magnetoresistance	3
	1.3	Thermal Predictions	4
		1.3.1 Thermal Conductivity	4
		1.3.2 Thermoelectric Effects	5
2	Cha	apter 2: The Sommerfeld Theory of Metals	6
	2.1	Introduction	6
		2.1.1 Fermi-Dirac Statistics	6
		2.1.2 Free Electrons	6
	2.2	Calculations	7
		2.2.1 Fermi Momentum, Energy, and Temperature	7
	2.3	Implications	7
		2.3.1 Sommerfeld Theory of Conduction	7
	2.4	Failures of the free electron model	8
3	Cha	apter 3: Crystal lattices	9
	3.1	Introduction	9
		3.1.1 Bravais Lattices	9
		3.1.2 Primitive Unit Cell	9
		3.1.3 Wigner-Seitz Primitive Cell	10
4	Cha	apter 4: The Reciprocal Lattice	11
	4.1	Role of Reciprocal Lattice	11
	4.2	Definitions and Examples	11
	4.3	First Brillouin Zone	11
	4.4		11
	4.5	Miller Indices	

1 Chapter 1: Drude Theory of metals

1.1 Assumptions

1.1.1 Basic Assumptions

The basic assumptions of the Drude model are as follows:

- 1. Independent electron approximation: Between collisions, the interaction of a given electron with other electrons and ions is neglected. Therefore, in the absence of external electromagnetic fields, each electron moves uniformly in a straight line. When external fields are present, each electron's motion is governed by Newton's laws, influenced only by those external fields, while ignoring the additional complex fields produced by other electrons and ions. Neglecting electron-electron interactions between collisions is referred to as the independent electron approximation. Similarly, ignoring electron-ion interactions is called the free electron approximation.
- 2. Collisions, akin to those described in kinetic theory, are treated as instantaneous events that abruptly change an electron's velocity. Drude attributed these collisions to electrons bouncing off impenetrable ion cores, rather than electron-electron collisions, which are the main collision mechanism in a typical gas. It is found that electron-electron scattering is generally one of the least significant scattering mechanisms in metals, except under unusual conditions.
- 3. We shall assume that an electron experiences a collision (i.e.. suffers an abrupt change in its velocity) with a probability per unit time $\frac{dt}{\tau}$. We mean by this that the probability of an electron undergoing a collision in any infinitesimal time interval of length dt is just $\frac{dt}{\tau}$. The time τ is variously known as the relaxation time, the collision time, or the mean free time. and it plays a fundamental role in the theory of metallic conduction. It follows from this assumption that an electron picked at random at a given moment will, on the average, travel for a time τ before its next collision, and will on the average, have been travelling for a time τ since its last collision. In the simplest applications of the Drude model the collision time t is taken to be independent of an electron's position and velocity. We shall see later that this tums out to be a surprisingly good assumption for many (but by no means all) applications.
- 4. Electrons are assumed to reach thermal equilibrium with their surroundings only through collisions. These collisions maintain local thermodynamic equilibrium in a simplified manner: immediately after a collision, an electron's velocity is not correlated with its pre-collision velocity, but is randomly directed with a speed appropriate to the local temperature at the collision site. Consequently, the higher the temperature of the region where the collision occurs, the faster the typical post-collision electron speed.

1.2 Electrical Predictions

1.2.1 DC Electrical Conductivity

The drude model provides an estimate of the relaxation time where:

$$\tau = \frac{m}{\tau m e^2}$$

thus the mean relaxation time should have the inverse temperature dependence compared to the resistivity. Additionally using room temperature resistivities of order of microohm-centimetres, we get mean free paths of around 1 to 10 angstrom, quite consistent with the interatomic spacing. However, we shall see in Chapter 2 that this classical estimate of τ is an order of magnitude too small at room temperatures.

Fortunately, the Drude model can still be utilized without a precise understanding of the causes of collisions. Without a theory for the collision time, it becomes crucial to identify predictions of the Drude model that do not depend on the relaxation time τ . Several such τ -independent quantities exist and remain of fundamental interest today. In many ways, the exact quantitative treatment of the relaxation time remains the weakest aspect of modern theories of metallic conductivity. Therefore, τ -independent quantities are highly valued, as they often yield much more reliable information.

