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Module 4: Introduction to Alloys and Application of Spectroscopy in Metal Analysis.

Introduction

Learning Outcomes

Upon completion of this topic, you will be able to,

1. **Understand Ferrous Alloys & Plain Carbon Steels:** Grasp their composition, properties, and industrial applications.
2. **Analyze Effects of Alloying Elements (Cr, Ni, W, Co, V)** Explain how each element modifies steel's strength, toughness, corrosion resistance, and high-temperature performance.
3. **Explore Shape Memory Alloys (SMAs)** Define SMAs, describe their unique properties, and identify key applications in biomedical, aerospace, and robotics fields.
4. **Apply Spectroscopic Methods for Metal Analysis-** Understand spectroscopy basics, principles of AAS and colorimetry, and use Beer-Lambert's Law for quantitative determination.
5. **Evaluate Purpose & Applications of Common Alloys**: Recognize why alloys are made and describe composition, properties, and uses of Duralumin, Magnalium, German silver, and Gun metal.

Introduction

Definition of Alloys
An alloy is a homogenous mixture of two or more elements one of which must be a metal.

<div align="center">OR</div>

An alloy is a substance made by combining together two or more elements where the primary element is a metal. Alloys are basically a homogeneous mixture of two or more than two metals, or a metal or a non-metal.

Properties of Pure Metals
1) Pure metals often lack the ideal combination of mechanical properties—such as hardness, ductility, and tensile strength—necessary for specific applications.
2) Working with pure metals can be challenging, often requiring specialized techniques and tools for shaping, fusing, or combining them.
3) While high thermal conductivity can be beneficial in certain contexts, it can be disadvantageous in applications requiring thermal insulation.

Limitations of Pure Metals:
1) Compared to alloys, pure metals typically have lower hardness and tensile strength, making them less suitable for structural applications that require high strength.
2) Many pure metals have poor wear resistance, leading to faster degradation in applications involving friction or abrasion.
3) Numerous pure metals are prone to corrosion when exposed to air, moisture, or chemicals. For example, iron readily rusts when in contact with oxygen and water.

Purpose of Making Alloys:
1) ***To Increase Hardness:*** *Alloys are generally harder than their pure metal components. For instance:*

- *Gold and Silver:* Pure gold and silver are soft, but alloying them with a small amount of copper enhances their hardness and wear resistance, making them suitable for jewelry and coins.
- *Iron:* Pure iron is often unsuitable for many uses, while steel, made by combining iron with carbon, is much stronger. Additional metals like chromium, nickel, and manganese can further enhance specific properties.
- *Copper:* Alloying copper with zinc or tin results in brass or bronze, which are both harder than pure copper.

2) **To Lower Melting Point:** *Alloys typically have lower melting points than their individual components, as the alloying elements act as impurities.*
- *This property is utilized in low-melting alloys, such as Solders, which are now often lead-free and based on SnCu or SnAgCu compositions.*
- *Wood's Metal an alloy of bismuth, tin, lead, and cadmium melts at 71°C, much lower than its individual components.*

3) **To Modify Color:** *Alloying can change the color of a base metal, allowing for the creation of visually distinct alloys. For example:*
- *Aluminium and Tin: When alloyed with copper, aluminium bronze exhibits a striking golden hue, despite aluminium and tin being silvery white.*
- *Brass: This yellow alloy results from combining red-brown copper and silvery-white zinc.*
- *Electrum: A natural alloy of gold and silver, its color varies from pale to bright yellow depending on the proportions of its components. Man-made versions are often referred to as green gold.*

4) **To Enhance Corrosion Resistance:** *Pure metals like iron and copper are reactive and susceptible to corrosion.*
- *Iron: While pure iron corrodes easily in moisture, stainless steel (an alloy of iron with carbon, chromium, and nickel) resists corrosion effectively.*
- *Copper Alloys: Brass, an alloy of zinc and copper, shows greater resistance to sulfuric acid than pure zinc, while other copper-based alloys like naval brass exhibit strong corrosion resistance.*

5) **To Improve Casting Properties:** *Alloys often have better casting characteristics, allowing them to fill molds more precisely. Unlike pure metals, which shrink upon solidification, many alloys expand slightly, improving dimensional accuracy in castings.*
- *For instance, adding manganese to aluminium and copper enhances tensile strength.*
- *Gun metal (88% Cu, 10% Sn, and 2% Zn) and phosphor bronze are examples of copper alloys with excellent casting properties.*

6) **To Alter Chemical Reactivity:** *The reactivity of metals can be modified through alloying, either increasing or decreasing it.*
- *For example, aluminum amalgam (Al-Hg) is more reactive than pure aluminum, whereas sodium amalgam (Na-Hg) is less reactive than pure sodium.*
- *Adding silicon to aluminum can enhance oxidation resistance, slowing the oxidation rate compared to pure aluminum.*

7) **To Reduce Malleability and Ductility:** *Pure metals are highly malleable, which can be a disadvantage in certain applications.*

- *For example, pure gold is too soft for making durable ornaments. However, alloying it with copper or silver enhances its hardness, making it suitable for various designs.*
- *Tool Steel: Alloys of iron with high carbon content and elements like chromium and molybdenum are very hard and wear-resistant but have reduced ductility and malleability.*

Non-Ferrous Alloys
Non-ferrous alloys do not contain iron as a primary element. Common elements in non-ferrous alloys include aluminum, copper, lead, zinc, tin, and nickel.

Main Properties of Non-Ferrous Alloys:
1) *Lower melting points compared to ferrous alloys.*
2) *Excellent formability.*
3) *Attractive and appealing colors.*
4) *Good cold working characteristics.*
5) *Special electrical conductivity properties.*
6) *Magnetic properties.*
7) *Easy to cast.*
8) *Low friction coefficient.*
9) *High resistance to atmospheric corrosion.*
10) *Low density.*

Important Non-Ferrous Alloys are:

Aluminium alloys *are popular in the engineering industry because they are:*
- *Lightweight and easy to handle.*
- *Highly resistant to corrosion, so they last longer.*
- *Good conductors of heat and electricity.*
- *Malleable and ductile, meaning they can be shaped and stretched without breaking.*
- *Can be cast, forged, welded, extruded, and rolled into different shapes.*
- *Four times stronger than the same weight of mild steel.*

Aluminium alloys-Duralumin

Alloy	Composition	Characteristics	Uses
Duralumin	Al = 95%, Cu = 4%, Mn = 0.5%, Mg = 0.5%	Light in weight, tough, highly ductile, easily castable, good conductor of heat and electricity, corrosion resistant.	Commonly used in the aircraft industry (as Alclad), automobile and locomotive parts, surgical instruments, cables, and fluorescent tube caps.

