SOLID STATE PHYSICS
LECTURE

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CHAPTER ONE
CRYSTAL STRUCTURE AND CRYSTALLOGRAPHY

INTRODUCTION

SOLID CRYSTAL

Crystal structures may be conveniently specified by describing the arrangement within the solid of a small representative group of atoms or molecules, called the ‘unit cell.’ By multiplying identical unit cells in three directions, the location of all the particles in the crystal is determined. In nature, 14 different types of crystal structures or lattices are found. The simplest crystalline unit cell to picture is the cubic, where the atoms are lined up in a square, 3D grid. The unit cell is simply a box with an atom at each corner. Simple cubic crystals are relatively rare, mostly because they tend to easily distort. However, many crystals form body-centered-cubic (bcc) or face-centered-cubic (fcc) structures, which are cubic with either an extra atom centered in the cube or centered in each face of the cube. Most metals form bcc, fcc or Hexagonal Close Packed (hcp) structures; however, the structure can change depending on temperature. These three structures will be discussed in more detail on the following page.

CRYSTALLINE

The regular repeating pattern that the atoms arrange in is called the crystalline lattice.

ORDERED, LONG RANGE ORDER.

EXAMPLES: metal like iron, copper, aluminum OR semiconductor like silicon, germanium.

AMORPHOUS

means none crystalline, disordered, not ordered, short range order.

EXAMPLES: GLASS
THE LATTICE

Fig. (2): a) Point lattice with unit cell outlined. b) Unit cell with lattice vectors indicated.
BRAVAIS LATTICE

simple cubic  body-centered cubic  face-centered cubic

simple tetragonal  body-centered tetragonal

simple orthorhombic  body-centered orthorhombic  base-centered orthorhombic  face-centered orthorhombic

rhombohedral  hexagonal

simple monoclinic  base-centered monoclinic  triclinic
<table>
<thead>
<tr>
<th>System</th>
<th>Axial lengths and angles</th>
<th>Unit cell geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>cubic</td>
<td>$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$</td>
<td><img src="image" alt="cubic cell" /></td>
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<tr>
<td>tetragonal</td>
<td>$a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$</td>
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<td>hexagonal</td>
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<td><img src="image" alt="monoclinic cell" /></td>
</tr>
<tr>
<td>triclinic</td>
<td>$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$</td>
<td><img src="image" alt="triclinic cell" /></td>
</tr>
</tbody>
</table>

Figure 3: 14 Bravais lattices, and seven geometrical systems.
**Unit cell**
The crystal structure of a material is often discussed in terms of its unit cell. The unit cell is a spatial arrangement of atoms which is tiled in three-dimensional space to describe the crystal. The unit cell is given by its lattice parameters, the length of the cell edges and the angles between them, while the positions of the atoms inside the unit cell are described by the set of atomic positions \((x_i, y_i, z_i)\) measured from a lattice point. For each crystal structure there is a conventional unit cell, which is the smallest unit that has the full symmetry of the crystal (see below). However, the conventional unit cell is not always the smallest possible choice. A primitive unit cell of a particular crystal structure is the smallest possible unit cell one can construct such that, when tiled, it completely fills space. This primitive unit cell does not, however, display all the symmetries inherent in the crystal. A Wigner-Seitz cell is a particular kind of primitive cell which has the same symmetry as the lattice.

**Number of lattice points for unit cell:**

To calculate the total number of atoms per unit cell \((N_{total})\) which is called the number of atoms / unit cell. There are different types of unit cell, each have different number of atoms. For cubic, the relation:
\[ N_{\text{total}} = \frac{N_i}{1} + \frac{N_c}{8} + \frac{N_f}{2} \quad ; \text{where} \]

- \( N_i \): number of atom inside the unit cell.
- \( N_c \): number of atom at the corners of unit cell.
- \( N_f \): number of atom at the faces of unit cell.

The total number of lattice points for unit cell (\( N \)) calculated by counting that bound and are interior to the cell and considering the sharing of points by adjacent cells.

**EXAMPLE:**

8 lattice points at the corners in unit in figure of simple cubic, are each shared by 8 adjacent cells (\( N_c \)); the points on the face of a cell shared by 2
cells \((N_f)\) and of course, the interior points \((N_i)\) belong to the cell in equation:

\[
N_{\text{total}} = N_i / 1 + N_c / 8 + N_f / 2 \tag{1}
\]

1. Simple cubic lattice (S.C): simple cubic structure (U.C), have 8 atoms at the corners only.

2. Face center cubic (F.C.C): have 6 atoms at the faces only.

3. Body center cubic (B.C.C): one atom at the center of the cubic.

For 2 adjacent unit cells sharing one atom at the face, give half atom in each unit cell.

To calculate the density of unit cell. This depends on the type of unit cell (S.C, FCC, and BCC), they have three different number of atoms; so they have different density:

\[
\text{Density (}\rho\text{)} = \frac{\text{number of atoms per unit cell x M (g/mole)}}{\left[a\_o^3 \times N_A \text{ (avogadro's number)}\right]}
\]

**CLOSE-PACKING STRUCTURES**

At each lattice position imagine a sphere of atoms or molecules at the basis of radius \(R\), (it is one or more atoms / molecules called basis).

For simplicity, consider all the spheres to be equivalent. Now imagine each of the cell dimension shrinking uniformly (but not the radius of the spheres) until the spheres just touch. Where \(R\) is the atomic radius and \(a\_o\) is the lattice parameter or called lattice constant.

Atomic packing factor = \(f\), which is also called fractional volume factor:

\[
F = \text{atomic packing factor} = A.P.F = \frac{N_{\text{atom}} \times V_{\text{atom}}}{V_{\text{crystal}}} \tag{2}
\]

\(N_{\text{atom}}\) = NUMBER OF ATOMS PER UNIT CELL, DEPENDS ON TYPE OF UNIT CELL (SC, BCC, FCC)

\(V_{\text{atom}} = \frac{4}{3} \pi R^3\) represented as spherical shape.

\(V_{\text{crystal}}\) (VOLUME OF CRYSTAL) = \(a\_o^3\) (lattice constant)
How to calculate the total number of atoms per unit cell (N_{total})

For simple cubic

In simple cubic, we have 8 corners atoms only and each of these atoms is a number of 8 cells enclosing the corner, so there is $8 / 8 = 1$ atom per unit cell.