1.2.2 Hall Effect and Magnetoresistance

The equation of motion of any particular electron based on the effect of any time dependent force on it is as follows:

$$\frac{dp(t)}{dt} = -\frac{p(t)}{\tau} + f(t)$$

This essentially means that the effect of individual electron collisions introduces a frictional damping term into the equation of motion for the momentum per electron. The magnetoresistance, which is the ratio of the electric field along the x-axis to the current density in the same direction, has been observed to be independent of the field. The strength of the transverse field is also of interest, as it is proportional to the applied field H and the current density along the wire. Consequently, we can define a quantity known as the Hall coefficient, expressed as

$$R_H = \frac{E_y}{J_x H}$$

In terms of other known quantities we can find the Hall coefficient to be

$$R_H = -\frac{1}{nec}$$

This is a very striking result, as it indicates that the Hall coefficient is dependent solely on the density of carriers, with no other parameters of the metal playing a role. Given that we have already calculated n by assuming the atomic valence electrons become the metallic conduction electrons, measuring the Hall constant provides a direct test of this assumption.

When attempting to determine the electron density from measured Hall coefficients, one encounters the issue that, contrary to the Drude model prediction, the Hall coefficients generally depend on the magnetic field. Additionally, they are influenced by temperature and the quality of sample preparation. This outcome is somewhat unexpected because the relaxation time τ can significantly depend on temperature and the condition of the sample. However, at very low temperatures in extremely pure, well-prepared samples subjected to very high fields, the measured Hall constants tend to approach a limiting value. The more sophisticated theory presented in later chapters predicts that for many (but not all) metals, this limiting value precisely corresponds to the simple Drude result.

1.3 Thermal Predictions

1.3.1 Thermal Conductivity

One of the most remarkable achievements of the Drude model upon its introduction was its ability to explain the empirical Wiedemann-Franz law (1853). This law states that the ratio K/σ of thermal conductivity to electrical conductivity in numerous metals is directly proportional to temperature, with a proportionality constant that is approximately the same for all metals. This striking regularity is evident in conductivity tables, where the measured thermal conductivities are provided for various metals at temperatures of 273 K and 373 K, alongside the corresponding ratios $\frac{K}{\sigma}$ (referred to as the Lorenz number) at these temperatures.

To account for this phenomenon, the Drude model posits that the majority of the thermal current in a metal is carried by the conduction electrons. This assumption stems from the empirical observation that metals exhibit much higher heat conductivity compared to insulators. Consequently, thermal conduction by the ions (present in both metals and insulators) is significantly less significant than thermal conduction by the conduction electrons (found exclusively in metals).

It was natural for Drude to apply the classical ideal gas laws to evaluating the electronic specific heat and mean square velocity. He therefore in effect took C_v to be $1.5*nk_B$ and $1_{\overline{2}}$ mv² to be $1.5*k_B*T$ where kb is Boltzmann's constant, $1.38X10^-16erg/K$ This leads to the result:

$$\frac{K}{\sigma} = \frac{3 * k_b^2 * T}{2 * e^2}$$

The right side is proportional to T and depends only one universal constants in complete agreement with the Wiedemann and Franz. and this gives us a lorenz number as $1.11x10^-8watt - ohm/K^2$

This success. though wholly fortuitous. was so impressive as to spur further investigations with the model. It was, however, quite puzzling, since no electronic contribution to the specific heat remotely comparable was ever observed. Indeed, at room temperature there appeared to be no electronic contribution to the specific heat measured at all.

1.3.2 Thermoelectric Effects

This leads us to consider another physical phenomenon: When a temperature gradient exists in a long, thin bar, it should be accompanied by an electric field directed opposite to the temperature gradient, a phenomenon known as the thermoelectric field (or the Seebeck effect). Conventionally, this field is expressed as:

$$E = Q\nabla T$$

Observed thermoelectric voltages in metals at room temperature are typically on the order of microvolts per degree, which is about 100 times smaller. This discrepancy mirrors the 100-fold error encountered twice in Drude's derivation of the Wiedemann-Franz law. However, in this case, the error is not compensated, providing clear evidence of the inadequacy of classical statistical mechanics in describing the behavior of the metallic electron gas.

