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Predicting of glass transition temperature of tellurite oxide glasses using Support vector regression

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In front of the jury members:

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Dedication

In the name of Allah, first and foremost, and with your support, I dedicate this work to the cornerstone of my life, to the best people in my life, to my dear parents; without whom I cannot imagine life, to the most precious person in existence, my beloved mother. I ask Allah to guide me in honoring her, prolong her life, and heal her from every illness. To the one who removed thorns from my path and illuminated the way of knowledge for me, my dear father, may Allah grant him continued support. To those without whom the world loses its sweetness, my dear siblings, the flame of hope in my life and the source of strength, you are my family. You have provided me with unconditional support and continuous encouragement throughout my life, believing in my abilities. Here I am today, capable of achieving accomplishments and overcoming challenges.

to my large family, uncles, and aunts, and to my companions on the journey, to my friends whom I will never forget, for their presence beside me during the toughest moments of my life. Thanks to your support, I am here today.

To all those who i meet them in my academic journey, and to those who gathered around the study table, to everyone who contributed to my academic journey, I dedicate this work and express my gratitude to each and every one of you

Aib Elkansa

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General Introduction

General Introduction

The history of glass manufacturing dates back to ancient times, and over the centuries, glassmaking techniques have continuously evolved. In the Middle Ages, glass gained significant importance in architecture and other fields. In the 17th century, new techniques were developed for glassmaking, leading to improvements in the physical and chemical properties of glass. In the 20th century, the glass industry witnessed a major revolution in technology and design. Advanced techniques were developed to produce glass with precise and diverse specifications. A wide range of innovative glass products emerged, such as heat-insulating glass, soundproof glass, safety glass, tempered glass, and smart glass that interacts with the environment. Glass has become an integral part of our daily lives. It is used in windows, doors, furniture, and household items like dishes and cups. It is also utilized in chemical, electronic, medical, and construction industries. Modern glass technologies are present in various fields such as technology screens, optical fibers, and solar panels. Thanks to technological advancements and innovation, glass continues to offer new and creative applications, remaining a fundamental material in our daily lives and modern industry Glass is an amorphous solid characterized by a transparent window in the electromagnetic spectrum and a glass transition temperature. Its structure is disordered, similar to that of a liquid, showing only short-range order. It is a non-equilibrium material, possessing excess internal energy. It is more or less stable against devitrification, the process of returning to equilibrium during which its atoms rearrange to crystallize.

Additionally, when heated above its glass transition temperature, it exhibits sufficient viscosity for easy shaping (such as fiber drawing or molding), a property not found in crystalline solids. The three main categories of glass typically distinguished are oxide, halide, and chalcogenide glasses, with the addition of metallic glasses and organic glasses. The properties of materials in their glassy state have been a subject of extensive scientific interest. This unique state occurs when the liquid form of a material is cooled below its melting point, but it does not undergo crystallization. The resulting glassy solid can exhibit intriguing mechanical and electrical properties that differ from those present in the crystalline state. By studying the glassy state and glass transition processes, we can improve our understanding of the properties and physical behavior of glassy materials, polymers, and related substances. This understanding contributes to the development of new and enhanced applications in various fields, ranging from windows to electronics, making research in this area highly valuable One of the methods used to predict the glass transition temperature in glass is the utilization of machine learning algorithms, such as

Support Vector Regression (SVR). SVR relies on leveraging machine learning techniques to build a model capable of predicting future values based on historical data. The use of SVR in this study to predict the glass transition temperature of tellurite oxide glasses involves utilizing a set of available variables that can affect the glass transition temperature, such as glass composition, manufacturing temperature, and chemical element compatibility. The SVR model is trained using known experimental data, where the relationship between the independent variables and the glass transition temperature is established.. The use of machine learning algorithms in glass development and understanding the glassy state and glass transition offers several advantages. It allows for data-driven analysis and prediction, which accelerates the research and development process. It also enables the exploration of complex relationships between various factors and glass properties that may not be readily apparent through traditional methods.

Moreover, machine learning algorithms can uncover novel correlations and patterns that may lead to the discovery of new glass compositions or optimization of existing ones. This can facilitate the design of different types of glasses tailored for specific applications, such as optical fibers, displays, or energy-efficient windows. The application of machine learning algorithms in glass development and understanding the glassy state and glass transition provides powerful tools for analysis, prediction, and optimization. It accelerates research, enables data-driven decision-making, and opens up new possibilities for innovative glass materials and applications.

In this study, we examined the effectiveness of Support Vector Regression (SVR) in predicting the glass transition temperature (Tg) using different kernel functions, including the Radial Basis Function (RBF), polynomial, sigmoid, and linear kernels. Their performance was evaluated using metrics such as R2 and RMSE This memorandum is divided into three chapters, in addition to a general introduction and a conclusion.

Chapter I: This is a theoretical study in which generalities about glass will be presented. One of the key elements of this work will be discussed, which is the glassy state and the glass transition temperature.

Chapter II: In this chapter, we introduced the concept of machine learning and discussed its techniques. Additionally, we provided an explanation of Support Vector Regression (SVR), which was utilized in our study.

Chapter III: In the final chapter, the obtained results will be presented, followed by their discussion, analysis, and interpretation.

Chapter I

Generalities about glass

1) Introduction

Glass carries both historical and practical significance as it is one of the oldest and most important materials produced by humans[1]. In ancient times, glass was highly valued and considered one of the precious metals, as evidenced by the discovery of a glass bead decorated with golden masks in the tombs of the Pharaohs. In modern times, glass has become one of the most widely used materials in various applications, including household items, fiber-optic communications[2],screen and laser production, The high value of glass is attributed to its exceptional and unique properties, such as transparency, hardness (resistance to scratches and holes), and high chemical resistance. Glass can be made in different shapes and sizes, making it suitable for a wide range of applications. It can also be mixed with rare earth ions and microcrystals to meet specific requirements. Glass materials have unique structural and thermal properties, giving them an advantage over crystalline materials.

Researchers' opinions vary on the origin, uses, and history of glass due to the lack of accurate evidence. Nevertheless, the history of industrial glass manufacturing dates back to 3000 BC and developed slowly over the ages. It significantly developed during the Roman period, where glass production reached advanced levels. The fourth century AD was considered the first golden age of glassmaking, and since then, the technology of glass production and its uses has continued to evolve in many different applications in daily life[3].

2) States of matter

The material in the four known states (solid, liquid, gaseous, and plasma) is composed of atoms or molecules that move permanently. These states differ from each other due to the nature of the interactions between the material's atoms and molecules[4]. Each state can be physically distinguished by its flow or fluidity property, where the material flows freely in its gaseous and liquid states and takes the shape of the container in which it is placed. On the other hand, gaseous or liquid material loses its ability to flow when it transforms into the solid state after being cooled and takes on a fixed shape and size. Materials can be classified into two main types.

2.1)Crystalline material:

Crystalline materials are substances that exhibit a regular arrangement of atoms in space, forming a periodic geometric pattern. If this pattern extends throughout the material, it forms a single crystal. However, if the periodicity of the geometric pattern is disrupted, resulting in

boundaries between small groups of atoms or small single crystals in different orientations, the material is referred to as polycrystalline. The defining characteristic of crystalline materials is the presence of long-range order in the spatial distribution of atoms or molecules. This is evidenced by the diffraction peaks representing the different atomic planes, which can be observed using X-ray diffraction techniques. These materials consist of atoms, ions, or molecules arranged in organized geometric structures, with a fundamental unit called the unit cell.

2.2) Amorphous materials

Non-crystalline materials, also known as amorphous materials, lack a regular and repeating arrangement of atoms or molecules in space. Instead, they exhibit a disordered, random arrangement, which prevents them from forming a well-defined crystal lattice structure. Non-crystalline materials are characterized by the absence of sharp diffraction peaks in X-ray diffraction patterns, in contrast to crystalline materials. Examples of non-crystalline materials include glass, certain plastics, and some metals and alloys that are rapidly cooled from the molten state.