Copper alloys *are known for excellent corrosion resistance, electrical and thermal conductivity, and formability.*
- *Brass (copper and zinc) is stronger than pure copper, and adding other metals improves properties like ductility and machinability.*
- *Bronze (copper and tin) is stronger and harder than brass, but it is more expensive and superior in performance.*

Comparison between brass and bronze:

Brass	Bronze
Alloy of copper and zinc	Alloy of copper and tin
Lower corrosion resistance than bronze	Superior corrosion and shock resistance
Cheaper due to zinc	More expensive due to tin
Less strong and hard than bronze	Stronger and harder than brass
Toughness makes it difficult to machine	Easier to machine
Used in hardware, musical instruments, and fasteners	Used in valves, gears, bearings, and chemical equipment

Alloys of Copper (Brass)-German Silver / Nickel Silver

Alloy	Composition	Characteristics	Uses
German Silver/Nickel silver	Cu = 60%, Zn –=20%, Ni =20%	Good strength and corrosion resistance to salt water. Ductile, malleable, and looks like silver.	Used in utensils, tableware, bolts, screws, ornaments, cutlery, corrosion-resistant implements, coinage, decorative articles.

4.1 Ferrous Alloys

4.1.1 Plain Carbon Steel

a) What is Plain Carbon Steel?

Plain Carbon Steel is a type of steel that primarily consists of iron and carbon, with no significant amounts of other alloying elements. Principal hardening element is carbon in steel. It increases tensile strength, hardness, raises wear and abrasion resistance, lowers ductility, toughness, machinability.

b) Give the basic classification of Plain Carbon Steel - Based on Carbon Content:

Steel Type	Carbon Content (%)	Key Characteristics	Common Applications
Low carbon content (Mild Steel)	0.15-0.30%	Good balance of strength and ductility	Structural applications, MS roundbar in RCC, construction, Rail tracks
Medium Carbon Steel	0.3-0.8%	Higher strength, moderate hardness	Machine parts, gears, axles, clutch plates, hydraulic fittings
High Carbon Steel	0.8-1.50%	Maximum hardness, wear resistance	Cutting tools, lathes, drills, chisels

MILD STEEL (M.S.) ROUND BARS ARE USED FOR REINFORCEMENT IN REINFORCED CEMENT CONCRETE (RCC).

HYDRAULIC FITTINGS LIKE CYLINDERS, RAMS, SHAFTS, TURBINE ROTORS ETC.

c) Drawbacks of Plain Carbon Steel

1) Corrosion Vulnerability
   ● High susceptibility to rust and corrosion.
   ● Lacks chromium coating like stainless steel (10-12% chromium).
   ● Requires additional protective measures (e.g., painting or coating).
2) Manufacturing Challenges
   ● Difficult to bend or mold due to high strength.
   ● Needs specialized machinery and techniques.
   ● Increases potential for costly waste and rework.
3) Temperature Limitations
   ● Lower heat resistance than stainless steel alternatives.
   ● Prone to damage at elevated temperatures.
4) Material Property Drawbacks
   ● Reduced weldability with higher carbon content.
   ● Decreased ductility as carbon content increases.
5) Maintenance Considerations
   ● Requires regular maintenance to prevent corrosion.

4.1.2 Alloy Steel
a) What is Alloy Steel? : Alloy steel is a type of steel that is alloyed with various elements to improve its properties, such as strength, hardness, resistance to wear and corrosion, and durability. Unlike plain carbon steel, which primarily contains iron and carbon, alloy steel contains additional elements like Ni, Cr, Co, W, V, Mo, Mn in varying amounts.

b) Write a note on Stainless Steel.

Stainless steel prevents rust through a simple but effective process:

1. The Protective Layer
   - When chromium (at least 10.5%) is exposed to air, it instantly forms a thin, invisible layer.
   - The film prevents moisture from reaching the underlying metal so rust cannot form. This layer is like a protective shield that covers the entire surface.
   - The layer is made of chromium oxide and is extremely thin, about 2-3 nanometers (1 nanometer is 1 billionth of a meter!)

2. Self-Repairing
   - If the protective layer is damaged (scratched or worn away) the chromium reacts with air to immediately form a new protective layer.
   - This self-repairing process happens automatically as long as there's enough chromium and oxygen present.

c) Explain the effect of alloying elements in steel.

Element	Primary Effects	Practical Applications
Nickel (Ni)	• Improves tensile strength, hardness, toughness -fatigue resistance without loss in ductility. Corrosion resistance	• Marine hardware, low temperature, heavy duty applications. • Chemical processing equipment • High-strength structural components
Chromium (Cr)	• Up to 18% addition possible • Below 1.5%: Enhanced tensile strength • At 12%: High corrosion resistance • Improves hardness and toughness simultaneously	• Ball bearings • Metal working rolls • Gears and axles • Springs
Cobalt (Co)	• Enhances strength and thermal stability • Improves wear resistance • Maintains high performance at elevated temperatures	• Aerospace applications • Nuclear industry components • High-speed cutting tools
Tungsten (W)	• Improves toughness and hardness • Increases shock resistance • Promotes fine grain structure • Maintains strength at high temperatures	• High-speed cutting tools • Wear-resistant parts • Rocket nozzles
Vanadium (V)	• Promotes fine grain structure • Increases hardenability • Imparts strength and toughness to heat-treated steel	• High-speed tool steels • Spring steel • Turbine blades

What are the uses of alloy steels?

Due to their advantageous characteristics, alloy steels have multiple uses, especially in industry. They fall into two main categories: construction and tool steels.

Alloy steels for construction

The construction industry relies on certain alloys to provide the material properties they need. Examples include high hardness and strength, ductility, toughness, low corrosion, and resistance to wear and high temperatures, among many other things. In the main, these are

steels alloyed with nickel, chromium, chromium-molybdenum, chromium-nickel and chromium-nickel-molybdenum.