The application of quantum statistical mechanics helps resolve this discrepancy. However, in certain metals, the sign of the thermoelectric voltage—the direction of the thermoelectric field—opposes the prediction of the Drude model. This inconsistency is as perplexing as the discrepancies observed in the sign of the Hall coefficient. While the quantum theory of solids can explain a reversal in the thermoelectric voltage's sign, the absence of a truly quantitative theory for the thermoelectric field tempers one's sense of achievement in this regard.

2 Chapter 2: The Sommerfeld Theory of Metals

2.1 Introduction

2.1.1 Fermi-Dirac Statistics

In the era of Drude and for subsequent years, it was deemed reasonable to assume that the electronic velocity distribution, akin to that of an ordinary classical gas with density n = N/V, was governed in equilibrium at temperature T by the Maxwell-Boltzmann distribution.

As discussed in Chapter I, this assumption, when coupled with the Drude model, resulted in reasonably accurate predictions, notably aligning with the Wiedemann-Franz law. However, it also predicted an additional contribution to the specific heat of a metal, k_B per electron, which was not observed. This paradox cast doubt on the Drude model for a significant period, until the advent of quantum theory, which recognized that for electrons, the Pauli exclusion principle necessitated replacing the Maxwell-Boltzmann distribution with the Fermi-Dirac distribution:

$$f(v) = \frac{m^3}{4h^3\pi^3(1 + e^{(0.5mv^2 - k_B T_0)/k_B T})}$$

To justify both the application of the Fermi-Dirac distribution and its integration into an otherwise classical theory, a thorough examination of the quantum theory of the electron gas is required.

For simplicity, we shall initially focus on the ground state (i.e., T=0) of the electron gas before exploring its behavior at nonzero temperatures. Surprisingly, the properties of the ground state are inherently significant in themselves. At room temperature, the electron gas at metallic densities behaves akin to a very low temperature, nearly indistinguishable from T=0. Consequently, many electronic properties of a metal hardly deviate from their values at T=0, even under room temperature conditions.

2.1.2 Free Electrons

The task at hand is to compute the ground-state properties of N electrons confined within a volume V. Due to the assumption of independent electron approximation, we can determine the electron system's ground state by initially identifying the energy levels of a single electron within volume V, and subsequently filling these levels in accordance with the Pauli exclusion principle, allowing at most one electron per energy level.

A single electron's description involves its wave function $\psi(\mathbf{r})$ and specification of its spin orientation. In the absence of interactions, the wave function associated with an energy level E satisfies the time-independent Schrödinger equation:

$$H\psi = E\psi$$

where H represents the kinetic energy term constructed from the Laplacian operator.

2.2 Calculations

2.2.1 Fermi Momentum, Energy, and Temperature

The expressions for Fermi momentum, energy, and temperature can be derived as follows:

$$n = \frac{k_F^3}{3\pi^2}$$

$$\epsilon_F = \frac{h^2 k_F^2}{2m}$$

$$T_F = \frac{\epsilon_F}{k_B}$$

These expressions are obtained from the observation of density states in momentum space, where energy exhibits quadratic dependence on momentum and a fixed number of particles per unit volume n.

2.3 Implications

2.3.1 Sommerfeld Theory of Conduction

Sommerfeld revisited the Drude model, replacing the classical Maxwell-Boltzmann velocity distribution with the Fermi-Dirac distribution. The use of a quantum-mechanical velocity distribution within a classical framework requires justification. The behavior of a metallic electron is well described by classical mechanics if its position and momentum can be specified with sufficient accuracy, without violating the uncertainty principle.

However, it is not immediately obvious that the dynamics of N electrons can be described classically, given the profound impact of the Pauli exclusion principle on their statistics. Despite this, an elementary theorem, though not proved here due to its cumbersome notation, demonstrates that the dynamics of N electrons are not as profoundly affected by the exclusion principle as their statistics.

The use of Fermi-Dirac statistics only affects predictions of the Drude model that rely on knowledge of the electronic velocity distribution. If the collision rate $1/\tau$ does not depend on energy, then the estimation of electronic mean free path and calculations of thermal conductivity and thermopower are the only affected quantities.