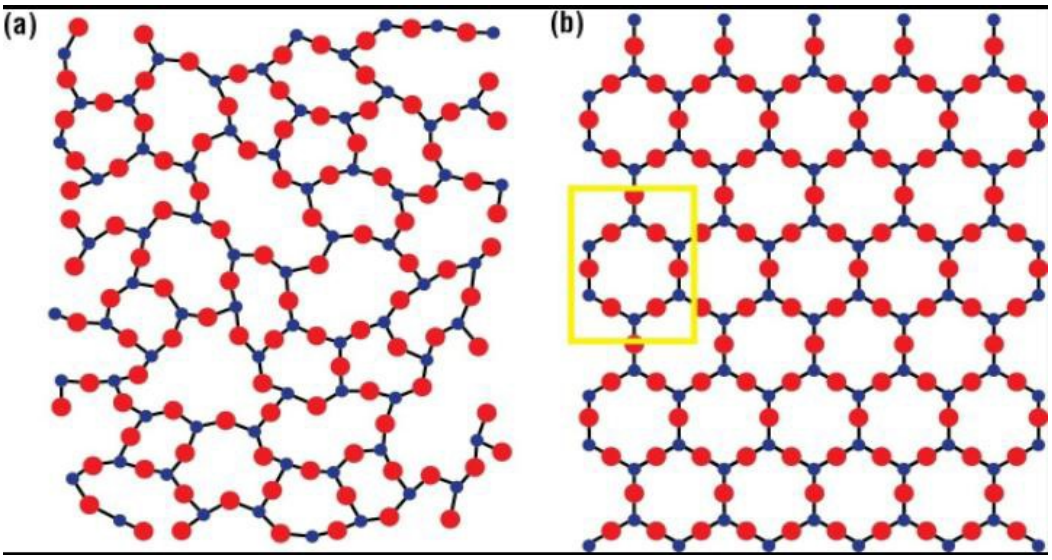


fig (1.I): a) Non-crystalline solid material, (b) Crystalline solid material

3) The definition of glass

Glass is a non-crystalline and homogeneous solid material,with its atoms randomly distributed at equal distances. It is characterized by the phenomenon of glass transition or vitrification , where it transforms from a liquid state to a solid state without crystallizing, and it is obtained by rapidly cooling the molten glass liquid[5] .Glass melts at very high temperatures, and it does not have a specific melting point, but rather gradually evolves from a solid state to a plastic state of viscosity. Glass is manufactured from different components, which are heated to high until they become viscous and then cooled. Glass is known for its transparency and ease of

refraction, as well as its excellent mechanical and chemical properties, making it a desirable material for many industrial and technological applications.

4) Glass Transition and glassy state

Regardless of the states of matter (liquid, solid, gas), substances can exist in other forms such as the glassy state, in which ordinary glass serves as an example. It is possible to convert almost any substance into the glassy state. The glassy state is usually obtained by cooling a system from the liquid state, for which the molecular mobility is important, to low temperature, at which the system can be considered as a solid obtained by avoiding the crystallization process. The glass transition corresponds to the temperature at which the system can be considered as frozen on the time scale of the experiment. Although this phenomenon is ubiquitious in nature and known for a long time, the molecular process by which liquids acquire rigidity upon cooling remain an open question in condensed matter science. This glass transition phenomenon, which is not a classical phase transition, is associated with both thermodynamics and kinetics processes,[6], In a structural definition, glass is described as a non-crystalline solid , in which each atom retains its characteristic environment of the crystalline state, more or less distorted, while the arrangement of the second neighbors is very disturbed compared to that of the crystal. We can also say that the glass is formed by a disordered three-dimensional assembly of fundamental structural groupings, similar to those of the crystalline state. But this description is too broad, as it encompasses amorphous materials which are not usually classified as glasses. A thermodynamic presentation describes glass as a non-equilibrium material , therefore presenting an internal energy content greater than that of the corresponding crystallized products, but whose return to a situation of stable equilibrium, i.e. the crystallization cannot take place even after considerable periods of time.

In a last definition, of phenomenological type, which involves a kinetic factor, the glassy state will be characterized by the presence of a glass transition , which is a characteristic transformation observed on cooling, during the passage from a supercooled liquid phase to a vitreous phase, or, conversely, to the heating of the glass with the supercooled liquid.[7]

Glasses are amorphous solids. The most common way to obtain amorphous solids is by rapidly cooling them from the liquid state so that they solidify without crystallization. The continuous increase in viscosity during the cooling of a liquid results in the liquid freezing until solidification. To study this process, the evolution of a thermodynamic variable (often the specific volume) is typically tracked as a function of temperature, as shown in Figure (2*I).

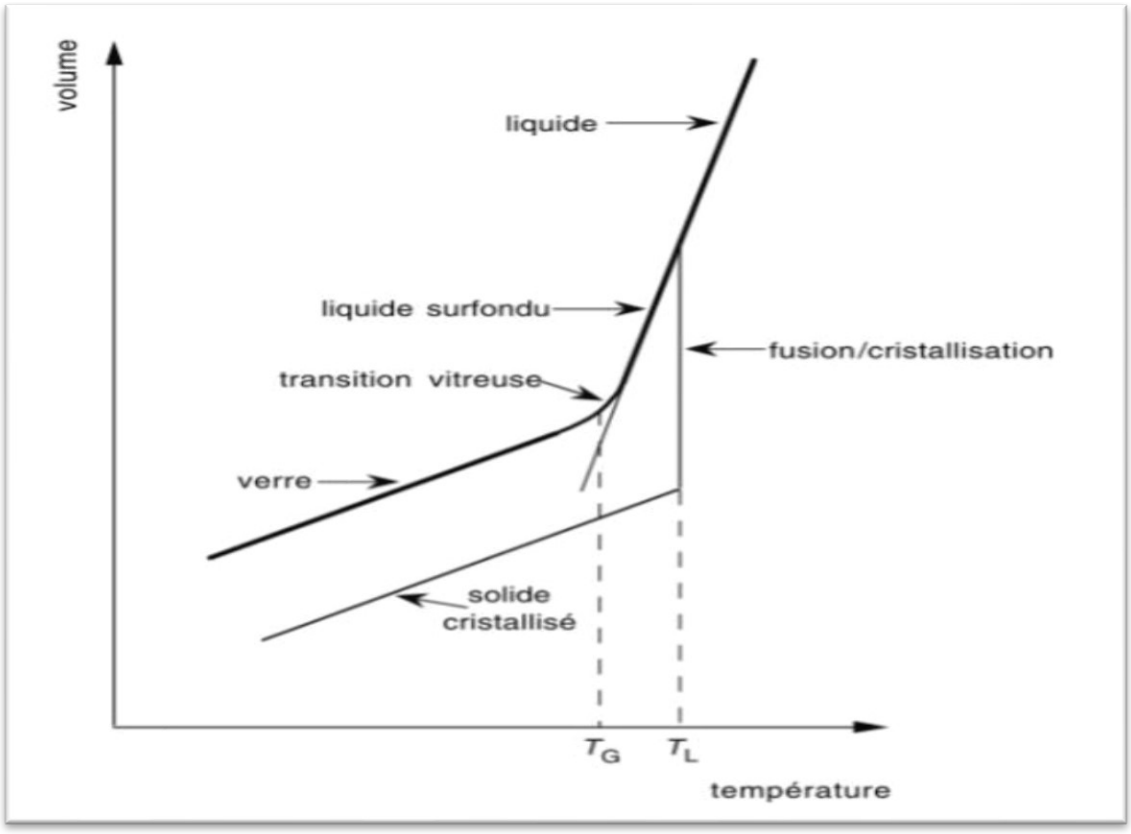


fig (6.I): Glass formation through rapid cooling

The temperature at which this process occurs is referred to as the glass transition temperature (Tg), which is significantly lower than the melting temperature (Tf);

This figure schematically shows the example of a sufficiently viscous liquid at TL to cross this temperature without crystallization. It can be observed that the volume below TL initially lies within the extrapolation of the values it takes above TL. However, at the temperature TG, where the viscosity reaches approximately 10^{12} Pa·s, there is a significant decrease in the slope of the curve, becoming similar to that of a crystalline solid. On the other hand, at this TG temperature, there is no abrupt change in volume as observed during the transition from the liquid to the solid state. This indicates that there is no structural variation during the TG transition. The substance obtained below TG, which has the structure of a liquid but the properties of a solid, is referred to as glass[8], The glass transition is also observed by tracking the variations, as a function of temperature, of various properties such as refractive index, enthalpy, and electrical conductivity. Consistently, a change in the slope of the curve representing the property as a function of temperature (T) is observed at TG.