Alloy tool steels

Other steels are more suitable for the manufacture of tools. These often contain nickel, chromium, tungsten, vanadium or molybdenum. The following properties are important in these applications:

- Wear resistance
- Oxidation/rust resistance
- High impact and shock resistance
- Resistance to high temperatures
- Resistance to deformation
- Suitability for non–high speed cutting

Examples are hammers, pliers, standard wrenches, Allen wrenches, files, saws, clamps, and gouges, among many others.

4.2 Spectroscopic Determination of Metals from Metal ion solutions

4.2.1 Interaction of Electromagnetic Radiation with Molecules-Introduction and Pre-requisite

When electromagnetic radiation strikes a molecule, it can undergo various wave-based and particle-based interactions:

Wave Nature Effects

- Reflection: Light bounces off the surface.
- Refraction: Light bends when passing through different media.
- Interference: Overlapping waves create patterns of constructive/destructive intensity.
- Diffraction: Light bends around edges or through slits (special case of scattering).
- Scattering: Light changes direction due to interaction with particles (e.g., Rayleigh scattering makes the sky blue).
- Optical Rotation: Rotation of polarized light by chiral molecules.

Particle Nature Effects

- Absorption: Molecules absorb photons, promoting electrons to higher energy levels.
- Emission: Excited molecules release photons as they return to lower energy states.
- Transmission: Light passes through the substance without being absorbed.

Color and Perception

- The color of an object depends on the wavelengths of light that are reflected, transmitted, emitted, or scattered.
- A green leaf reflects green light and absorbs other wavelengths.
- An object that absorbs all wavelengths appears black.
- An object that reflects all wavelengths appears white.
- A transparent object appears colored based on the light it transmits.

Real-World Examples

- Rainbow: Caused by refraction and dispersion of sunlight in water droplets.
- Blue Sky: Due to scattering of short-wavelength light.
- Sunset Redness: Longer wavelengths dominate as shorter ones scatter away.
- Sodium Lamps: Emit monochromatic yellow light due to atomic emission.

Definition of Spectroscopy: Spectroscopy is the scientific study of the interaction between matter and electromagnetic radiation. It involves observing how atoms or molecules absorb, emit, or scatter light (or other types of radiation) to gain information about their structure, composition, and properties.

Definition of Spectrum: A spectrum is a graphical or visual display of the different wavelengths or frequencies of electromagnetic radiation that are absorbed, reflected, scattered, transmitted, or emitted by an object, atom, or molecule.
When radiation interacts with matter, certain wavelengths are affected differently depending on the material's properties. This variation is recorded by a detector and plotted as intensity versus wavelength (or frequency), forming a spectrum.

Types of Spectroscopy - Based on Radiation-Matter Interaction
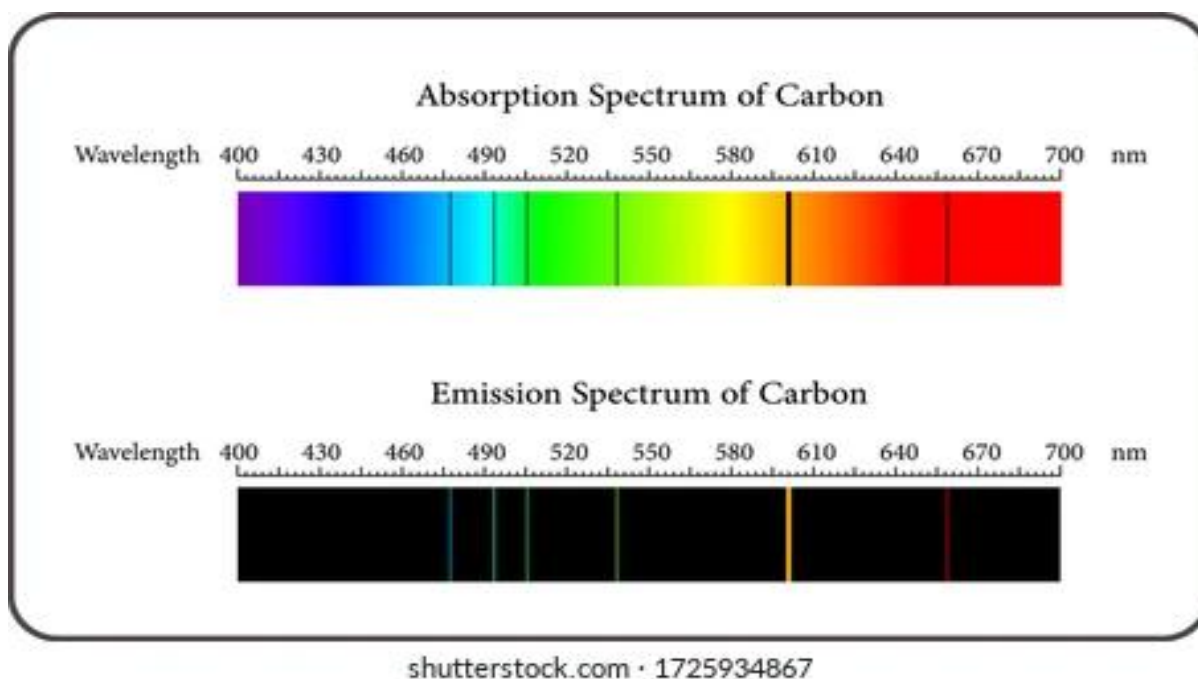### 1) Absorption Spectroscopy
In absorption spectroscopy, the focus is on the absorption of radiation by atoms or molecules as a function of wavelength. When light passes through a sample, certain wavelengths are absorbed by the sample's atoms or molecules, reducing the intensity of light at those wavelengths.
- When gases are placed between a light source and the detector, they absorb light at specific narrow wavelengths corresponding to their energy transitions.
- This absorption creates a pattern called an absorption spectrum, which appears as a series of dark lines (missing wavelengths) on a continuous background of light.
- Each atom or molecule produces a unique absorption spectrum, which can be used to identify and quantify substances.