While Drude's overestimation of thermal conductivity is rectified by Sommerfeld's theory, thermopower is similarly overestimated, requiring a reduction by a factor of 100. The predictions of the Drude model regarding DC or AC conductivities, Hall coefficient, and magnetoresistance remain unchanged regardless of whether Maxwell-Boltzmann or Fermi-Dirac statistics are employed.

However, incorporating an energy-dependent relaxation time into calculations, as suggested by Lorentz, results in temperature dependence in DC and AC conductivities, non-vanishing magnetoresistance, and field- and temperature-dependent Hall coefficient. Yet, when employing the correct Fermi-Dirac velocity distribution, the impact of energy-dependent relaxation time on most quantities of interest in metals is minimal, as these quantities are primarily determined by electron scattering near the Fermi level.

2.4 Failures of the free electron model

- 1. Inadequacies in Free Electron Transport Coefficients:
 - (a) Hall Coefficient: According to free electron theory, the Hall coefficient should have a constant value of $R_H = -1/ne$ at metallic electron densities, independent of temperature, relaxation time, or magnetic field strength. However, observed Hall coefficients typically vary with magnetic field strength and temperature, sometimes dramatically. In many cases, such as aluminum, the observed Hall coefficient is significantly different from the free electron theory prediction and may even have the opposite sign at high magnetic fields. Alkali metals are the only ones that closely adhere to the predictions of free electron theory.
 - (b) Magnetoresistance: Free electron theory predicts that the resistance of a wire perpendicular to a uniform magnetic field should not depend on the field strength. However, in almost all cases, it does. In some metals, like copper, silver, and gold, the resistance can increase seemingly without limit as the field strength increases. The behavior of resistance in a magnetic field varies significantly depending on the preparation of the metallic specimen and its orientation with respect to the field.
 - (c) Thermoelectric Field: The sign of the thermoelectric field, similar to the Hall coefficient, does not always match the prediction of free electron theory, although the order of magnitude is generally correct.
 - (d) Wiedemann-Franz Law: While the Wiedemann-Franz law is successful at high and very low temperatures, it fails at intermediate temperatures, leading to a temperature dependence of K/σ .
- 2. Linear Term in Specific Heat: Sommerfeld theory reasonably explains the linear term in the low-temperature specific heat of alkali metals, less accurately for noble metals, and poorly for transition metals like iron and manganese, as well as for bismuth and antimony.
- 3. Compressibility of Metals: Although free electron theory provides good estimates for the bulk moduli of many metals, more attention to ions and electron-electron interactions is necessary for a more accurate equation of state estimation.
- 4. Determining the Number of Conduction Electrons: The assumption that valence electrons become conduction electrons while others remain bound to ions raises questions about its validity, especially in elements like iron with multiple chemical valences.
- 5. Why Some Elements Are Nonmetals: The presence of insulators challenges the rule of thumb for determining the number of conduction electrons. The discrepancy in behavior, such as boron being an insulator while aluminum is a good conductor, or carbon being an insulator in diamond form and a conductor in graphite form, raises questions about the underlying mechanisms.

The presence of a periodic lattice of ions is fundamental to modern solid-state physics, providing the basis for its analytical framework. The absence of a periodic ion array in liquids compared to their presence in solids is a key reason for the disparity in the development of theories between the two states of matter. To advance the theory of solids, whether metallic or insulating, further investigation into periodic arrays is essential.

3 Chapter 3: Crystal lattices

3.1 Introduction

3.1.1 Bravais Lattices

A fundamental concept in the description of any crystalline solid is that of the Bravais lattice, which specifies the periodic array in which the repeated units of the crystal are arranged. The units themselves may be single atoms, groups of atoms, molecules, ions, etc., but the Bravais lattice summarizes only the geometry of the underlying periodic structure, regardless of what the actual units may be. We give two equivalent definitions of a Bravais lattice:

- 1. A 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.
- 2. A (three-dimensional) Bravais lattice consists of all points with position vectors R of the form:

$$R = n1a1 + n2a2 + n3a3$$

where al a2, and a3 are any three vectors not all in the same plane, and n1,n2 and n3 range through all integral values.