The total number of atoms per unit cell as represent in relation (1), now this calculated as below:

A) FOR S.C : $N_{total} = 1$ atoms per U.C (unit cell)

B) FOR B.C.C : $N_{total} = 2$ atoms per U.C

C) FOR F.C.C : $N_{total} = 4$ atoms per U.C

How to calculate the fractional volume of U.C:

1. Suppose $f$ is represent the fractional volume, so for S.C, the total number of atoms per UC = 1

2. Calculate the total volume of the atoms = $(4/3) \pi R^3 = (4/3) \pi (a_o/2)^3$

   \[= (\pi a_o^3) / 6\]

3. Calculate the total volume of U.C = $a^3$

4. Calculate the fractional volume ($f$):
   \[f = [\pi /6 a^3] / a^3 = \pi / 6\]

HOME WORK:

1. Calculate the fractional volume for B.C.C = $\pi (3)^{1/2} / 8$.

2. Calculate the fractional volume for F.C.C = $\pi (2)^{1/2} / 6$. 
(a) Primitive, (b) Body–centered, and (c) face–centered cubic unit cells
MILLER INDICES

How to index hkl?

   remember that miller indices (hkl) are always integers (1,2,3,………etc.) .

Method to obtain Miller indices:

1. determine the interception of planes with axis x,y,z respectively interms of a,b,c.

2. take the reciprocal .

3. evaluate to obtain an integer values of hkl as integer values in bracket (hkl).this value represent the plane.

Planes (123), (111), (222) .....etc

Representation:*Plane (hkl)

* Family of planes {hkl}

* Direction [hkl]

* Family of directions ≤ ≥?????

Miller index system:

How to index planes?????

1. The intercepts on the fig. are : 3a, 2b, 2c respectively.

2. Recprocals of 3 2 2 are 1/3 , 1/2 , 1/2

3. Evaluation 2 3 3 where the denominator is = 6 , now the plane indices is (233).

Q ) determine the planes of the shadow areas in figures shown.

(110), (321), (111), (642), (020)
**Translation vector:**

A lattice contains a large number of planes of atoms. We name these planes using the Miller indices \( (n_i, n_j, n_k) \). Defined with the convention that the vectors \( \mathbf{R} = n_i \mathbf{a}_1 + n_j \mathbf{a}_2 + n_k \mathbf{a}_3 \). Where \( \mathbf{R} \) is a translation vector and is a normal vector to the plane. \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \) are basis vectors and \( n_i, n_j, n_k \) are integers.

**TRANSLATION VECTORS**

This is defined by the formula: \( \mathbf{T} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c} \)

For any type of lattice, there exist three fundamental transition vectors \( \mathbf{a}, \mathbf{b}, \mathbf{c} \), these are the shortest vectors, which satisfy the condition that if we traverse any integer distances \( n_1 \mathbf{a}, n_2 \mathbf{b}, n_3 \mathbf{c} \), from a point in the crystal lattice, then we reach to a point which has identically the same environment as the original point. **HEXAGONAL**: indices with hexagonal are \( (hkil) \) see hexagonal.

**Crystal Planes**

Planes in a crystal can be specified using a notation called Miller indices. The Miller index is indicated by the notation \([hkl]\) where \( h, k, \) and \( l \) are reciprocals of the plane with the \( x, y, \) and \( z \) axes. To obtain the Miller indices of a given plane requires the following steps:

1. Step 1. The plane in question is placed on a unit cell.
2. Step 2. Its intercepts with each of the crystal axes are then found.
3. Step 3. The reciprocal of the intercepts are taken.
4. Step 4. These are multiplied by a scalar to insure that is in the simple ratio of whole numbers.

For example, the face of a lattice that does not intersect the \( y \) or \( z \) axis would be \( (100) \), while a plane along the body diagonal would be the \( (111) \) plane. An illustration of this along with the \( (111) \) and \( (110) \) planes is given in figure.
Examples of Miller indices notation for crystal planes.

Crystal Directions

Figure shows some examples of the various directions in the unit cell. The crystal direction notation is made up of the lowest combination of integers and represents unit distances rather than actual distances. A \([222]\) direction is identical to a \([111]\), so \([111]\) is used. Fractions are not used. For example, a vector that intercepts the center of the top face of the unit cell has the coordinates \(x = 1/2, y = 1/2, z = 1\). All have to be inversed to convert to the lowest combination of integers (whole numbers); i.e., \([221]\) in. Finally, all parallel vectors have the same crystal direction, e.g., the four vertical edges of the cell shown all have the crystal direction \([hkl] = [001]\).

SEE FIG. BELOW
Procedure to index a direction: (a) the direction desired to be indexed (?) with a line (1) drawn parallel to the desired line and with the intercepts; (b) several directions with associated planes.

[SOME DIRECTION DETERMINATION EXAMPLES]
**SYMMETRY IN CRYSTALS**

There are various types of crystals SYMMETRY which is classified into certain groups depending on their symmetry. These are **EXTERNAL** and **INTERNAL** symmetry.

1. **EXTERNAL SYMMETRY**

   A. **Center of Symmetry:**

   When it has a point such that all straight lines drawn through it will pass through a pair of similar points lying on opposite sides of the center of symmetry and at the same distance from it.

   B. **Axis of Symmetry:** Axis pass through the crystal, this axis rotated from ascertain point and returned to the same point. Rotation of the crystal around the axis of symmetry with a certain angles. Started from point by rotation around axis with angle $360/n$, where n are called fold axis $2, 3, 4, 6...$ then return to the same point.

   $$360/2 = 180 \; ; \; 360/3 = 120 \; ; \; 360/4 = 90 \text{ degrees}$$

   C. **Plane of Symmetry:** When we draw plane pass through the center of plane, which represent the center of crystal, this plane is called plane of symmetry.

2. **INTERNAL SYMMETRY:** These are rotation, reflection, inversion, rotation inversion, gliding, screw axis.

   A. **Rotation:** operated with $2, 3, 4, 6$ fold of symmetry.

   B. **Reflection:** operation produces the same effect as a plane of symmetry.

   C. **Inversion Center:** every point located at a distance $(r)$ relative to the center, there exists similar point at $r$ and on the same line through this center.

   D. **Gliding Plane:** exists in crystal (when it couples are reflection plane with a translation parallel to this plane so that the structure is brought into self-coincidence by the movement and reflection across the specified plane.)
E. **Screw Axis**: combines rotation with translation parallel to the axis like the working of a screw, the direction of rotation may be clockwise or anti-clockwise, and existence of 2, 3, 4, …… rotation.

F. **Rotation Inversion**.
CHAPTER TWO

Crystal bonds

2.1 Types of bonds in crystal:

Types of binding interaction which causes the atom and molecules to attract at relatively large distances and which join atoms together to form molecules and other structures.