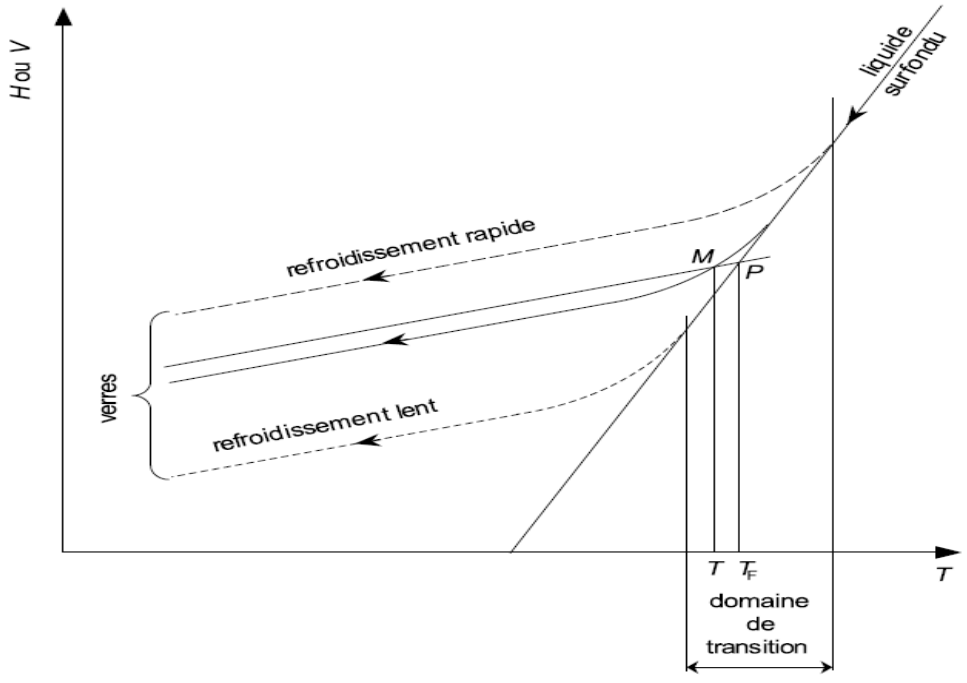
To understand the glass transition, we mention the third basic concepts:

. • A liquid is characterized by its structure, which refers to the molecular arrangement specific to each temperature, becoming more compact as the temperature decreases

. • The time required for a liquid to reach equilibrium in its structure at a given temperature, known as the "relaxation time" or more accurately the "delay time," is proportional to the viscosity.

• The glass transition occurs when the structure no longer has enough time to adapt to the temperature change.[9]

In a first approximation, the glass transition occurs when the viscosity is on the order of 10^{12} Pa·s, which corresponds to a structural relaxation time of around 10^{3} s. However, the notion of relaxation time implies that TG should decrease as the cooling rate decreases. Indeed, a closer examination reveals that the glass transition occurs at higher viscosities, or lower temperatures, when the cooling (or heating) process is slower. Therefore, the glass transition for a given liquid, unlike a true phase change, does not occur at a fixed temperature but varies depending on the cooling (or heating) rate within a temperature range known as the "glass transition interval" or "transition domain" (Figure 3*I).



fig(7.I):Schematic representation of the glass transition region and the fictive temperature (Tf) of a glass.

The supercooled liquid is in equilibrium at each temperature. Within the glass transition interval, it is indeed referred to as the "equilibrium liquid," and its properties are independent of its

thermal history. On the other hand, a glass is, from a thermodynamic perspective, an out-of-equilibrium system, and its properties depend, albeit marginally, on its thermal history[10]

In 1946, Tool following numerous experiments he conducted on glass annealing at the NBS laboratories, suggested that the structural state of a glass is fully determined by knowing, on one hand, its actual temperature T, and on the other hand, the temperature at which the glass would be in equilibrium, which he referred to as its "fictive temperature." It is accepted that this fictive temperature TF is the temperature of the liquid from which the glass in question would be obtained through instantaneous cooling. If the actual temperature of a glass and the value of one of its properties, such as refractive index or specific volume V, are known, its fictive temperature can be easily graphically estimated in the (T, V) diagram (Fig. 3)[5]

The abscissa TF corresponds to the intersection point P between the line representing the variation of volume of the supercooled liquid and the line drawn from point M representing the glass, parallel to the line describing the variation of volume of the solid with temperature. The concept of fictive temperature applies only to glasses. Above the glass transition interval, TF is necessarily equal to T. If a glass is held at a temperature T within the glass transition interval, its fictive temperature TF will tend towards T. Such a thermal treatment, referred to as stabilization or structural relaxation, gradually transforms a glass into an equilibrium liquid[10]

4.1)Thermal analysis

Thermal analysis involves measuring the physical and chemical changes that occur in a substance when it is subjected to heating. These changes include energy loss or absorption, weight fluctuations, dimensional alterations, and variations in durability. These transformations occur within specific temperature ranges, which differentiate various material types and are influenced by their thermal history. Consequently, thermal analysis helps in elucidating the underlying nature of the glassy state.

Among the thermal analysis methods, we can mention the following techniques:

Determination of the glass transition temperature by Differential Scanning Calorimetry (DSC)

Determination of the glass transition temperature by Dynamic Mechanical Analysis (DMA)

Determination of the glass transition temperature by Dilatometry (DIL)

Thermo mechanical Analysis (TMA)

Among the mentioned methods, we will focus on the Differential Scanning Calorimetry (DSC) technique in our study.

- **Differential Scanning Calorimetry (DSC):**

Calorimetry is one of several analytical techniques collectively known as thermal analysis methods. Differential Scanning Calorimetry (DSC) is a thermal analysis procedure designed to measure the energy absorbed or emitted by a sample as a function of temperature or time. In this context, the term "differential" refers to measurements that involve determining the relative behavior of a selected substance compared to a reference material. When a thermal transition occurs in the sample, DSC provides a direct calorimetric measurement of the enthalpy change at the reaction temperature. The fundamental principle of using DSC as a thermal analysis tool is the need to measure, as a function of temperature, the difference in heat required to increase the temperature of the sample relative to the reference material.[11]

5)Properties of glass

5.1) Optical Properties

- **Transparence**

The concept of light transmittance is closely related to glass, which is characterized by clear and homogeneous transparency that allows all wavelengths of light to pass through, from ultraviolet to infrared. Glass also possesses the property of retaining thermal radiation. Transparency is defined by the Beer-Lambert law[12],. as follows:

$$I=I_0 exp(-\alpha x) \quad \text{.....(1)}$$

I: Radiation intensity emitted

I_0 : Incoming radiation intensity.

x : Glass sample thickness

α: Absorption coefficient

- **Refractive index**

The refractive index(n) represents the speed of light propagation in glass and is the ratio between the speed of light(c) in a vacuum and the speed of light in glass cv.

$$n=c/cv \quad \text{.....(3)}$$

The refractive index varies with the frequency of the optical radiation and hence the wavelength changes, causing a decrease in the refractive index with an increase in the wavelength λ . This change is called dispersion and is given by the following relationship.

$$Dv=dn/d\lambda \quad \text{.....(4)}$$

When a bundle of light falls perpendicularly on a homogeneous glass sample, a part of this bundle is reflected on the interface, with a reflection coefficient R given by the following relationship:

$$R=(1-n)^2/(1+n)^2 \quad \text{.....(5)}$$

The other part penetrates into the sample, with a portion of it being absorbed, hence the term light transmission in glass is defined by the transmission coefficient T given by the following relationship:

$$T=I/I_0 \quad \text{.....(6)}$$

5.2) Thermal Properties

- **Thermal conductivity**

Glass has a weak thermal conductivity, where the rate of heat flow in it is much lower compared to metals. Regardless of any changes in the composition of glass, its thermal conductivity will not change significantly. The type of glass that has the highest thermal conductivity is silica glass.