2) Emission Spectroscopy
Emission spectroscopy involves observing the emission of radiation from atoms or molecules as they return from an excited state to a lower energy state.
- When atoms or molecules are energized (e.g., by heating or electrical excitation), they emit light at specific wavelengths characteristic of their energy transitions.
- The resulting emission spectrum can be of three types:
  - Line Spectrum: Produced by isolated atoms. The emitted radiation appears as sharp, well-defined lines at precise wavelengths.
  - Band Spectrum: Occurs when small molecules or radicals emit light. The emission lines overlap to form bands of light instead of discrete lines.
  - Continuous Spectrum: Observed from hot solids, stars, or the sun, where radiation is emitted over a continuous range of wavelengths without interruption.
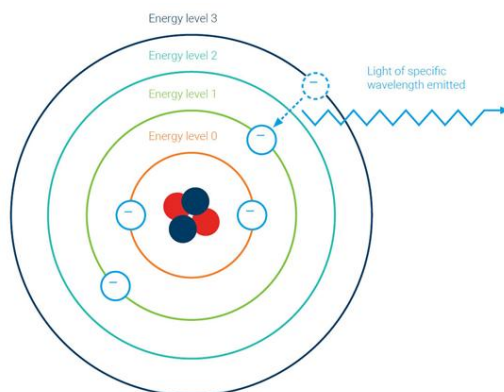
Absorption Spectrum of Carbon

Emission Spectrum of Carbon

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Summary:

Type	Observed Interaction	Appearance of Spectrum	Source
Absorption Spectroscopy	Absorption of specific wavelengths	Dark lines on continuous background (absorption lines)	Gases absorbing light
Emission Spectroscopy	Emission of radiation	Line spectrum (sharp lines), band spectrum (overlapping lines), or continuous spectrum	Excited atoms, molecules, hot solids

4.2.2 Atomic Absorption Spectroscopy
What is Atomic Absorption Spectroscopy (AAS)?

AAS is an analytical technique used to determine how much of certain elements are in a sample. It uses the principle that atoms (and ions) can absorb light at a specific, unique wavelength. When this specific wavelength of light is provided, the energy (light) is absorbed by the atom. Electrons in the atom move from the ground state to an excited state. The amount of light absorbed is measured and the concentration of the element in the sample can be calculated.
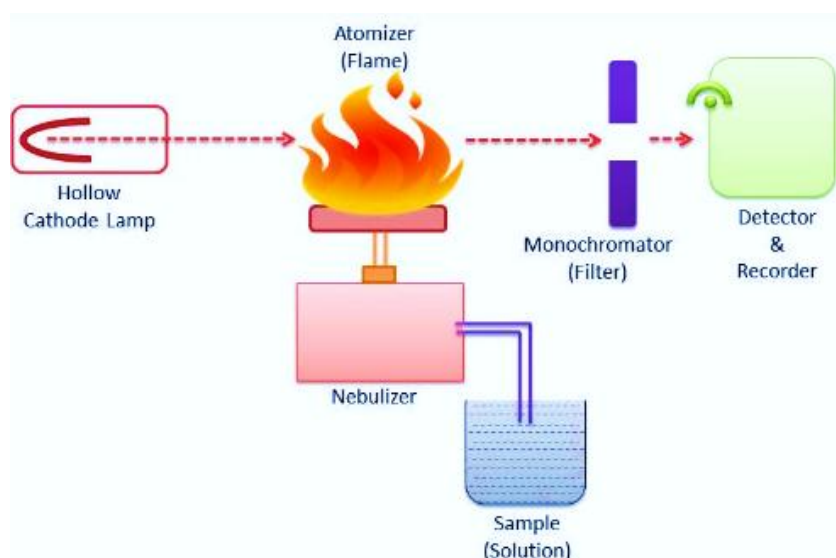

The Beer-Lambert Law describes the relationship between light absorption and concentration of the element. According to the law, the amount of light absorbed is proportional to the number of atoms excited from the ground state in the flame.

Atomic Absorption Spectroscopy (AAS)

Atomic Absorption Spectroscopy (AAS) is an analytical technique that measures the concentration of elements by analyzing the light absorbed by free atoms in the gaseous state.

1) In this method, a sample—typically a liquid containing metal ions—is first atomized using a flame or graphite furnace, converting it into free atoms.

2) A light beam of a specific wavelength, usually emitted by a hollow cathode lamp that matches the element of interest, is then passed through the atomized sample.

3) The atoms absorb this light, and the amount of light absorbed is directly proportional to the concentration of the specific element present.

4) AAS is especially useful for detecting and quantifying metals and trace elements such as lead, iron, copper, and zinc. It offers high sensitivity and specificity, with detection limits often reaching parts per billion (ppb). Because each element absorbs light at a unique wavelength, AAS provides reliable and accurate results even in complex sample matrices.

5) However, AAS requires sophisticated instrumentation, including a radiation source, atomizer, monochromator, and detector, as well as a high level of operator expertise.

6) The instruments are costly, and the analysis process can be more time-consuming due to sample preparation and calibration.
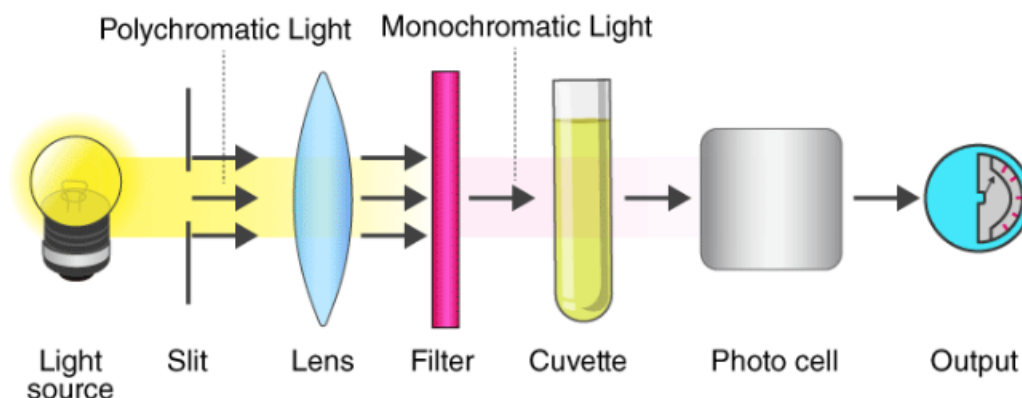

Applications: AAS is commonly used in environmental monitoring, clinical diagnostics, food and drug safety, mining, and industrial quality control—especially when precise trace metal detection is required.