BONDS are CLASSIFIED as:

1. Strong Bonds
   a. Covalent bond
   b. Ionic bond
   c. Metallic

2. Weak Bonds
   a. Van-der-waals
   b. Hydrogen bond

1. Strong Bonds:

These are results from the exchange or sharing of electrons and occur, because the bonded system has a lower potential energy than the separate atoms.

a. Covalent Bonds:

Electrons are shared between different atoms. The bond energy is electrostatic in origin. In diamond, the individual atoms of carbon are linked by covalent bond to form a rigid crystal lattice.

b. Ionic Bonds:

Electrons are transferred from one neutral atom to another, and the resulting positive forces. Example: Na⁺Cl⁻

c. Metallic Bond:

Electrons have greater freedom of movement.

2. Weak Bonds:

a. Van der Waals:
These are weak attractive forces acting over short distances outside a molecule and enable it to attract both polar and non-polar neighbours.

b. Hydrogen bonding:

Hydrogen bonds are basically, electrostatic interactions between molecules. These bonds are particularly important in determining the properties of H₂O molecules.

**TYPES OF ATOMIC INTERACTION**

**A. Van der Waals – London Interaction:**

Consider two identical inert gas atoms at a separation (R), large in comparison with the radii of the atoms. The attractive interaction which varies as the minus sixth power of the separation of the two atoms oscillators. This is the Van der Waals interaction, known also as the London – interaction.

\[ \Delta U = -\frac{A}{R^6} \]

**B. Repulsive Interaction:**

As the two atoms are brought together, their charge distribution gradually overlap as shown in figure, thereby changing the electrostatic energy of the system. At sufficiently close separation, the overlap energy is repulsive, in large part because of the "Pauli exclusion principle". It is usually to write the total potential energy of two atoms at separation (R) as:

\[ U(R) = 4\epsilon \left[ (\sigma / R)^{12} - (\sigma / R)^6 \right] \]

Where \( \epsilon, \sigma \) are new parameters, with \( 4 \epsilon \sigma^6 = A \), and \( 4 \epsilon \sigma^{12} = B \).

This U(R) is called Lennard – Jones potential. The force between the two atoms is given by \(-dU/dR\).
2.2 Crystal Diffraction of Solids and Reciprocal Lattice:

**Incident Beam:**

To study crystal structure through diffraction of photons, neutrons, and electrons. The diffraction depends on the crystal structure and on the wavelength ($\lambda$), where $\lambda$ lattice constant of the crystal.

For optical system, $\lambda \approx 5000$ angstrom.

Large enough compared with any lattice parameter (constant) of the solid.

X-ray photons is the energy of x-ray photons, it is:

Where $h = 6.62 \times 10^{-27}$ erg.s = $6.62 \times 10^{-34}$ J.s (Plank's constant), so, energies needed for x-ray photons $10\text{ - }50 \text{ KeV}$ range.

Neutron: $\lambda_n = 0.28 \div [E \text{ (ev)}]$

Electron: $\lambda_e = \frac{12}{[E \text{ (ev)}]^{1/2}}$, where $E = \frac{h^2}{2m\lambda^2}$

These values of the x-ray wavelength are so small, smaller than the lattice parameters of materials, so, it will be possible to use x-ray for diffraction.

To derive and calculate the wavelength's for electrons

?? H.W.

so we can obtain a very small electrons wavelength for crystal diffraction of solids which is comparable to the materials lattice constant.

**Bragg's Law:**

To derive and satisfy Bragg's law, suppose an incident beam on a planes of solids (arrangement of atomic layers) as shown below:
\( \sin \theta = \frac{BC}{d} \), or \( BC = d \sin \theta \), where \( BC = BD = d \sin \theta \).

The total path difference = \( BC + BD = d \sin \theta + d \sin \theta = 2d \sin \theta \),

Constructive interference of the radiation from successive planes occurs when the path difference is an integral number (\( n \)) of wavelength \( \lambda \), so that:

\[
( n \lambda = 2d \sin \theta ) , \quad \text{where } n = 1, 2, 3, \quad \text{etc.}
\]

This is called Bragg's law used in a diffraction of crystals with x-ray or electron beam, etc.

**Experimental Diffraction Methods:**

1. **Laue Method:**:

A diffraction technique used with single crystal samples. This is typically used to determine the orientation of ase/face of a crystal relative to the incident beam. This technique uses many wavelength's.
2. Rotating Crystal Method:

This is used for determining the entire crystal structure: in particular, the shape and size of unit cells and atom positions. The technique uses monochromatic x-ray and require a single crystal of materials.

3. Powder Method

This method uses monochromatic x-ray but in this method the sample is finally grounded.

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**Figure 3** Sketch of a monochromator which by Bragg reflection selects a narrow spectrum of x-ray or neutron wavelengths from a broad spectrum incident beam. The upper part of the figure shows the analysis (obtained by reflection from a second crystal) of the purity of a 1.16 Å beam of neutrons from a calcium fluoride crystal monochromator. (After G. Bacon.)

**Figure 4** X-ray diffractometer recording of powdered silicon, showing a counter recording of the diffracted beams. (Courtesy of W. Parrish.)
LATTICE GEOMETRY

Planer spacing formula d - interplaner spacing (the distance between atomic planes).

\[ \frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2} \]

Where \( d_{hkl} \) is perpendicular to the plane of atoms shaded as shown in the geometry below.

Then: \( a \) is the atomic distance called atomic constant.

\( d \) : is the distance between parallel planes.

\[ 2d \sin \theta_{hkl} = n \lambda \]
INTRODUCTION

Definitions:

Waves:

Is a disturbance that propagates. Apart from electromagnetic radiation, which can travel through vacuum, waves exist in a medium through which these travel and can transfer energy from one plane to another without any of the particles of the medium being displaced permanently, with no associated mass transport. Instead, any particular points oscillate around a fixed position.

Type of Waves:

1. Longitudinal waves: Vibrations along the wave's direction of travel.

2. Transverse Waves: Waves vibrations perpendicular to the wave direction of travel.

SOUND:

Is a mechanical wave that propagates through air, liquid and solid of a frequency detected by the auditory system.

PHONONS:

Are especially relevant in the behavior of heat and sound in crystals. In a crystal, the atoms are nearly arranged in a uniform, repeating structure, when heated the atoms can oscillate at specific frequencies. The bonds between the individual atoms in a crystal behave essentially like a springs. SEE FIG below:
2D – LATTICE / nth ball of atoms a distance equal to a (lattice constant) with springs.

**PHONON:**

Is a quantized mode of vibration occurring in a rigid crystal lattice, such as atomic lattice of solids.