- **Viscosity**

Viscosity is one of the most important properties of glass and a key factor in its shaping process. Viscosity is related to the temperature and chemical composition of the glass, as well as the liquid's resistance to shear stress. In other words, the higher the viscosity, the higher the shear stress on the glass. Glass can be considered a Newtonian fluid, meaning that the shear and normal stresses follow linear functions with respect to the strain(εij). Therefore, the viscosity coefficient of glass can be determined using the following equation[10]

$$\eta = dy/\tau dt \quad \text{.....(7)}$$

τ:Shear stress.

dy/dt: Angular deformation rate

- **Thermal expansion**

When a material is heated, it leads to an increase in its thermal energy and thus an increase in its atomic vibrations. If the bond strength between atoms is not strong enough, these vibrations lead to an increase in the length of atomic bonds and, consequently, an increase in the sample's volume. This phenomenon is called thermal expansion. The thermal expansion of a material is characterized by a factor that relates the change in length with temperature, called the linear thermal expansion coefficient or the coefficient of linear expansion, denoted by α, and a factor that relates the change in volume with temperature, called the volumetric thermal expansion coefficient, denoted by β. The linear thermal expansion coefficient is given by the equation[10]

$$\alpha\Delta T = L/L_0(\Delta L/\Delta T) \quad \text{.....(8)}$$

$\alpha_{\Delta T}$: The linear thermal expansion coefficient in the range.

$\Delta L/\Delta T$: The relative elongation of a sample with an initial length L0

ΔT: The thermal range considered.

The volumetric thermal expansion coefficient is given by the approximate relation:

$$\beta = 3\alpha \quad \text{.....(9)}$$

5.3)Electrical properties

At normal temperatures, glass is an electrical insulator and is considered a dielectric material in this state. The electrical resistance of glass varies with its composition, and at high temperatures, the resistance decreases, and the humidity increases the conductivity of the glass to electric current. Moreover, the rough surface of the glass reduces the resistance to current flow[10].

6) glass structure

Several hypotheses have been proposed to study the glass structure since the beginning of the twentieth century, including the crystal theory developed by a group of scientists: Lebedev, Valuenkov, and Oshitz-Poraik. This theory suggests that glass is formed from many small and organized atomic domains called crystals. The second theory, proposed by the scientist Zachariazen in 1932 (the random network model), suggests that the glass structure does not depend on

organized atomic domains, but rather on the nature and proportion of the oxides it is composed of [13], The glass structure is divided into two types:

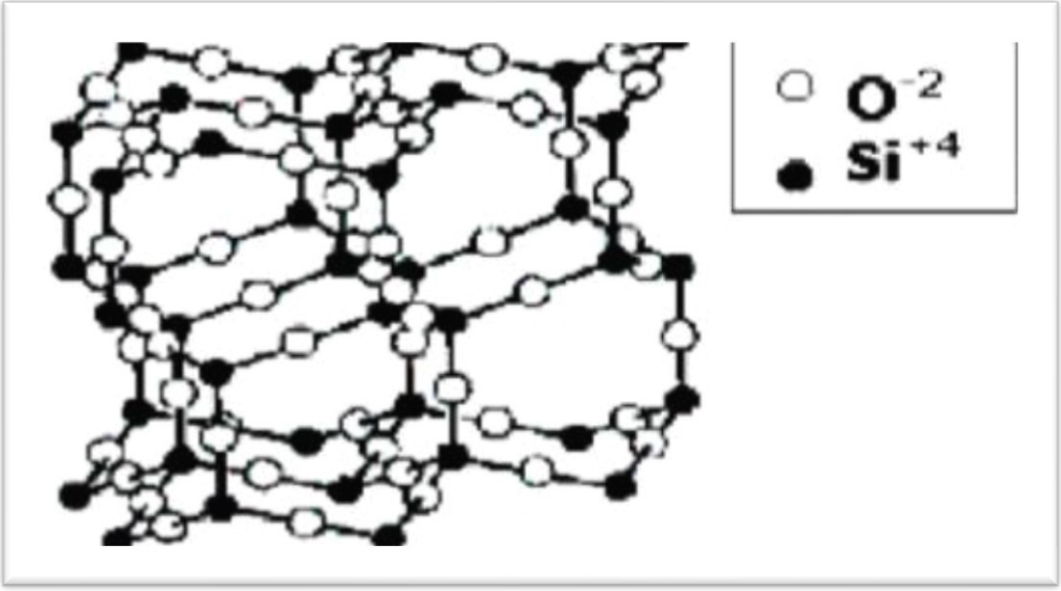
6.1)The simple structure

The simple glass is composed of only one oxide, often with a chemical formula of either SiO_2, Al_2O_3, or B_2O_3, where the molecules arrange themselves into multiple-faced shapes that depend on the chemical makeup of the constituent molecules[10]

-Silica glass composed of SiO_3 molecules.

-Phosphate glass P_2O_5.

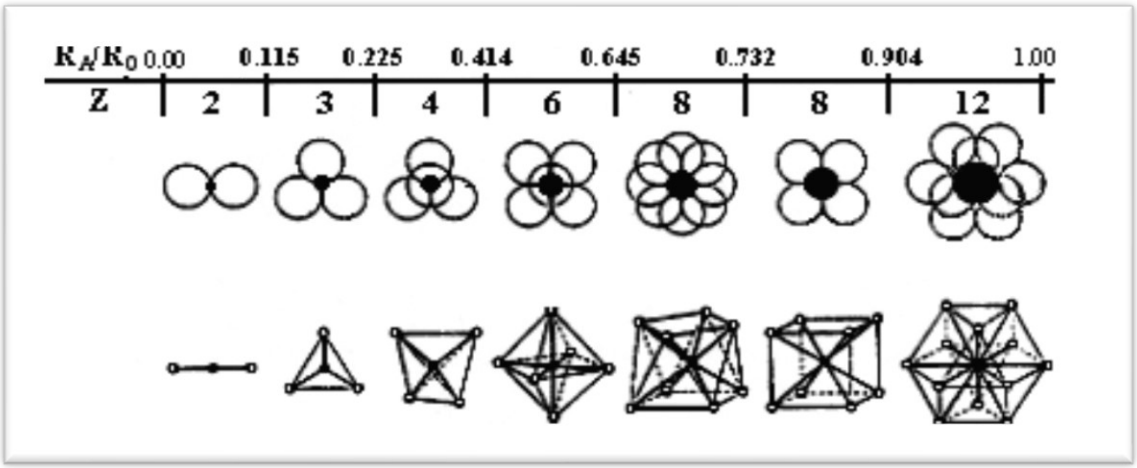
-Borosilicate glass composed of B_2O_3.



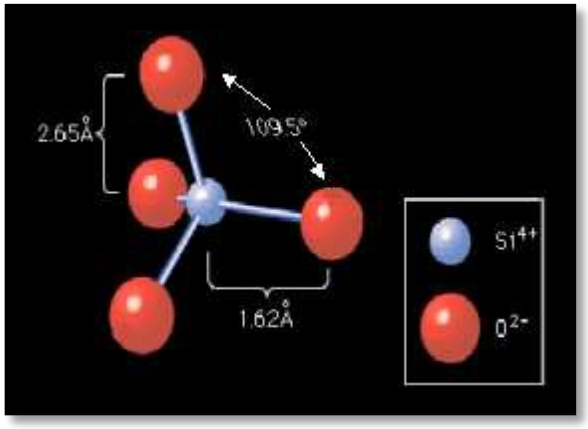
fig(8.I):The atomic structure of simple silica glass.