4.2.3 Colorimetry for Metal Detection

Colorimetry can detect certain metal ions in solution by reacting them with specific reagents to form colored complexes. The intensity of the resulting color is then measured using a colorimeter or UV-visible spectrophotometer, and it is directly proportional to the metal ion concentration in the sample.

How It Works:
1. Metal ions (like Fe^{2+}, Cu^{2+}, Pb^{2+}, Ni^{2+}, etc.) are dissolved in water or an appropriate solvent.
2. A color-forming reagent is added that reacts selectively with the metal ion to form a colored compound.
3. The absorbance of this solution is measured at a specific wavelength.
4. A calibration curve (absorbance vs. known concentrations) is used to determine the unknown concentration.

Light source — Slit — Lens — Filter — Cuvette — Photo cell — Output

Polychromatic Light   Monochromatic Light

Examples of Colorimetric Metal Detection:

Metal Ion	Reagent Used	Color Produced	Application
Iron (Fe^{2+}/Fe^{3+})	1,10-Phenanthroline or Thiocyanate	Orange-red complex	Water and soil testing
Lead (Pb^{2+})	Dithizone or Sodium rhodizonate	Pink to red complex	Paint, water testing (field kits)
Nickel (Ni^{2+})	Dimethylglyoxime (DMG)	Red/pink precipitate	Industrial wastewater analysis

Unlike AAS, colorimetry does not require atomization or specialized lamps. It is simple, rapid, and cost-effective, making it ideal for routine applications. However, it is generally less sensitive and less specific, with detection limits in the parts per million (ppm) range. It is also more susceptible to interference from other colored substances, turbidity, or light-scattering particles in the sample.

Applications: Colorimetry is widely used in areas such as water quality testing (e.g., measuring chlorine, nitrates, or phosphates), food and beverage industry (e.g., sugar or dye content), pharmaceutical analysis, and clinical laboratories (e.g., estimating glucose or protein levels). Its low cost and portability also make it valuable for fieldwork and educational purposes.

Distinction Between Atomic Absorption Spectroscopy (AAS) and Colorimetry

Criteria	Atomic Absorption Spectroscopy (AAS)	Colorimetry
Principle	AAS is based on the absorption of light by free atoms in the gaseous state. A sample is atomized (converted to atoms), typically by a flame (or graphite furnace), and a beam of light at a specific wavelength (characteristic of the element being analyzed) is passed through it. The amount of light absorbed is directly proportional to the concentration of the element in the sample.	Colorimetry is based on the absorption of light by colored solutions or compounds. When certain chemicals react, they form colored products. The intensity of the color is measured using a colorimeter or spectrophotometer, and is proportional to the concentration of the substance producing the color.
Nature and State of Sample	AAS requires the sample to be converted to free atoms in the gaseous phase, typically through thermal atomization (using a flame or graphite furnace).	Colorimetry is used for liquid samples, specifically solutions that are either naturally colored or become colored after a chemical reaction.
Type of Analytes Measured	AAS is element-specific and is primarily used for detecting and quantifying metallic elements and some metalloids (e.g., lead, copper, iron, zinc, mercury).	Colorimetry is used for a broader range of substances, including inorganic ions, organic compounds, and biomolecules, provided they can form colored compounds.
Sensitivity and Detection Limits	AAS is highly sensitive, with detection limits in the parts per billion (ppb) range, making it ideal for trace analysis of metals.	Colorimetry has moderate sensitivity, usually with detection limits in the parts per million (ppm) ranges.
Specificity	AAS provides high specificity because each element absorbs light at a unique wavelength. Monochromatic light is used, often generated by a hollow cathode lamp specific to the element of interest.	Colorimetry can be less specific since multiple compounds might produce similar color responses. Interfering substances can affect color intensity unless proper reagents or masking agents are used.
Instrumentation	Requires a sophisticated Atomic Absorption Spectrophotometer, which includes: - a radiation source (hollow cathode lamp) - atomizer (flame or furnace) - monochromator - detector	Uses a colorimeter or UV-Visible spectrophotometer which includes: - a light source (tungsten filament lamp) - filter (monochromator) - cuvette (sample holder) - detector. These are simpler and more affordable instruments compared to AAS systems.

Cost and Accessibility	AAS instruments are expensive, require regular calibration, special gases, and trained personnel. Typically used in advanced laboratories.	Colorimetry is low-cost, easy to use, and more accessible in routine laboratories, field testing kits, and educational settings.
Applications	AAS is used in: - Environmental analysis (e.g., heavy metal contamination in water/soil) - Clinical diagnostics (e.g., measuring trace metals in blood) - Pharmaceuticals - Food safety - Mining and metallurgy	Colorimetry is applied in: - Water quality testing (e.g., nitrates, phosphates) - Food and beverage analysis (e.g., sugar content, color additives) - Pharmaceuticals (e.g., drug concentration) - Biochemistry (e.g., protein or glucose estimation in clinical samples)
Sample Preparation	Sample preparation for AAS may involve digestion with strong acids, filtration, and sometimes dilution, to bring the analyte into a suitable form for atomization.	Sample preparation is often simple—mixing the sample with reagents to produce a colored compound and then measuring absorbance.
Limitations	- Expensive and requires skilled operation - Cannot measure non-metallic elements - Requires calibration and correction for interferences	- Less sensitive and specific - Color may be affected by turbidity or impurities - Not suitable for colorless compounds without derivatization

4.2.4: Beer-Lambert's Law

What is the Beer-Lambert Law?

The Beer-Lambert law relates the concentration of a sample to the amount of light the sample absorbs as it passes through the sample. The equation for the Beer-Lambert Law is generally written as:

$A = \epsilon L c$

where

A = Absorbance

ϵ = Molar extinction coefficient
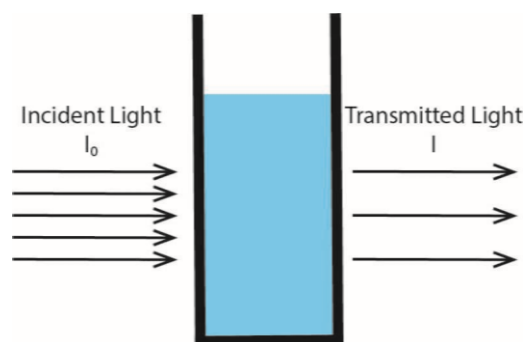
L = Path length

c = Concentration of the sample

The absorbance is related to the ratio of the intensity of light that enters the sample and leaves the sample.