الفونون: عبارة عن نموذج مكم من الاهتزاز يحدث في مشبك البلورة الصلب مثال: مشبك الذرات للمادة الصلبة.

The study of **phonons** is an important part of solid state physics, because phonons play an important role in many of the physical properties of solid, such as the **THERMAL CONDUCTIVITY** and the **ELECTRICAL CONDUCTIVITY**. In particular, the properties of **LONG λ**, phonons gives rise to **SOUND** in solid. In insulating solid, phonons are also the primary mechanism by which heat conduction takes place.

**PHONONS:**

Are quantum mechanical versions of a special type of vibrational motion, known as **NORMAL MODE**, in classical mechanics.
PHONON BEHAVIOR AND PROPERTIES:

Dispersion Relation: $\omega$ versus $k$ (wave vector) = $2\pi / \lambda$.

If $\omega_k$ is the frequency of phonon to its wave number $k$.

The speed of propagation of phonon, which is also the speed of sound in the lattice, is given by the slope of the dispersion relation. **SEE FIG. BELOW**

1. At low values of $k$ (i.e. long $\lambda'$ s), the dispersion relation is almost linear, and the speed of sound is approximately $=\omega a$, independent of the phonon frequency. As a result, packets of phonons with different (but long $\lambda'$ s) can propagate for large distances across the lattice without breaking apart. This is the reason that sound propagates through solids without significant distortion.

2. This behavior fails at large values of $k = 2\pi/\lambda$, small $\lambda$ (short $\lambda$) due to the microscopic details of the lattice.

* It should be noted that the physics of **SOUND IN AIR** is different from the physics of sound in **SOLID**, because sound waves in air propagate in a gas of randomly moving molecules rather than a regular crystal lattice.
ONE DIMENTIONAL LINEAR CHAIN

To understand the thermal and physical properties associated with atomic (lattice) vibrations in a solid, it is useful to consider two simple cases:

1. One – dimensional (1D) **Monatomic Linear Chain**.

2. One – dimensional (1D) **Diatomic Linear Chain**.

1. The Monatomic Linear Chain

In 1D monatomic linear chain, there is one atom per unit cell. If only the nearest-neighbor interaction is considered, then the linear chain can be represented by a string of identical masses connecting to one another by the same massless spring, as illustrated in the fig. below.
In this case, the equation of motion for the atomic displacement can be easily derived using **HOOK'S LAW** ----> \( F = -kx.\text{or} \quad F= -CU. \)

According to this classical law, the force acting on the \( n \)th atom with mass \( M \) can be expressed as:

\[
F = -C_{nm} (U_n - U_{nm}) \quad \ldots \ldots (1)
\]

\[
F_n = M \left( \frac{d^2 U}{dt^2} \right) = -C (U_n - U_{n+1}) - C (U_n - U_{n-1})
\]

When \( C \) is the force constant between two adjacent atoms and \( U_n, U_{n-1}, U_{n+1} \) denote the displacements of the \( n \)th atoms.

The solution of eqn. (1) has the form of travelling wave, which is given by:

\[
U_n = U_k \cdot e^{j(nka-wt)} \quad \ldots \ldots (2)
\]

\( k = \) wave vector \( = 2\pi/\lambda \) of the lattice wave, \( \mathbf{k} \) is a vector.

\( a = \) lattice constant

\( n = \) integer number

\( U_k = \) amplitude as a function of \( k \).
**ω = \((4C/M)^{1/2}\). |\sin (ka/2) | = \omega_m .|\sin (ka/2)|**

Eqn. (3) Called the Dispersion Relation.

Where \(\omega_m = (4C/M)^{1/2}\) is the maximum frequency.

To obtain the maximum value of the frequency from (10) as follows:

when \(\sin(ka/2) = 1\); \(\omega = \omega_m\). Or means: \(\omega = \omega_m\) at \(\sin(ka/2) = 1\)

**Conclusion:**

This frequency \((\omega = \omega_m)\) is independent of the position \((n)\) of any atom, so all atoms vibrate with this frequency; these are called **NORMAL MODES**.

To draw the dispersion relation from (3):

\[
\omega^2 = 4C/M \sin^2 (ka/2) \text{ or } \\
\omega = 2.(C/M)^{1/2}.|\sin (ka/2)|
\]

This is the dispersion relation for an elastic wave vector \(k\) and frequency \(\omega\). As shown in fig. below:
Discussion

(1) Starting from zero of k axis, this function rises up to maximum value $\omega = \omega_m$ at $k = \pi/a$; then drops to larger value of $k$.

There are no new features in the regions other than between $k = \pi/a$ and $k = -\pi/a$. This is connected by reciprocal lattice vector $[G]$ are equivalent. This region is called: **FIRST BRILLOUIN ZONE**

(2) For small values of $k$

So, $\omega$ versus $k$ is linear (dashed line).
Debye’s assumption is valid in this region: long $\lambda$ approximation:

$$\omega = 2 \sqrt{C/M} \sin(ka/2)$$

$$ka/2 = \pi/2; \quad k = \pi/a = \pi/(\lambda/2) = 2\pi/\lambda \quad \text{where a=\lambda/2}$$

$$\omega = 2 \sqrt{C/M} \cdot ka/2 \quad \text{at small} \ k \ (\text{long} \ \lambda)$$

For long $\lambda$ or small $k$; $\sin ka/2 \approx ka/2$

$$\therefore \omega = 2 \sqrt{C/M} \cdot ka/2 = a \sqrt{C/M} \cdot k = v \cdot k$$

Now $\omega = v \cdot k \therefore v = \omega/k$ is the phase velocity.

**Phase Velocity:**

In a dispersion-less medium such as air for sound waves, the velocity of any phase of a wave is:

$$v = \omega/k$$

**Group Velocity:**

If the medium is dispersive such as glass for light waves and solid for sound vibrations, parts of a group of waves could travel faster than the amplitude of this group

$$v_{\text{group}} = \frac{d\omega}{dk}$$

- For one dimensional chain of atoms $v_g = \frac{d\omega}{dk} = 0$; at the Brillouin zone boundary. [i.e. $k = \pi/a$; $k=2\pi/\lambda = \pi/a$ where $\lambda/2 = a$].
- For shorter wavelength's have no physical meaning.
- Bragg Reflection occurs at $k = \pi/a$.

An electron can propagate up to the region's edge.
Wigner – Seitz cell formation

In real space _2D_ lattice is shown with vectors drawn to nearest neighbors and next nearest neighbors. See two shaded primitive Unit cells from Wigner – Seitz drawing.