- **Goldsmith model**

Three negatively charged ions with a radius of RA=1 form a triangle, with a positively charged ion with a radius of RC= 0.155 located at the center. The chemical formula for this structure is CA3, which is triangular in shape and has a ratio of RC/RA.= 0.155, If the radius of the negatively charged ion is very large, then the stability of this structure is closest to 0.225, which corresponds to the chemical formula CA4, , a tetrahedral structure. If the ratio is equal to RC/RA= 0.414, then the structure is an octahedron. The corresponding stability regions for different values of the ratio between the radii of the negative and positive ions are shown in the figure below[14]



fig(9.I):The stability range of polyhedral is represented by a specific coordination number RC/RA.



fig(10.I): A spatial representation of the square pyramida sio4

- **Zachariasen model**

"Zachariasen" was able to establish conditions that must be met by oxide compounds with identical structural rules when comparing crystalline oxides and glassy oxides. These conditions should be met by oxide compounds with multiple faces to form a glassy structure upon assembly. These conditions are known as "Zachariasen's rules" and are as follows[15]

-The number of nearest neighboring cations is small, typically three or four.

-Each oxygen can bond to no more than two cations.

-Multiple faces share only vertices, not edges or faces.

-Each polyhedron has at least three vertices shared with other polyhedra.

These conditions are fulfilled for oxide compounds A_2O_3 ، AO_2 ، A_2O_5, And they are conducive to the formation of oxide glass, including SiO_2, P_2O_5, GeO_2, B_2O_3, and As_2O_3.

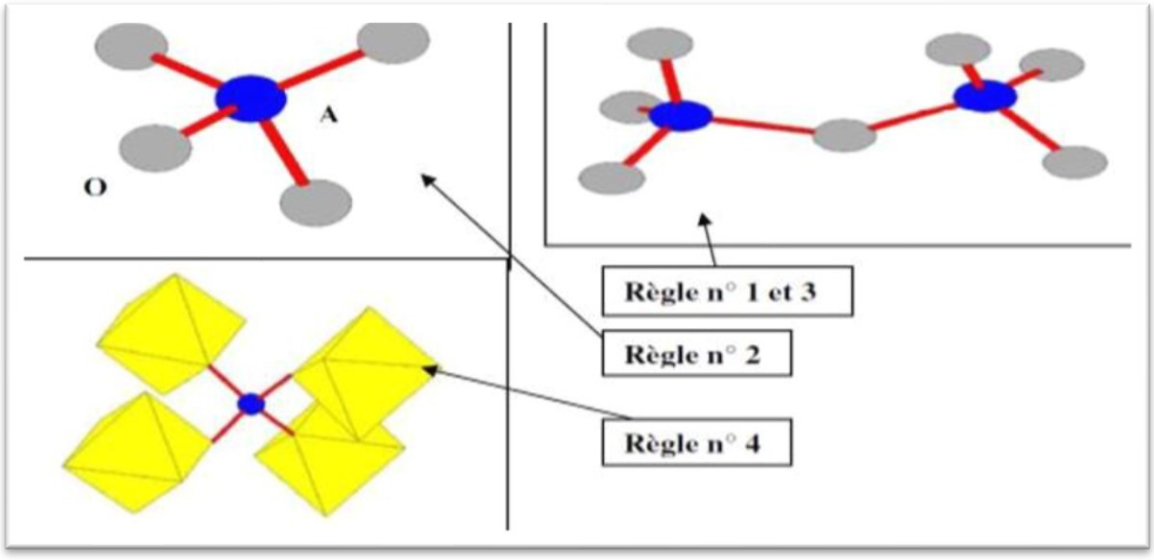


Figure (7*I): A diagram illustrating each of the rules that primarily define three categories of oxides.

6.2)The compound structure of glass:

Glass is usually composed of one or more oxide compounds. AO, A_2O ,A_2O_5 ,AO_2 ,A_2O_3 , Zachariasen reduced the roles of the cations and anions with varying sizes and charges in the glass network to three categories, summarized in the following table.

The formed oxides.	V_2O_5،AS_2O_3،AS_2O_5،P_2O_5،B_2O_3،GeO_2،SiO_2
The modifying oxides.	BaO،SrO،CaO،MgO،K_2O،Na_2O،Li_2O_3
Intermediate oxides	TiO_2,AL_2O_3 ، PbO ، ZnO ، CdO ،

Table (1-I): Zachariasen's classification of some oxides.

- **The network-forming oxides in glass**

The network-forming oxides are the oxides that form the basic structure of composite glass. Their percentage in the glass ranges from 55% to 94%. These oxides are classified according to their empty structural units into two categories: flat-building-unit oxides and spatial-building-unit oxides. The network-forming oxides are characterized by their high bonding energy and very high melting temperature[16].

The oxide of element A is AxOy.	The valence of element A.	The atomic number (Z) coordinance	The bond energy (O-A). [K.cal/mol]
Si	4	4	106
B	3	3.4	119.89
Ge	4	4	108
P	5	4	111 -88

Table (2-I): Bond energy of some network-forming oxides**.**

- **The network-modifying oxides**

Modified oxides are oxides that are added to the initial composition of glass to induce a change in its glass network structure in order to obtain specific physicochemical properties. Usually, alkali metal oxides with the chemical formula A_2O, such as K_2O, Li_2O, and Na_2O, or alkaline earth metal oxides with the chemical formula AO, such as CaO, MgO, and BaO, are used as modifying oxides[16]. Their entry percentages into the glass composition range from 1.5% to 22%

The oxide of element A is AxOy.	The valence of element A.	The atomic number (Z) coordinance	The bond energy (O-A). [K.cal/mol]
Na	1	8 -6	15 -20
K	1	8	13
Li	1	6 -4	? -36
Ca	2	8 -6	43 -32

table(3-I):Bond energy for some common modified oxides

- **The intermediate oxides**

Intermediate oxides are oxides that can perform both previous functions, either as forming oxides or as modifying oxides, depending on their added proportion to the glass composition. One of the most important intermediate oxides is aluminum oxide (Al_2O_3)[16]. Its percentage in glass ranges from 2% to 30%. According to the chemical composition of the glass, it belongs to one of the previous two categories, such as Al_2O_3, PbO, and TiO_2. These oxides work to stabilize the glass network by giving it properties of resistance to change and dissolution [13]

The oxide of element A is AxOy	The valence of element A.	The atomic number(Z) coordinance	The bond energy (O-A). [K.cal/mol]
Al	3	6 -4	79،101 - 53،67
Pb	2	6	39
Zn	2	4	72

Table (4-I): Bond energy for some intermediate oxides

7) Types of Glass:

There are five types of glass ceramics:

7.1) Oxide glass

The vast majority of glass includes oxygen as an ion that acts as a binding tool between bonds. Silica glass occupies a significant position among oxide glasses in terms of its compositions and technological applications. The main characteristic of silica-based glass is its transparency in the visible light range from 3 to 5 micrometers. It has a Tg greater than 1000 degrees Celsius and also possesses great thermal stability and extremely high resistance to corrosion. The main oxide glass-forming agents are GeO_2, B_2O_3, SiO_2, and P_2O_5. [17]

7.2) Chalcogenide glass

Chalcogens can form glass by themselves or with bonding to other chalcogen elements such as Se, Te, and S. They can form binary glasses (Sb, As) or with the fifth group (Sn, Si, Ge) of the periodic table, and also with other elements from the fourth group such as B_2S_3, Li_2S, and As_2S_3, as well as ternary glasses such as As_2S_3, As_2Se_3, and GeS_2.[17]