It's crucial that not only the arrangement, but also the orientation, remains consistent from every viewpoint within a Bravais lattice. For instance, examining the vertices of a two-dimensional honeycomb (Figure 4.3), the array appears identical when viewed from adjacent points only if the page is rotated 180° each time one moves from one point to the next. While structural relations are clearly consistent, orientational relations are not, indicating that the vertices of a honeycomb do not constitute a Bravais lattice.

An example that satisfies the structural but not the orientational requirements of definition (a) is the three-dimensional hexagonal close-packed lattice, as described below.

Given the equivalence of all points, the Bravais lattice must extend infinitely. Although actual crystals are finite, their vast majority of points are far enough from the surface to be unaffected by it. The notion of an infinite system serves as a useful idealization. However, if surface effects are relevant, the concept of a Bravais lattice remains pertinent, albeit with the understanding that the physical crystal occupies only a finite portion of the ideal lattice.

Often, finite crystals are considered not because of significant surface effects, but for conceptual convenience. Similar to Chapter 2 where the electron gas was placed in a cubic box of volume $V = L^3$, one typically selects the finite region of the Bravais lattice to have the simplest form. Given three primitive vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 , the finite lattice of N sites is commonly regarded as the set of points of the form $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$.

3.1.2 Primitive Unit Cell

A primitive cell, or primitive lattice cell, of a Bravais lattice is a volume of space that, when translated through all the vectors in the lattice, fills all of space without overlapping itself or

leaving voids. There isn't a unique way to select a primitive cell for a given Bravais lattice, and multiple choices of primitive cells for a two-dimensional Bravais lattice can be illustrated.

3.1.3 Wigner-Seitz Primitive Cell

One can always opt for a primitive cell that exhibits the full symmetry of the Bravais lattice. The most common choice is the Wigner-Seitz cell. The Wigner-Seitz cell surrounding a lattice point defines the region of space that is closer to that point than to any other lattice point. Due to the translational symmetry of the Bravais lattice, the Wigner-Seitz cell around any lattice point encompasses the Wigner-Seitz cell around any other lattice point when translated through the lattice vector that connects the two points. Each point in space has a unique lattice point as its nearest neighbor, thus belonging to the Wigner-Seitz cell of precisely one lattice point. Consequently, when translated through all lattice vectors, a Wigner-Seitz cell fills space without overlapping, making it a primitive cell. Since the definition of the Wigner-Seitz cell doesn't specify any particular choice of primitive vectors, the Wigner-Seitz cell exhibits the same symmetry as the Bravais lattice.

4 Chapter 4: The Reciprocal Lattice

4.1 Role of Reciprocal Lattice

The reciprocal lattice plays a pivotal role in the analytical investigation of periodic structures, with its significance stemming from various fields such as crystal diffraction theory, the study of functions exhibiting the periodicity of a Bravais lattice, and the examination of momentum conservation when transitioning from the full translational symmetry of free space to that of a periodic potential. In this concise chapter, we aim to elucidate fundamental aspects of the reciprocal lattice from a general perspective not bound to any specific application.

4.2 Definitions and Examples

Consider a collection of points \mathbf{R} forming a Bravais lattice and a plane wave $e^{(\mathbf{k}\cdot\mathbf{r})}$. While such a plane wave generally lacks the periodicity of the Bravais lattice for arbitrary \mathbf{k} , certain special choices of wave vectors yield periodic plane waves. The set of all wave vectors \mathbf{K} that produce plane waves with the periodicity of a given Bravais lattice constitutes its reciprocal lattice. Mathematically, \mathbf{K} belongs to the reciprocal lattice of a Bravais lattice of points \mathbf{R} if the relation

$$e^{i(\mathbf{k}(\mathbf{R}+\mathbf{r}))} = e^{i\mathbf{K}\cdot\mathbf{r}}$$

holds for any \mathbf{r} and all \mathbf{R} in the Bravais lattice. It's important to note that a reciprocal lattice is defined in reference to a specific Bravais lattice, which is often termed the direct lattice in relation to its reciprocal. Additionally, while it's feasible to define a set of vectors \mathbf{K} satisfying $e^{i\mathbf{K}\cdot\mathbf{R}} = 1$ for any arbitrary set of vectors \mathbf{R} , such a set of \mathbf{K} is referred to as a reciprocal lattice only if the set of vectors \mathbf{R} forms a Bravais lattice. It's trivially shown that the reciprocal of the reciprocal lattice is the direct lattice itself, rendering each pairing unique.