W.S.cell formation is similar to B.Z. in R.L.

A: Nearest neighbor vector.

B: Next nearest neighbor vector.

C: Center atoms lattice (chosen).
1/2 A vectors \( \perp \) r to the vector 1/2 B vectors

This U.C. must contain the **Symmetry** of the lattice and full the space by **Translation**.

**VIBRATIONAL MODES OF ADIATOMIC LINEAR LATTICE**

The dispersion relation for the case of a 1D diatomic linear chain will be derived. Figure below shows a 1D diatomic linear chain, which contain two types of atoms (M) and (m) with different masses per unit cell. If one assumes that only the nearest – neighbor interactions are important, then the force constant C, between the two different mass atoms is the same through the entire linear chain.

M : mass of atoms. (1\(^{st}\) type)

m : mass of atoms. (2\(^{nd}\) type)

One dimensional chain with two different masses m and M.

U : is the displacement, where F = - C.U → F= - kx

(a) Force acting on atoms of mass M = F

\[
F_1 = - C[(U_{2n} - U_{2n+1}) + (U_{2n} - U_{2n-1})]
= - C[U_{2n} - U_{2n+1} + U_{2n} - U_{2n-1}]
\]

M . \( d^2U_{2n}/dt^2 \) = + C[\( U_{2n-1} + U_{2n+1} - 2U_{2n} \)]. . . . . . . (1)
b. Force acting on atoms (m) = \( F_2 \)

\[
F_2 = m \frac{d^2U_{2n+1}}{dt^2} = -C[(U_{2n+1} - U_{2n+2}) + (U_{2n+1} - U_{2n})]
\]

\[
m \frac{d^2U_{2n+1}}{dt^2} = + C[U_{2n} + U_{2n+2} - 2U_{2n+1}] \ldots \ldots (2)
\]

\[
\therefore \omega^2 = k(1/M + 1/m) \pm k[(1/M + 1/m)^2 - 4\sin^2ka/M.m]^{1/2}
\]

This is Called the Dispersion Relation for a Diatomic Linear Lattice in 1D.

Now to draw this relation to obtain the modes of vibrations.

SEE REF. For more details if you wish. Solid physics

A.J DEKKER
**LATTICE VIBRATIONS AND SPECIFIC HEAT OF SOLIDS**

**Crystal Lattice** ----> Crystal in solids are either crystalline or amorphous as previously described in Ch.1.
We are talking about the crystalline solids which have a crystal lattice of atoms in an ordered system. This system reveals a symmetry which gives lattice vibrational modes which is either Longitudinal Mode or Transverse Mode; these vibrations are responsible to transfer an energy.

The theories describe these energies of vibrations are started from these points.

If vibrational energy of N atoms arranged in a linear chain as follows:

1D O-------O-------O-------O<... atom

so, it can be expressed as a one-dimensional system.

In 1D energy of N Harmonic Oscillator (H.O).

In 3D Extending to 3D case.

This leads to vibrational energy of crystal, with N atoms

Is equal to the energy of a system of 3D-H.O.

THE VARIOUS THEORIES OF LATTICE SPECIFIC HEAT

Crystal lattice of atoms

A<----------------------------------------->B

Classical Theory Quantum Theories

(Dulong and Petite Theory) (Quantized)

1. Einstein's theory
2. Debye's theory

**A) Classical Theory**: The total energy for single 3D-isotropic Harmonic Oscillator is:

\[ E_{Tot.} = \varepsilon = K.E + P.E. = P^2/2m + V(r) \]

\[ V(r) = 1/2m \omega_0^2 (x^2 + y^2 + z^2) = 1/2m \omega_0^2 r^2 \]
Where \( m \) : mass of atom; \( \omega \) : frequency of oscillators of atoms.

For an assembly of \textbf{N-independent oscillators}, so, the total internal energy \( U \) is equal to:

\[
U_{\text{tot}} = 3N<\varepsilon> = 3NkT
\]

And the specific heat capacity per gram (or per unit volume):

\[
C_v = (dU/dT)_v = 3Nk
\]

\( C_v = \text{constant value} \), independent on temperature as shown.

\[
C_v = 3Nk \quad \text{constant value}
\]

So, for amole of any substance of \( N \) atoms, is equal to Avogadro's number \((N_A)\) and the molar heat capacity \((C_v)_m\) is a function of \( T \):

\[
C_v = f(T) \quad \text{for typical solid substance}.
\]

\[
\text{This is known as Dulong and Petite.}
\]

The law of Dulong and Petite, fairly well with experimental results for most substances, at and \textbf{above room T.}, but the \textbf{breaks at low T.}.

\textbf{At low T. range} \text{------> } C_v \text{ for all substances} \approx \text{zero}.

\textbf{Being} \( \alpha T^3 \) \text{ as } T \text{ approaches to zero as shown in the above curve for } C_v.
According to the Classical Theory, each atom vibrates independently.

B) Quantum Theories:

1. Einstein's Theory of the Specific Heat:

Einstein in 1911 considered as independent harmonic oscillators with single natural vibrational frequency ($\omega$), but they are regarded as quantum harmonic oscillator, which may have only discrete energy values such as:

$$\varepsilon_n = (n+1/2) \hbar \omega_0 ; \quad n=0,1,2,...$$

$$U_{Tot} = 3N<\varepsilon>$$

$$C_v = (dU_{tot}/dT)_v = 3Nk (\hbar \omega/kT)^2 \left[ e^{\hbar \omega/kT}/(e^{\hbar \omega/kT} - 1)^2 \right]$$

This is the specific heat [according to Einstien].

NOW DISCUSSION

(A) At high Temp. $T > \theta_E$; so.

$$e^{\theta E/T} = 1 + \theta_E/T \quad \text{or} \quad e^x = 1 + x + ....$$

So; substitute for $e^{\theta E/T}$ in $C_V$.

$$C_V = 3R \quad \theta_E = \hbar \omega/k$$

This value is similar to the classical result.

(B) At low $T$; or $T < \theta_E$

$$C_v = 3R(\theta_E/T)^2 e^{\theta E/T} ; \quad C_v \propto 1/T^2 \quad \text{where} \quad R = Nk$$

$C_v$ decrease gradually until it is approaches to zero.

وعلى الرغم من أن النظرية فسرت النتائج عند درجات الحرارة الواطئة ولكنه كانت اقل بكثير من النتائج التجريبية. وتبقي هذه النظرية قاصرة عند تفسير هذا الاختلاف.
2. Debye Theory of $C_v$ in 1912:

Since, the atoms of the crystal no longer vibrate independently of one another.