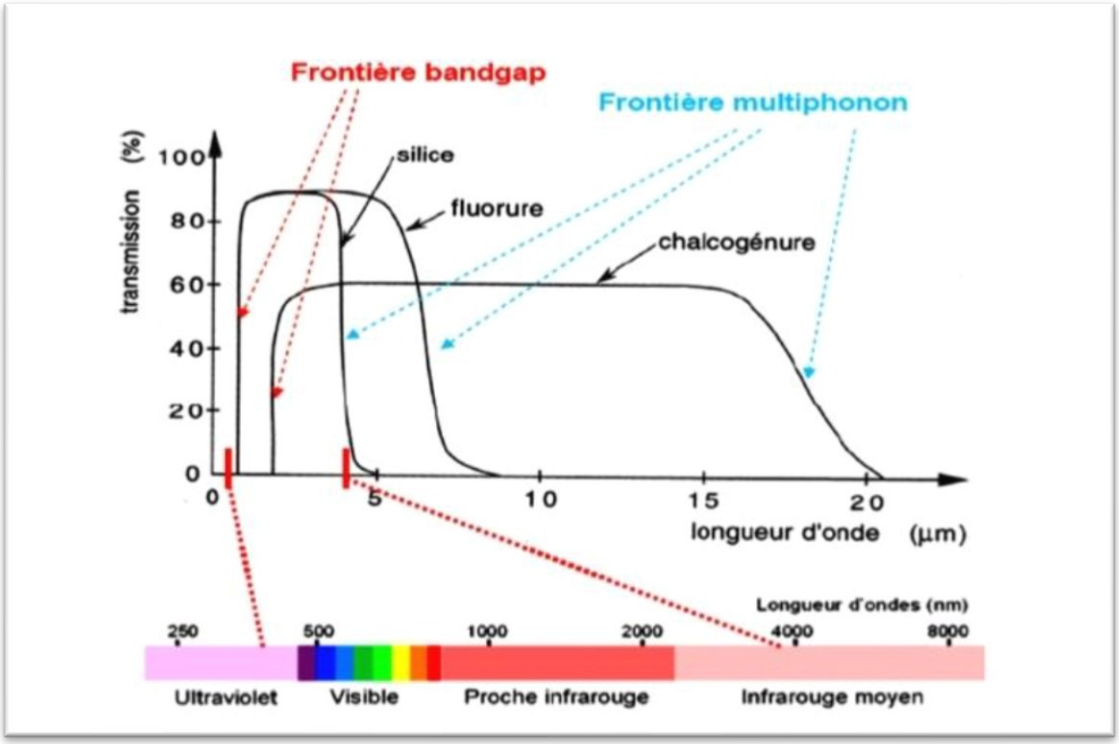
7.3)Halogenated glass

Halogenated glass is based on salts.(Chlorine Cl; Iodine, Br (Bromine), and Fluorine (F)), Most types of it are not chemically stable except for fluoride glass, which has good mechanical and chemical properties, which include ZnC_{l2} ,BiC_{l3},$ZnBr_2$,Pb_{I2} . [18]

7.4)Fluoride glass

The fluoride glass revolution began in 1975 with the discovery of a new series of fluoride glasses by the brothers Michel and Marcel Poulain. Most of these glasses have good visible transmission up to 1 μm in the infrared region. These features place the glasses at the top of the list

as serious filters for optics and materials for optical fibers. These glasses are characterized by their high optical transparency (200-10000 nm) [19]

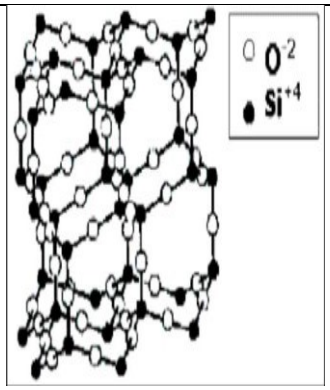


fig(11.I):The optical window for the three glass families includes oxides, fluorides, and halides

7.5)Metallic glass

It has been observed that some metal alloys in the liquid state can be converted into glass by rapid cooling. Metallic glasses have been the subject of much research due to their hardness, which differs from the brittle nature of conventional glasses. Metallic glass made by rapid solidification was discovered in 1960 and 1961 (where strips with a maximum thickness of 0.1 mm were formed) by extremely fast cooling. One of the features of metallic glass is its ordered structure, good mechanical properties, and high hardness. Interestingly, these glasses have high corrosion resistance and can be used as anti-corrosion coatings[18]

8)Let's take an example of a type of glass and highlight its features

Chemical survival	Glass	Structure	Specific volume	The density.	The viscosity	Thermal expansion	Refraction index
It is considered a chemical binder due to the strength of its bridging bonds.	SiO2		1.44	0.6364	It has a very high viscosity due to the strength of the bridging bonds . Si-O-Si	A thermal shock factor is weak, and therefore, it has a high resistance to thermal shock due to the strength of the bridging bonds Si-O-Si.	The refractive index is very weak due to the weak electronic polarization of the bridging oxygen ions present in it.

Table(5-I):Glass features SiO2.

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9) Conclusion

In this chapter, we attempted to provide some basic concepts about glass, defining it as a non-crystalline body that exhibits the glass transition phenomenon. We also introduced several hypotheses for studying the structure of glass, some of which rely on the nature and proportion of its basic components. We also mentioned some of its optical, electrical, thermal, and mechanical properties, among others.

References

[1] زينهم and محمد, *تكنولوجيا فن الزجاج*. الهيئة المصرية العامة للكتاب, 1995.

[2] H. E. Skallevold, D. Rokaya, Z. Khurshid, and M. S. Zafar, 'Bioactive glass applications in dentistry', *Int. J. Mol. Sci.*, vol. 20, no. 23, p. 5960, 2019.

[3] أسامة زيد وهبة الصيادي and دار الساقي, *أهم الاختراعات والاكتشافات في تاريخ الإنسانية*. Dar al Saqi, 2017.

[4] C. Hammond, *The basics of crystallography and diffraction*, vol. 21. International Union of Crystallography texts on crystallography, 2015.

[5] J. E. Shelby, *Introduction to glass science and technology*. Royal society of chemistry, 2020.

[6] A. Faivre, 'Les verres et la transition vitreuse', *Matér. Tech.*, vol. 103, no. 4, p. 404, 2015.

[7] I. M. Kalogeras and H. E. Hagg Lobland, 'The nature of the glassy state: structure and glass transitions', *J. Mater. Educ.*, vol. 34, no. 3, p. 69, 2012.

[8] N. R. Jadhav, V. L. Gaikwad, K. J. Nair, and H. M. Kadam, 'Glass transition temperature: Basics and application in pharmaceutical sector', *Asian J. Pharm. AJP*, vol. 3, no. 2, 2009.

[9] E. D. Zanotto and J. C. Mauro, 'The glassy state of matter: Its definition and ultimate fate', *J. Non-Cryst. Solids*, vol. 471, pp. 490–495, 2017.

[10] A. K. Varshneya, *Fundamentals of inorganic glasses*. Elsevier, 2013.

[11] N. Gao, M. J. Starink, and T. G. Langdon, 'Using differential scanning calorimetry as an analytical tool for ultrafine grained metals processed by severe plastic deformation', *Mater. Sci. Technol.*, vol. 25, no. 6, pp. 687–698, 2009.

[12] E. D. Palik, *Handbook of optical constants of solids*, vol. 3. Academic press, 1998.

[13] F. Rehouma, 'Étude de l'échange d'ions a l'argent dans un verre aluminoborosilicate: application a un procède d'enterrage sélectif des guides', 1994.

[14] W. Vogel, 'Classical theories of glass structure', *Glass Chem.*, pp. 41–56, 1994.

[15] J. C. Mauro, 'Topological constraint theory of glass', *Am. Ceram. Soc. Bull.*, vol. 90, no. 4, p. 31, 2011.

[16] W. H. Zachariasen, 'The atomic arrangement in glass', *J. Am. Chem. Soc.*, vol. 54, no. 10, pp. 3841–3851, 1932.

[17] W. Liang and J. Cheng, 'New Phosphate Glass for Precision Molding.', *Am. Ceram. Soc. Bull.*, vol. 80, no. 3, pp. 62–64, 2001.

[18] J. D. Musgraves, J. Hu, and L. Calvez, *Springer handbook of glass*, no. Part A. Springer, 2019.

[19] J. Lucas, 'Zirconium-Free Fluoride Glasses', *Halide Glas. Infrared Fiberoptics*, pp. 321–330, 1987.

Chapter II

Machine Learning

1)Introduction

Machine learning has emerged as a powerful field in computer science and data analysis. By enabling computers to intelligently perform specific tasks, machine learning has become an advanced field that aims to teach computers to simulate the human brain. Machine learning is based on statistics and produces fundamental statistical theories for computer learning processes. It involves creating algorithms that allow computers to learn from data and discover statistical rules or other patterns within it. These algorithms can be used to represent the way humans learn certain tasks[1].