$A = \log_{10}(I_0/I)$

where

I_0 = Incident Light- Intensity of light before sample

I = Transmitted Light- Intensity of light after sample
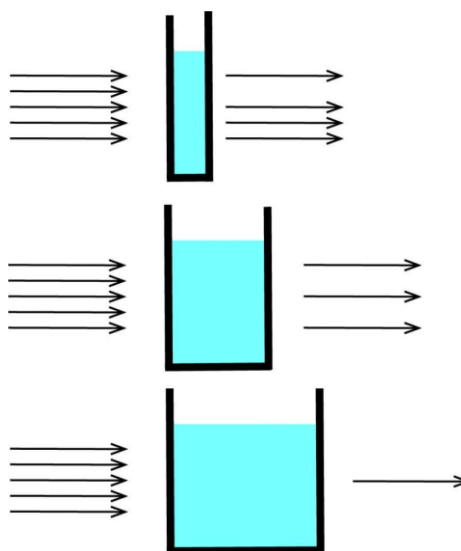
As light passes through a sample some of the light will be absorbed by the sample.

The Beer-Lambert Law is commonly used in <u>absorption and transmission measurements</u> on samples and can be used to determine the concentration of a sample.

In an absorption measurement, light passes through a cuvette filled with a sample. The intensity of the light after the cuvette is compared to the light before passing through the cuvette. The size of the cuvette determines the path length (L). (A cuvette is a special piece of <u>glassware</u>.) The wider the cuvette, the more sample the light will pass through, and the transmitted light will be lower. This explains why the equation is dependent on path length (L).

As the path length (L) gets larger, the amount of transmitted light decreases. Therefore, the absorption increases.
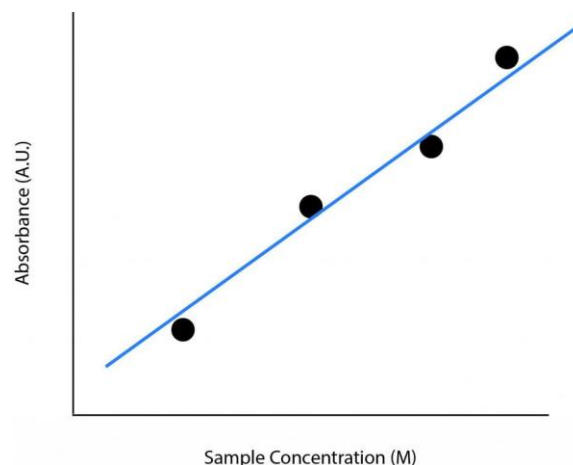
What is the Molar Extinction Coefficient?

The molar extinction coefficient is specific to every chemical and an important variable in the Beer-Lambert law. The molar extinction coefficient measures how much light a substance absorbs and is wavelength specific. It is also sometimes referred to as the molar absorption coefficient or molar absorptivity. In equations, it is most often symbolized as epsilon, ϵ.

The units of the molar extinction coefficient are most commonly $M^{-1}cm^{-1}$. The units should match the units of the path length and sample concentration. That way the absorbance results in a unitless number. On a graph, the absorbance is often written with units of A.U., which stands for arbitrary units.

Beer-Lambert Law Graph

A typical graph illustrating the Beer-Lambert law will be linear and positively correlated. The x-axis will have units of concentration and the y-axis will be absorbance. This indicates that the other two variables in the equation, molar extinction coefficient and path length, are held constant.

As the concentration increases, the absorbance will also increase. This pattern makes sense because if the concentration increases, there are more molecules present to absorb light and cause an increase in absorption.

Limitations of the Law

The law tends to become inaccurate at high concentrations. This is due to a combination of different factors. The refractive index of the solution may deviate. There are saturation and aggregation effects possible due to the molecule of interest interacting with each other (not just solvent as is the situation at low concentrations). An excellent way to test the limitations of the Beer-Lambert Law is to make a plot of concentration verse absorption at increasingly high concentrations for a sample. The plot should be linear, but at high concentrations will stop being linear. At this point, high concentrations are causing the law to be inaccurate.

4.2.5: Numerical

Example Problem 1: A chemist has a sample of Adenine with an absorbance of 0.67 at a wavelength of 260 nm. The Molar absorption coefficient ε_{260} is 7100 M⁻¹cm⁻¹. The path length of light is 1.00 cm. What is the concentration of the sample?

Solution1:

Step 1: In the example problem we are given the absorbance of the sample, the Molar absorption coefficient, and the path length of light. Concentration of the sample needs to be calculated.

Step 2: Using the Beer-Lambert Law equation, we can rearrange to solve for concentration (c): or

$$A = \varepsilon c l$$

or

$$c = \frac{A}{\varepsilon l} = \frac{0.67}{(7100 M^{-1}cm^{-1})(1.00cm)} = 9.4 \cdot 10^{-5} M$$

Example Problem 2: A chemist has a sample of Phenylalanine with an absorbance of 0.81 at a wavelength of 257 nm. The Molar absorption coefficient ε_{257} is 8850 M⁻¹cm⁻¹. The path length of light is 3.00 cm. What is the concentration of the sample?

Solution2:

Step 1: In the example problem we are given the absorbance of the sample, the Molar absorption coefficient, and the path length of light. Concentration of the sample needs to be calculated.

Step 2: Using the Beer-Lambert Law equation, we can rearrange to solve for concentration (c):

$$A = \varepsilon c l$$

or

$$c = \frac{A}{\varepsilon l} = \frac{0.81}{(8850 M^{-1}cm^{-1})(3.00cm)} = 3.1 \cdot 10^{-5} M$$

Example Problem 3: A solution of rhodamine dye of unknown concentration. Using a spectrometer you measure the absorption to be 9048. You know the molar extinction coefficient of rhodamine is 116000 cm⁻¹ M⁻¹. The cuvette you used has a path length of 1 cm. What is the concentration of your sample?