For one dimensional $\longrightarrow$ he saw for $N$-atoms chain $\longrightarrow$ there are essentially $N$-normal modes of vibrations.

For 3D $\longrightarrow$ crystal of $N$-atoms, each atom can vibrate independently along 3-coordinate. So, for this system, there are 3 $N$-possible normal modes.

Internal vibrational energy: $\epsilon_n = (n+1/2)\hbar\omega_0$

$$\langle\Delta U/\Delta T\rangle_v = C_v = (12/5)\pi^4/Nk (T/\Theta_D)^3$$

**HOMEWORK?? DERIVE THE ABOVE RELATION.**
The essential differences between Debye model and Einstein model is that, Debye considers the vibrational modes of crystal as a whole. whereas Einstein starting points was to consider the vibration of single atom, assuming the atomic vibration to be independent of each other.

In fact , that the atomic vibrations in crystals are strongly coupled and cannot considered as independent simplicity of Einstein model used.
CHAPTER FOUR
THIN FILM DEPOSITION

Types of Defects:

1. grain boundaries: interfaces between two single crystal regions of different orientation, atom at grain boundaries tend to be loosely bound, more reactive and accelerated diffusion along grain boundaries.
   Generally: lower temp. ----- smaller grains ----- many bounds
   high temp. ---- larger grains ---- fewer bonds.

2. line defects – dislocations.

3. point defects ----- vacancy , interstitial atoms, impurity atoms, self interstitial atoms.

In principles you can eliminate all of these except vacancies.
Fraction of vacancies (f):

\[ f = \exp \left( -\frac{E_f}{k_B T} \right), \quad k_B = 1.381 \times 10^{-23}, \quad E_f = 1 \text{ ev}, \]

at room temp. \( f = 10^{-17} \)

Point defects often arise from:
1. Fast deposition,
2. Low substrate temp. (no time for atoms to move to crystal lattice sites).

**NUCLEATION AND GROWTH OF SOLID CRYSTALS**

**Transformation to solid phase:**

These are required:

1. Nucleation of new phase.
2. Growth of new phase.

That depends on:

- Liquid phase instability
- Driving force to equilibrium
- Increase as we move to lower temp's.

3. Diffusion of atoms into clusters, this increases to these two terms (multiplication) to determine the total nucleation rate.

The max rate of nucleation is at some \( T \) less than \( T_e \) (equilibrium temp).

**GROWTH:**

Growth of the phase is diffusion controlled ----- increases with temp.

**Transformation rate:**

Total rate of forming solid is product of nucleation rate and growth rate.

**NUCLEATION DETAILS:**
Two sources are related to that
1. thermodynamics: Is nucleation possible? (means energy minimization occur).

**Homogenous Nucleation:**
We can see the transformation of vapor to liquid (or solid) for a pure material without substrate.

**Energy minimization involves two terms:**
1. **Volume transition**.
   \[ \Delta G = \frac{4}{3} \pi r^3 . \ G_v \]  
   Where \( r \) is the radius of liquid phase atom, and \( G_v \) is the change in free energy per unit volume.

2. **Surface formation**.
   \[ \Delta G_{(surface)} = 4 \pi r^2 \gamma, \]  
   where \( \gamma \) is the surface energy per unit area

Change in surface energy is always positive, when forming surfaces.

**TOTAL ENERGY CHANGE:**
\[ \Delta G_{(TOTAL)} = \frac{4}{3} \pi \ r^3 . \ \Delta G_v + 4 \pi r^2 \gamma \]  
1. Initial formation of nuclei has increase in \( G \) ---- go to metastable.
2. If \( r \square r^* \) : then nuclei shrink to lower \( G \). [\( \square \) less than]
3. If \( r \square r^* \) : then nuclei grow to lower \( G \). [\( \square \) greater than]
4. \( r^* \) is a critical radius for nuclei which results at \( \Delta G = \Delta G^* \)

**HOME WORK**
Find \( r^* \) from \( \left(\frac{d \Delta G_{(total)}}{dr}\right) = 0 \) ; energy minimization
To get \( r^* = - \frac{3 \gamma}{(\Delta G_v)} \) and find \( \Delta G^* = \left(\frac{16\pi \gamma^3}{3(\Delta G_v)^2}\right) \)
**Nucleation Rate:**

How fast will the critical nucleus continue to grow?

Now consider the rate at which atoms will join the critical nuclei.

Expect nucleation rate to be given by:

\[ N = N^* A^* W \]

where \( N^* \) : concentration of critical nuclei (nuclei/cm\(^3\))

\( A^* \) : critical surface area of nuclei.

\( W \) : flux of atoms impingement (atoms/cm\(^3\).sec)

\[ N^* = n_s \exp\left[ -\frac{\Delta G^*}{kT} \right] \]

where \( n_s \) is the density of possible nucleation sites.

\[ A^* = 4\pi r^*^2 \]

\[ N = N^* A^* W \]

\[ W = \alpha (p_v - p_s) \frac{N_A}{[2 M R T]^{1/2}} \]

Substitute 2,3,4, in 1 as below:

\[ N = n_s \exp\left[ -\frac{\Delta G^*}{kT} \right] + 4\pi r^*^2 + \alpha (p_v - p_s) \frac{N_A}{[2 M R T]^{1/2}} \]

This is called total nucleation rate.

**FILM FORMATION II**

**a. Island growth (volmer–weber/V-W).** Form 3D islands

**Sources:**

1. Film atoms more strongly bound to each other than to substrate.

2. and or slow diffusion.
b. Layer by layer growth (F-V-M): Generally highest crystalline quality

Sources:
1. Film atoms more strongly bound to substrate than to each other.
2. And/or fast diffusion.

C. Mixed growth (SK):
initially grown layer by layer, then forms 3D islands. This is involved a change in energies.

Young's equation:

When would we expect to see each of these modes of growth?

We write Young's equation: \( \gamma_{sv} = \gamma_{fs} + \gamma_{vf}\cos \theta \)

1. For islands growth, when \( 0 \leq \theta \leq 90 \) or \( 0 \leq \cos \theta \leq 1 \)

\[ \frac{(\gamma_{sv} - \gamma_{fs})}{\gamma_{vf}} = \cos \theta \leq 1 \]

\[ \gamma_{sv} \geq \gamma_{fs} + \gamma_{vf} \]

2. For layer growth: \( \theta = 0 \) or undefined, \( \cos \theta \geq 1 \)

\[ \gamma_{sv} \geq \gamma_{fs} + \gamma_{vf} \]

3. For mixed growth:

\[ \gamma_{sv} \geq \gamma_{fs} + \gamma_{vf} \]
the layer growth condition with cosine greater than 1 look odd, this is the case where the angle theta is undefined because for layer growth there is really no point where the substrate, vapor and film come together and therefore no way to define the angle.