With the advancement of technology, increased processing power, and storage capacity, many machine learning algorithms have been developed and improved. The recent advancements in machine learning enable automatic application of a variety of complex mathematical computations on big data, contributing to increased computation speed, reduced computational costs, and shortened development cycles[2].

The goal of machine learning is to create mathematical models that represent the relationships between inputs and outputs. These models are trained using training data and can be used to predict desired variable values by measuring input variables[3]. The development of this field involves effectively utilizing large and diverse datasets, exploring fast learning methods, and analyzing application features based on the specific domain of application

2)Development of Machine Learning

Machine learning and artificial intelligence are not new ideas. For more than 60 years, they have been the focus of research, development, and invention involving computer scientists, engineers, academics, researchers, students, and business experts. Machine learning is based on mathematical principles that combine algebra, statistics, and probability. In the 1950s and 1960s, eminent researchers like Alan Turing, John McCarthy, Arthur Samuels, Alan Newell, and Frank Rosenblatt led the significant growth of machine learning and artificial intelligence. Through the Optimizing Checkers Program, Samuel provided the first practical machine learning model; meanwhile, Rosenblatt created the Perceptron, a popular machine learning method that was based on biological neurons and laid the groundwork for artificial neural networks[4]. The following Table provides an illustration of the significant and extensive development of machine learning

.

1950	Alan Turning created “Turning Test” to check a machine’s intelligence. In order to pass the Turning Test, the machine should be able to convince humans that there they are actually talking to a human and not a machine.
1958	Frank Rosenblatt created Perceptron, which laid the foundation stone for the development of Artificial Neural Network (ANN).
1981	Explanation Based Learning (EBL) was proposed by Gerald Dejong, whereby, a computer can analyze the training data and create rules for discarding useless data[5]
2006	The term “Deep Learning” was coined by Geoffery Hinton which referred to a new architecture of neural networks that used multiple layers of neurons for learning
2014	Facebook invented the “DeepFace” algorithm based on Deep Neural Networks capable of recognizing human faces in photos
2017	Google proposed Google Lens, Google Clicks, Google Home Mini and Google Nexus based phones which use Machine Learning and Deep Learning Algorithms. Nvidia proposed NVIDIA GPUs- The Engine of Deep Learning. Apple proposed Home Pod which is a Machine Learning Interactive device

table 2 :Development of ML

3) Machine Learning Paradigms

Machine learning paradigms can be categorized into two main groups based on the training approach of the algorithm and the availability of output during the training process: Supervised learning, unsupervised learning This will also allow us to state the basic terminology, building basic equipment to expose some of the basic tools of machine learning:

3.1) unsupervised learning

Unsupervised learning is a powerful method for extracting hidden structures and patterns from unlabeled data through inference. Unlike supervised and reinforcement learning, unsupervised learning does not depend on labeled instances for evaluating accuracy. Density estimation in statistics is a significant application of unsupervised learning.

The main objective of unsupervised learning is to leverage the input feature values in the training data to uncover concealed structures. It relies on clustering algorithms that group data into meaningful clusters. These algorithms find widespread use in diverse fields such as topic-based article categorization, bioinformatics analysis of microarray and gene expression, market segment

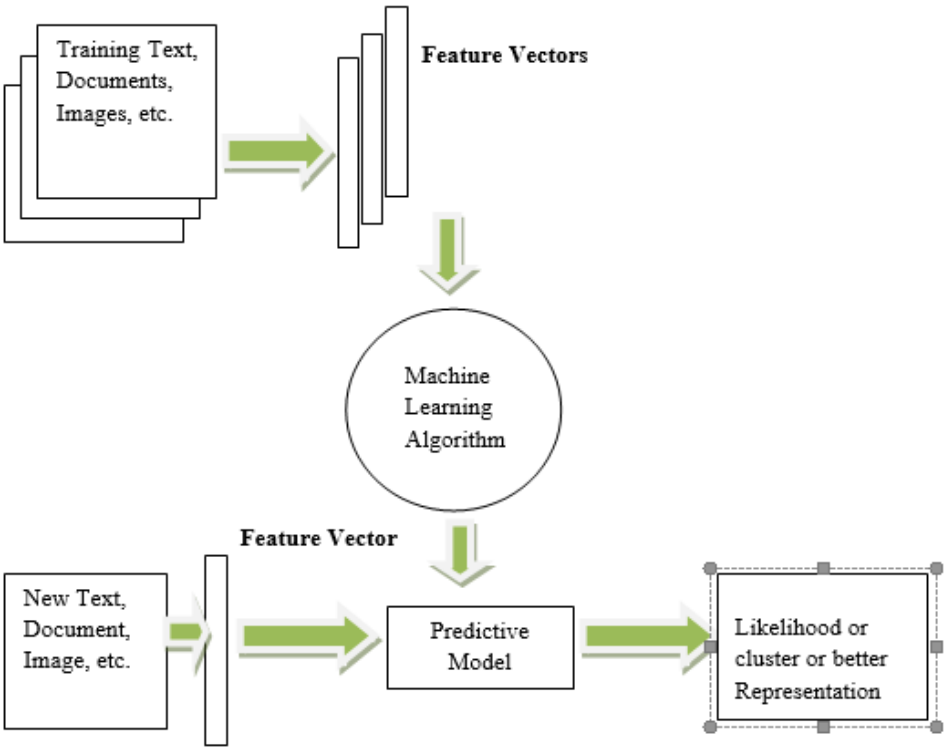
analysis, and social behavior grouping. Notable clustering algorithms include K-means, hierarchical clustering, and spectral clustering[6].

Evaluating the performance of clustering directly is challenging as the correct output labels are unknown. Instead, performance assessment focuses on identifying meaningful patterns within the data through the clusters discovered. Unsupervised learning benefits from the simplicity of collecting a large training dataset since output labels are not required.

When input data lacks labels, unsupervised learning offers a solution to address learning challenges. Its goal is to reveal hidden and potentially complex structures in the dataset. A common example of unsupervised learning is data clustering, which assigns data points to groups based on shared characteristics.

Generative modeling is a frequently used approach in unsupervised learning to search for a probability distribution that can generate samples resembling the observed data. This distribution can be explicitly or implicitly parameterized. Generative models incorporate latent variables to introduce unpredictability. In cases where the number of latent variables is significantly smaller than the data's dimensionality, dimensionality reduction techniques are employed. One strategy in unsupervised learning is to determine values for the latent variables that maximize the likelihood of the observed data[7].

At its core, unsupervised learning aims to discover previously unknown patterns in the data and derive rules from them. This approach is particularly valuable when the data categories are unknown and labels are absent in the training set[8]. Unsupervised learning is recognized as a statistical method for uncovering hidden structures in unlabeled data. For a more detailed explanation, refer to Figure(1.II)