Solution3:

Here we are trying to determine the value of C in the Beer-Lambert Law. So we start by rearranging the equation to solve for the variable we are looking for

A = εLc

c = A / εL

Then we can start plugging in values. Make sure to pay attention to units so that our concentration comes out with units of molarity.

c = 9048 / (1 cm * 116000 cm^{-1} M^{-1})

c = 9048 / 116000 M^{-1}

c = 0.078 M

The concentration of the unknown solution is 0.078 M.

PLEASE NOTE:

Both Terms Mean the Same Thing:
- *Name Variants:*
    - *Molar absorption coefficient*
    - *Molar extinction coefficient*
    - *Molar absorptivity*
- *Symbol: ε:(epsilon)*
- *Units :$M^{-1} \cdot cm^{-1}$*
- *Definition: It measures how strongly 1 mole of a substance absorbs light at a particular wavelength, per 1 cm of path length in a 1-liter solution.*
- *Used in: Beer-Lambert Law*

$$A = \varepsilon \cdot c \cdot l$$

  where
    - *A = absorbance*
    - *ε = molar extinction/absorption coefficient*
    - *c = concentration (mol/L)*
    - *l = path length (cm)*

Why the Different Names?
- *"Extinction" is more commonly used in physics and older literature.*
- *"Absorption" is preferred in chemistry and biochemistry.*
- *Functionally, they are identical when applied as ε\epsilonε in spectrophotometry.*

Bottom Line:

Yes, the molar absorption coefficient and molar extinction coefficient are the same thing — just different names for ε in Beer-Lambert's law.
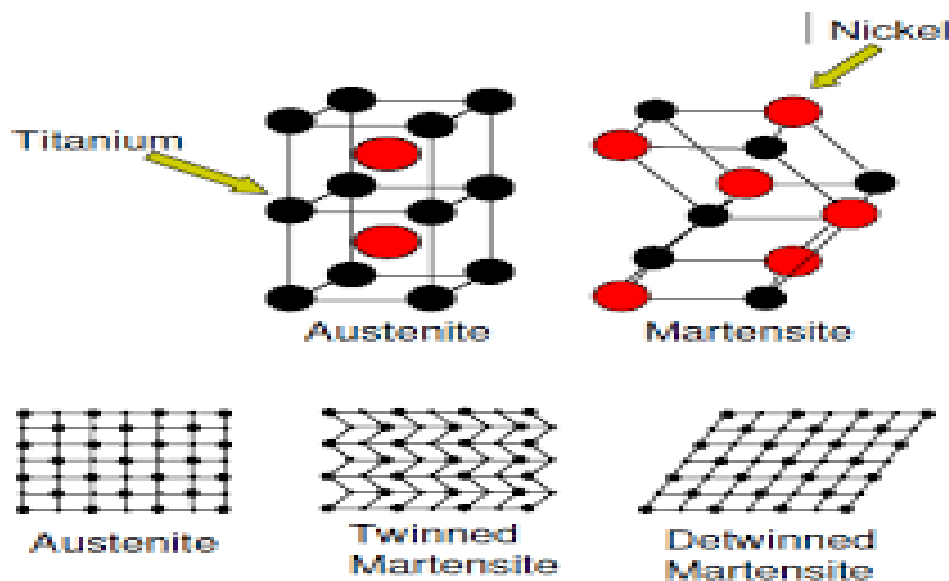
4.3 Shape Memory Alloys (SMA):

Alloys that have a "memory." These materials have the ability to remember and recover their original shapes with load or temperature. SMAs exhibit a solid-to-solid, reversible phase transformation.

Superelasticity is a remarkable property of shape memory alloys (SMAs) that allows them to undergo large elastic-like deformations and return to their original shape upon unloading. This behavior occurs through a unique mechanism involving martensitic phase transformations, making it fundamentally different from conventional metal elasticity.
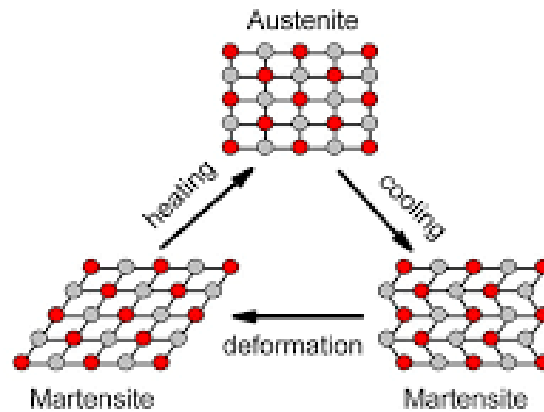
Mechanism of Superelasticity

Superelasticity operates through a stress-induced phase transformation between two main phases:

- **Austenite**: The high-temperature phase -CUBIC. **Austenite** is a phase that occurs at high temperature having a crystal structure and high degree of symmetry (cubic)
- **Martensite**: The low-temperature phase that forms under stress-MONOCLINIC . It is easily deformable phase which exists at low temperature (monoclinic)
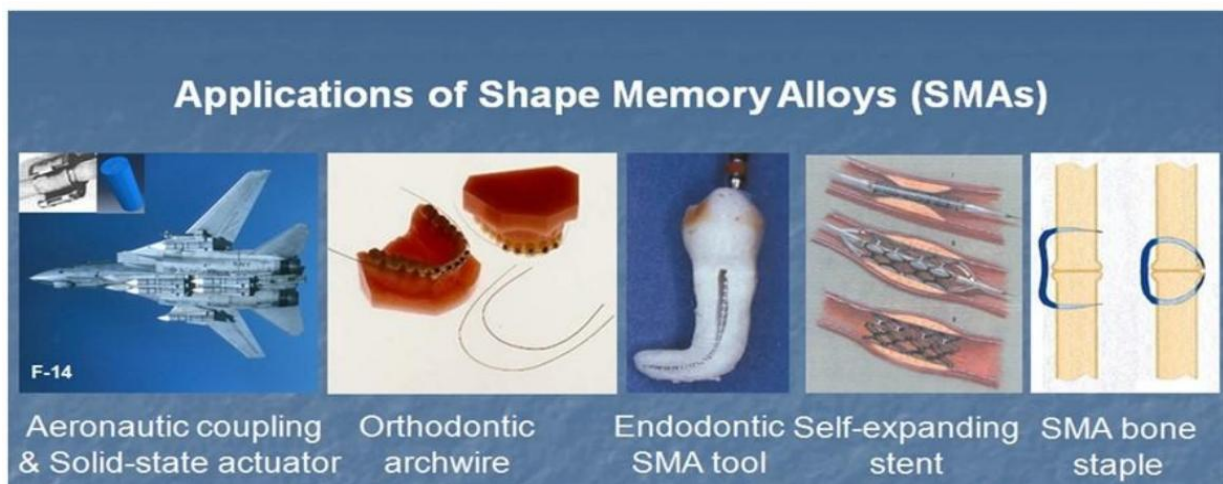