GAS ADSORPTION

Introduction

When a gas or vapor is brought into contact with a solid, part of it, is taken up by the solid. The molecules that disappear from the gas either enter the inside of the solid or remain on the outside attached to the surface. The former phenomena is termed **absorption** and the later is called **adsorption**. Adsorption is different from absorption, in which a substance diffuse into a liquid or solid to form a solution.

![Diagram of adsorption process](image)

The solid that taken up the gas is called the **adsorbent**, and the gas or vapor taken up on the surface is called **adsorbate**.

Molecules and atoms attach themselves onto surfaces in two ways:

1. **Physisorption**:
or called (Physical Adsorption);

Is a process that occurs when a gas or liquid (solute) accumulate on the surface of a solid or move rarely, a liquid (adsorbent) forming a monolayer or atomic film (adsorbate).

There is a weak Van der Waals attraction of the adsorbate to the surface. The attraction of the surface is weak but long ranged. The potential energy of an adatom in a physisorption state on a planer surface as a function of distance $z$ [$f(z)$] from the surface is shown in figure below:

$$Ed = Ea$$

P.E. vs. Z for Physisorption

The adsorption energy must be equal to the desorption energy, in case of physical adsorption.

2. CHEMISORPTION:

or called Chemical Adsorption;

the adsorbate sticks to the solid by the formation of a chemical bond with the surface. This interaction is much stronger than physisorption.
The potential energy diagram of chemisorption on a planar surface is shown below:

\[ E_a : \text{adsorption energy.} \quad E_b : \text{binding energy.} \]
\[ E_c : \text{chemisorption energy} \quad E_d : \text{desorption energy.} \]

Chemisorption occurs when \( E_d \) is greater than \( E_a \).

\[ E_d = E_a + E_c \quad \text{or} \quad E_c = E_d - E_a ; \quad \text{means} \quad E_d \geq E_a \]

When a molecule adheres to a surface through the formation of a chemical bond as opposed to the Van der Waal's forces which causes physisorption.

**In Chemisorption:**

It is characterized by:

1. High temperature.
2. Strong covalent bond.
3. Adsorption takes place only in a monolayer system.
4. Reversible only at high temperature.
5. Increasing in electron density in the interface of adsorbant and adsorbate.

**In Physisorption:**

It is characterized by:
1. low temperature.
2. weak bond.

Similar to surface tension, a desorption is a consequence of **SURFACE ENERGY**.

**SURFACE ENERGY:**

To define the surface energy (S.E) or surface free energy of a particular crystal face, we can think of the bulk solid as being divided along a plane parallel to that face to form two new surfaces. The energy required for such separation per unit area of surface formed is defined as the surface energy:

\[
E_s = E_v \cdot V + E_s \cdot S
\]

- \( E_s \): total surface energy of solid.
- \( S \): surface area of solid.
- \( V \): volume of solid.
- \( E_v \): energy due to volume of solid.
- \( E_s \): surface energy per unit area of solid.
CHAPTER FIVE
VAPORIZATION AND DRILLING BY LAZER

GENERAL INTRODUCTION

At the vicinity of the material, the laser beam is focused.

The incident flux and the time of the pulse gives a change in temperature that will give boiling temp. for the material in time less than the pulse length.

When these condition satisfied then vaporization established which has

\[ T(0,t) = 2 \varepsilon F/ K \left[ k t/ \pi \right]^{1/2} \quad (1) \]

Where \( k \), \( K \) are thermal constants of the substrate, as it's limiting speed (carlaw 1959).

\[ \varepsilon = \varepsilon F / (\lambda + \rho C T) \quad (2) \]

\( T \): vaporization temp. (°C)

\( F \): incident intensity (W/cm²)

\( \lambda \): Heat of vaporization (J/cm³)

\( C \): Specific heat(J/g°C)

\( \varepsilon \): emissivity at laser wavelength.

\( \rho \): density (g/cm³)

\( F \): assumed to be uniform at semi-infinite sheet, and all material is completely vaporized at equilibrium.

For good approximation: eqn. 2, is a function of time, then becomes:
The integral of the relation: \( \int dx = \int \nu dt \) (integral from 0 to \( t \))

\[ x(t) = \int \nu(t) dt = \left[ \frac{1}{\lambda + \rho C T} \right] \int \epsilon F(t) dt . \]  

(4)

where \( x(t) \): depth of penetration of the vaporization front at time \( t \).

So, the distance of the drilling depth, can be equated.

1. If the drilling depth is to be done at low intensity, long irradiated time are needed, and the fraction of available energy used for heating is very significant, especially when drilling metals.

2. If short, high power pulse are to be needed, then large fraction of the available energy can be used in the actual drilling process.

A. BULK HEATING AND VAPORIZATION:

If the heat equally dividing between the bulk heating and vaporization, if we equating the penetration distance of the heat \( x \) into the solid produced by half the flux, then we have:

The drilling depth relation:

\[ \nu \cdot t_p = (k t_p)^{1/2} \]  

(5)

Also called characteristic heat penetration.

\[ (k t_p)^{1/2} = \left[ \frac{C (F/2) t_p}{\dot{\lambda} + \rho C T_{vap}} \right] \]  

(6)

Solve for \( F \), results:

H.W

B. DRILLING WITH LOW INTENSITY PULSES
At LASER power $P = 10^6$ (watt/cm²) ; $T = T_b$ ( $T_b$ : boiling temp. )

$$P = \pi A K T_b/ C(T_b) \quad ---- \quad (8)$$

Minimum values of ($p/r$) for the production of boiling on the surface with 10.6 μm focused on circular area of radius $r$ (cm).

Copper and gold have high values amongst.

After the onset of boiling, the rate at which drilling proceed is determined by the concentration of energy equation:

$$\nu = C F / (\lambda + \rho CT) \quad (9)$$

Where we set $T = T_b$ ; $P = P_c$ ; and $C = C(T_b)$,

$$\nu = [C(P - P_c)] / [r^2\pi(\lambda + \rho CT_b)]$$

$F = P / r^2\pi$ (watt/cm²), $r$ is the radius of circular area.

where $P_c$ : is the conserved power. $T_b$ : boiling temp.

$$\nu = C F / (\lambda + \rho CT_b) \quad (10)$$

$$= C P / [(r^2\pi)(\lambda + \rho CT_b)] \quad (11)$$

Using the above equation to predict the velocity, and knowing the pulse time ($t_{\text{pulse}}$), the depth can be predicted as follows:

$$x = \nu (t_p - t_{\text{vap.}}) = [C(P - P_c)(t_p - t_{\text{vap.}})] / [(r^2\pi)(\lambda + \rho CT_b)]$$

----------(12)

The depth is:

$$x = \int [C(P - P_c)] / [(r^2\pi)(\lambda + \rho CT_b)] dt.----- \quad (13)$$

Where $P = P(t)$.