4.3 First Brillouin Zone

The Wigner-Seitz primitive cell of the reciprocal lattice is denoted as the first Brillouin zone. Higher Brillouin zones, representing primitive cells of a different type, emerge in the theory of electronic levels within a periodic potential. While the terms "Wigner-Seitz cell" and first Brillouin zone refer to identical geometric entities, the latter term primarily applies to the k-space cell in practice. Specifically, when discussing the first Brillouin zone of a particular r-space Bravais lattice associated with a specific crystal structure, it invariably denotes the Wigner-Seitz cell of the associated reciprocal lattice. Consequently, due to the reciprocal relationship between the body-centered cubic and face-centered cubic lattices, the first Brillouin zone of the bcc lattice corresponds to the fcc Wigner-Seitz cell, and conversely, the first Brillouin zone of the fcc lattice aligns with the bcc Wigner-Seitz cell.

4.4 Lattice Planes

Given a specific Bravais lattice, a lattice plane is defined as any plane containing at least three non-collinear Bravais lattice points. Due to the translational symmetry of the Bravais lattice, such a plane inherently contains infinitely many lattice points, thereby forming a twodimensional Bravais lattice within the plane.

A family of lattice planes denotes a set of parallel, equally spaced lattice planes encompassing all points of the three-dimensional Bravais lattice. Each lattice plane is a member of such a family. Notably, the decomposition of a Bravais lattice into a family of lattice planes lacks uniqueness. The reciprocal lattice offers a straightforward method to categorize all feasible families of lattice planes, as encapsulated in the subsequent theorem: For any family of lattice planes separated by a distance d, reciprocal lattice vectors exist perpendicular to these planes, with the shortest having a length of $2\pi/d$. Conversely, for any reciprocal lattice vector \mathbf{K} , there exists a family of lattice planes normal to \mathbf{K} and spaced by a distance d, where $2\pi/d$ corresponds to the length of the shortest reciprocal lattice vector parallel to \mathbf{K} .

The correspondence between reciprocal lattice vectors and families of lattice planes furnishes a convenient approach to specify the orientation of a lattice plane. Typically, plane orientation is described by providing a vector normal to the plane. Given that reciprocal lattice vectors are normal to any family of lattice planes, selecting the shortest reciprocal lattice vector to represent the normal is a natural choice. This methodology yields the Miller indices of the plane:

4.5 Miller Indices

The Miller indices of a lattice plane represent the coordinates of the shortest reciprocal lattice vector normal to that plane, relative to a designated set of primitive reciprocal lattice vectors. Consequently, a plane characterized by Miller indices h, k, l is orthogonal to the reciprocal lattice vector $hb_1 + kb_2 + lb_3$. Defined in this manner, the Miller indices are integers, as any reciprocal lattice vector is a linear combination of three primitive vectors with integral coefficients. Additionally, since the normal to the plane is determined by the shortest perpendicular reciprocal lattice vector, the Miller indices h, k, l have no common factors. It's worth noting that the Miller indices are contingent on the specific choice of primitive vectors.

The geometrical interpretation of the Miller indices in the direct lattice offers an alternative definition. Given that a lattice plane characterized by Miller indices h, k, l is perpendicular to the reciprocal lattice vector $hb_1 + kb_2 + lb_3$, it lies within the continuous plane $\mathbf{K} \cdot \mathbf{r} = A$, for a suitable constant A. This plane intersects the axes determined by the primitive vectors $\mathbf{a}_1, \mathbf{a}_2$, and \mathbf{a}_3 of the direct lattice at the points $x_1\mathbf{a}_1, x_2\mathbf{a}_2$, and $x_3\mathbf{a}_3$, where $x_1 = A/(2\pi h)$, $x_2 = A/(2\pi k)$, and $x_3 = A/(2\pi l)$. Consequently, the intercepts with the crystal axes of a lattice plane are inversely proportional to the Miller indices of the plane.

REFERENCES

References

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