Feature	One-Way SME	Two-Way SME
Number of remembered shapes	One (austenite)	Two (martensite and austenite)
Response to temperature	Shape recovery only on heating	Shape changes on both heating and cooling
Need for training	Not required	Required
Complexity	Simpler	More complex

Examples of Shape memory alloys

Generally, shape memory alloys are intermetallic compounds having super lattice structures and metallic ionic - covalent characteristics. Thus, they have the properties of both metals and ceramics.

- **Ni - Ti alloy (Nitinol)**
- **Cu - Al- Ni alloy**
- **Cu - Zn - Al alloy**

Applications of SMAs:

1) **Medical Applications:** Super elastic SMAs have revolutionized many medical tools and implants due to their biocompatibility, super elasticity, and thermal activation behavior.

   a) **Stents for Arteries and Vessels**
   - Function: Tiny tube-like structures inserted into narrowed or blocked blood vessels to keep them open.
   - How it works: The stent, made of Nitinol, is compressed into a small diameter and inserted into the body using a catheter. Once exposed to body temperature (~37°C), the SMA expands and regains its original (larger) shape.
   - Advantage: Minimally invasive surgery, self-expanding capability, long-term durability, and compatibility with MRI scans.
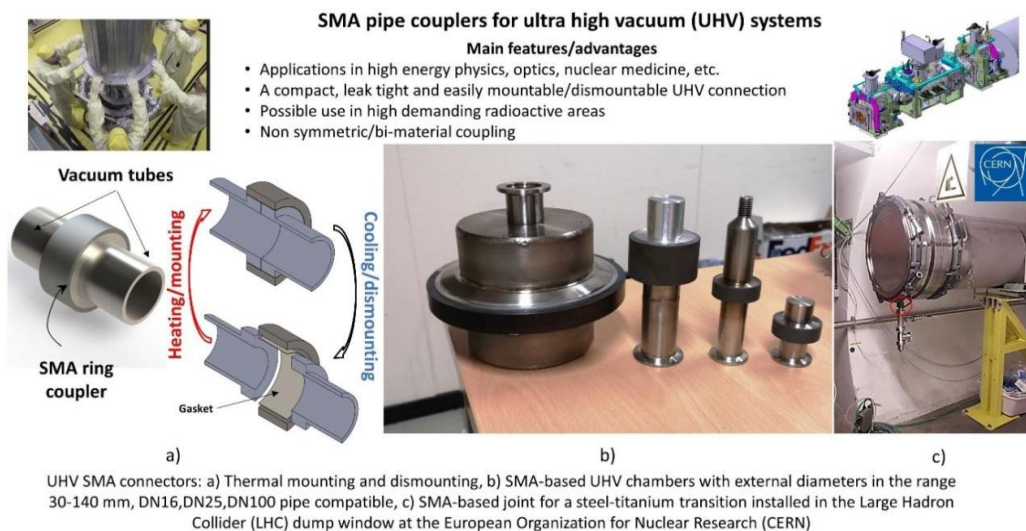
b) Orthodontic Wires (Braces)

- Function: Used in dental braces to apply constant pressure to teeth to realign them.
- How it works: Nitinol wires apply a gentle, continuous force as they try to return to their original shape, guiding teeth into correct alignment.
- Advantage: Less discomfort for patients, fewer adjustments needed, and more effective treatment.

2) Industrial applications:
SMA Pipe Couplings

- Function: SMA pipe couplings join two pipes by gripping them tightly without welding or adhesives.
- How it works: The coupling is expanded at a low temperature or mechanically to fit over pipe ends. When heated above its transformation temperature, the SMA contracts to its original size, creating a strong, leak-proof seal.
- Advantage: Provides a secure, durable joint that resists pressure and vibration, with quick and easy installation.
- Applications: Widely used in industries requiring reliable and corrosion-resistant pipe joints, such as oil and gas pipelines, chemical processing plants, aerospace systems, and water supply networks. Also suitable for marine environments, nuclear reactors, offshore platforms, and underground piping due to its resistance to harsh conditions and mechanical stresses.

UHV SMA connectors: a) Thermal mounting and dismounting, b) SMA-based UHV chambers with external diameters in the range 30-140 mm, DN16,DN25,DN100 pipe compatible, c) SMA-based joint for a steel-titanium transition installed in the Large Hadron Collider (LHC) dump window at the European Organization for Nuclear Research (CERN)

3) From Mars to Your Bike
SMA Tyres

- Shape Memory Alloy (SMA) tyres, originally developed by NASA for Mars rovers, are now being adapted for everyday use—starting with bicycles. The SMART Tire Company leads this innovation with its METL™ airless bike tyres, which use a nickel-titanium alloy called NiTinol+.

- Key Features:
  Airless Design: No inner tube, so they never go flat.
  Superelasticity: Can deform under pressure and return to their original shape.
  Durability: Withstand extreme terrain and temperatures.
  Sustainability: Use 50% less rubber than traditional tyres and are re-treatable.
- Origins in Space Exploration:
  NASA needed tyres that could survive the harsh Martian terrain—rocky, sandy, and extremely cold. Traditional rubber tyres weren't viable, so engineers turned to SMA materials. These tyres could flex and recover without damage, making them ideal for rovers like Curiosity and future lunar missions.

4) Eyeglass frames, Mobile phone antennas, Earthquake dampeners, Micro-actuators

Advantages

This unique combination of high strain recovery and mechanical stability makes super elastic shape memory alloys invaluable for applications requiring reversible deformation under load.