C. DRILLING WITH HIGH INTENSITY PULSES

For short irradiation times, eqn. below:
\[ T(0,0,t) = \left[ 2P \epsilon (kt)^{1/2} \right] \left[ 1/(\pi)^{1/2} - i \text{erfc}(t/2.\sqrt{kt}) \right] / r^2 \pi K \]  

\( (14) \)

For short irradiation times, the above eqn. reduced to:

\[ T = \left( 2P \epsilon / r^2 \pi^{3/2} K \right)(kt)^{1/2} \]  

\( (15) \)

One can predict \( t_{vap} \). To onset of vaporization, if \( T = T_b \)

\[ t_{vap} = \left[ \pi^3 r^4 KT_b^2 \right] / \left[ 4 P^2 \epsilon^2 k \right] \]  

\( (16) \)

so, \( t_{vap} \alpha 1/(\text{intensity})^2 \); typically \( \approx \text{ms (milliseconds)} \)

For KW–CW LASERS and much less for normal pulsed laser, but varies greatly from one metal to another.

TABLE shows time \( t_{vap} \) to onset of vaporization of metal surfaces of incident intensity \( F \) of 10.6\( \mu \)m radiation.

After the surface has reached the vaporization temperature, removal of material is governed by the conservation of energy equation:

\[ \psi = \epsilon P / r^2 \pi (\lambda + \rho C T_{vap}) \]  

\( (17) \)

And the thermodynamic eqn.:

\[ \psi = C \exp(-\lambda z / \rho N_A k_B T_{vap}) \]  

\( (18) \)

Where \( C \) : velocity of sound in the material;

\( \lambda \) : heat of vaporization (energy/unit volume); \( z \) : atomic number; \( \rho \) : density; \( N_A \) : Avogadro's number; \( k_B \) : Boltzman's constant.

\[ P / \pi r^2 = (C / \epsilon) (\lambda + \rho C T_{vap}) \exp(-z \lambda / \rho N k T) \]  

\( (19) \)

\( P / \pi r^2 \) is constant at low temperature. Temperature calculated is close to boiling temperature \( T_b \). \( T = T_b \) at low intensity pulse is justified.

At high intensity \( (Q \text{--} \text{switched}) \); temp. changes rapidly with intensity.

Now using:
\[ \psi = \frac{C P}{[r^2 \pi (\lambda + \rho C T_{vap.})]} \] (20)

and

\[ \psi = C \exp\left(-\frac{\lambda z}{\rho N_A k_B T_{vap.}}\right) \quad \text{(21)} \]

To predict the velocity (\(\psi\)) and knowing the duration of the applied pulse \(t_p\), the depth of drilling (\(x\)) can be predicted from the expression:

\[ x = \psi (t_p - t_{vap.}) \quad \text{(22)} \]

where \(t_{vap.}\) is obtained from:

\[ t_{vap.} = \frac{\pi^3 r^4 K^2 T_b^2}{[4 P^2 C^2 k]} \quad \text{(23)} \]

so, (\(x\)) can be evaluated by integration relative to the time.
CHAPTER SIX
LASER HEATING OF SOLIDS: THEORY

INTRODUCTION

SOLUTION OF BASIC HEAT EQUATION:

Heat equations:

\[ \Delta^2 T - (1/k) \frac{\partial T}{\partial t} = - \frac{A(x,y,z,t)}{K} \quad (1) \]

Or

\[ \frac{1}{k} \frac{\partial T}{\partial t} = \Delta^2 T + \frac{A(x,y,z,t)}{K} \quad (1) \]

The conduction of heat in three dimension solid is given in general by the solution to the eqn.:

\[ \rho C \cdot \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} (K \cdot \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (K \cdot \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (K \cdot \frac{\partial T}{\partial z}) + A(x,y,z,t) \quad (2) \]

where: \( \Delta^2 T = \frac{\partial}{\partial x} (\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (\frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (\frac{\partial T}{\partial z}) \)

and

\[ k = \frac{K}{\rho C} \quad \text{or} \quad \frac{1}{k} = \frac{\rho C}{K} \]

\( k \): Thermal diffusivity = \( K / \rho C \)

\( K \): Thermal conductivity; \( \rho \): density; \( C \): specific heat.

\( K, \rho, C \): are dependent on \( [T] \) and positions \( x,y,z \); \( A(x,y,z,t) \): heat supplied to the solid at the rate \( [A] \) per unit time per unit volume.

NOTE

Thermal properties of most materials do not vary greatly with \( T \). They can often be assumed independent of \( [T] \), and can be assigned an average value of the \( T – \text{rang of interest} \).

Assume the solid is taken to be homogenous and isotropic, then equation two reduced to:

\[ \Delta^2 T - (1/k) \frac{\partial T}{\partial t} = - \frac{A(x,y,z,t)}{K} \quad (1) \]
In steady state, when $\frac{\partial T}{\partial t} = 0$ ---(3)

Substitute equation (3) in (1) to obtain:

$$\Delta^2 T = - \frac{A(x,y,z,t)}{K} \quad ------ \quad (4)$$

*Eqn. (1) and (4) can be solved in a large number of cases as follows:

* If there is no heat is supplied to the material, then $A = 0$; and eqn. (1):

$$\Delta^2 T - \frac{(1/k)\partial T}{\partial t} = - \frac{A(x,y,z,t)}{K}$$

becomes:

$$\Delta^2 T - \frac{(1/k)\partial T}{\partial t} = 0 \quad \text{or} \quad \Delta^2 T = \frac{(1/k)\partial T}{\partial t} \quad ------ \quad (5)$$

[ Equation (5) is called time dependence case ].

*Also when $A = 0$; then equation (4):

$$\Delta^2 T = - \frac{A(x,y,z,t)}{K}$$

becomes:

$$\Delta^2 T = 0 \quad ------ \quad (6)$$

[ Equation (6) is called steady state case ].

In practice, cases in which heat sources are present or absent can be solved by imposing on the solution of (5) and (6), the appropriate boundary conditions of applied heat flux and transfer across the surface of solid.
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