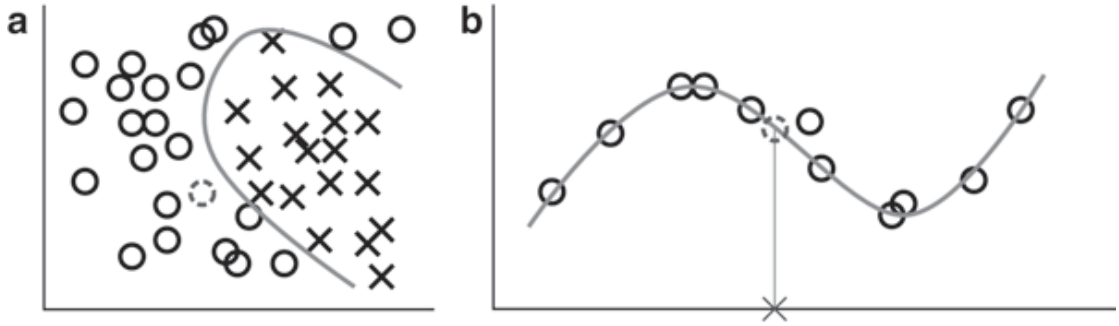


Fig(5.II) Unsupervised Learning

3.2)Supervised learning

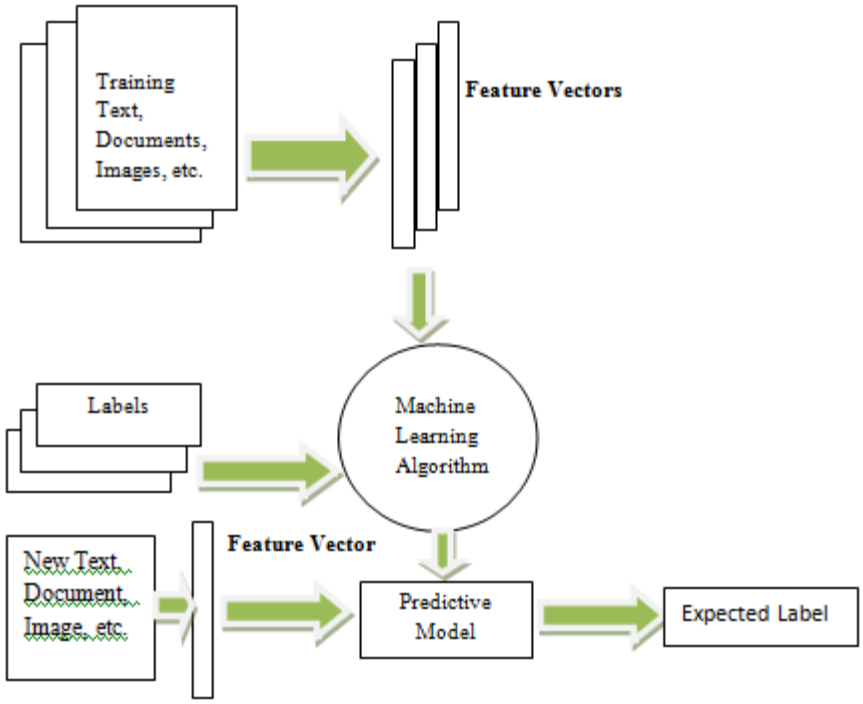
Supervised Learning involves inferring a function from labeled training data in the field of machine learning. The training data comprises a collection of training examples. Through the analysis of the training data, a supervised learning algorithm generates an inferred function that can be employed to map new examples.

Supervised learning methods necessitate knowing the value of the output variable for each training sample. Consequently, each training sample comprises input and output values. The algorithm then trains a model to forecast the output variable based on the input variables and defined features. When the output variables exhibit continuous values, the predictive model is denoted as a "regression function." For example, predicting the air temperature at a specific time of the year falls into the realm of regression. Conversely, if the output variables assume discrete values, the predictive model is known as a "classifier."[7] Automated medical diagnosis serves as an exemplar of a classification problem, where patient data is classified into specific diseases. Figure 2 provides an exemplification of these two types of problems.



Fig(6.II):Supervised machine learning problems. (a) In a classification problem (b) The goal in regression problems

In supervised learning, a set of examples or training instances is provided along with their corresponding correct outputs. Based on these training sets, the algorithm learns to respond more accurately by comparing its output with the given inputs[8]. Supervised learning is also known as learning from examples or learning from models. Figure 3 illustrates the concept.



Fig(7.II):Supervised Learning

4) Machine learning models

4.1) Classification and Regression Model

Classification is a supervised learning task where the output values are grouped into predefined categories. It is used when the output values are categorical variables. Regression, on the other hand, is another category of supervised learning where the output values are numeric. It is

employed when the output values are continuous variables[9], There are several classification and Regression algorithms in Machine Learning. Here are some common algorithms in this context:

- Linear and Logistic Regression
- Decision Trees
- Support Vector Machines
- K-Nearest Neighbors
- Naive Bayes
-support vector regression
- Artificial Neural Networks

These are just a sample of the available algorithms, and there are many more advanced and specialized algorithms for specific problems in Machine Learning. The choice of algorithm depends on the data and the problem you are trying to solve[10]

4.2) Clustering and Dimensionality Reduction

Clustering is an unsupervised machine learning technique used to divide a dataset into subgroups or clusters based on similarities and proximity between its elements.

On the other hand, dimensionality reduction is an unsupervised learning process that aims to reduce the number of variables or dimensions in a dataset while retaining important information.[11]

There are various clustering and dimensionality reduction algorithms used in unsupervised learning. Here are some commonly used algorithms

-PCA (Principal Component Analysis)

-t-SNE (t-Distributed Stochastic Neighbor Embedding)

-Hierarchical

-Density-Based

-K-Means

-UMAP (Uniform Manifold Approximation and Projection)

These are just some of the commonly used algorithms, and there are many more available based on the specific needs, nature of the data, and the problem at hand.[12]

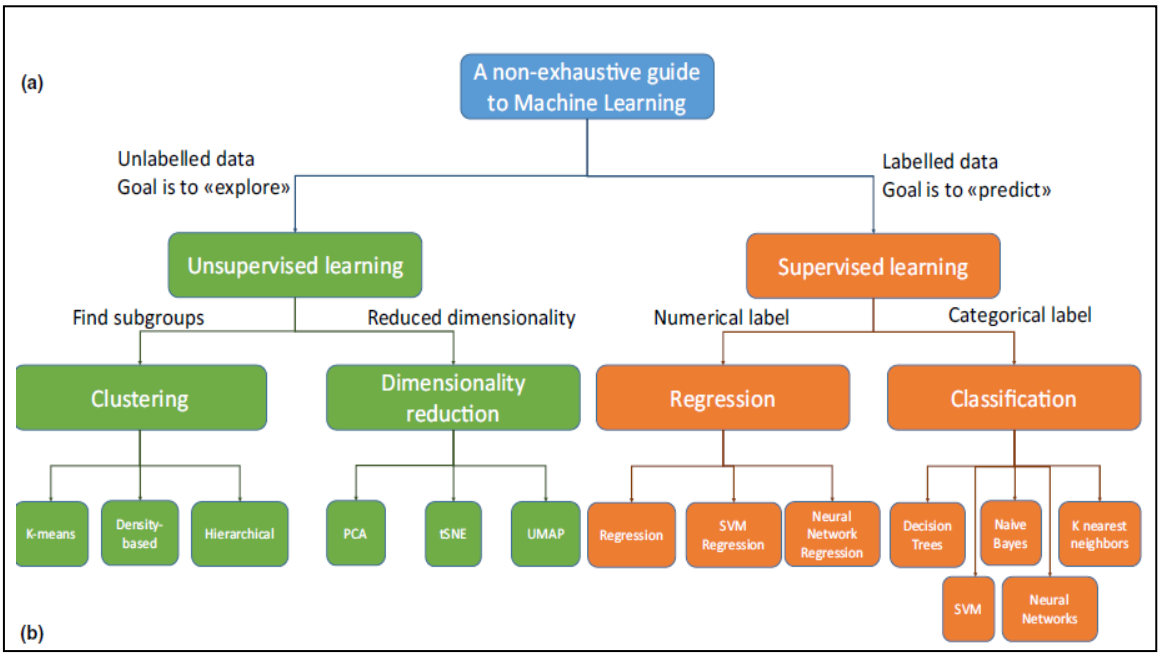


Fig (8.II):the different methods of machine learning

5)Machine Learning Algorithms

Data mining is a research field that has led to the development of numerous data mining algorithms. These algorithms can be directly applied to a dataset to create models or extract valuable insights and inferences from the data. Here are some popular algorithms in the field of data mining:

5.1) Linear and Logistic Regression

- **Linear Regression**

The goal of linear regression, as part of the regression algorithms family, is to discover relationships and dependencies between variables. Linear regression represents the modeling relationship between a continuous scalar dependent variable y (also known as label or target in machine learning terminology) and one or more explanatory variables (also called independent variables, input variables, features, observed data, observations, attributes, dimensions, data points, etc.)[13] denoted by X using a linear function. In regression analysis, the objective is to predict a continuous target variable, while in another area called classification, the goal is to predict a label

from a finite set. Linear regression also falls under the category of supervised learning algorithms, meaning that we train the model on a set of labeled data (training data) and then use the model to predict labels on unlabeled data (testing data)[11].

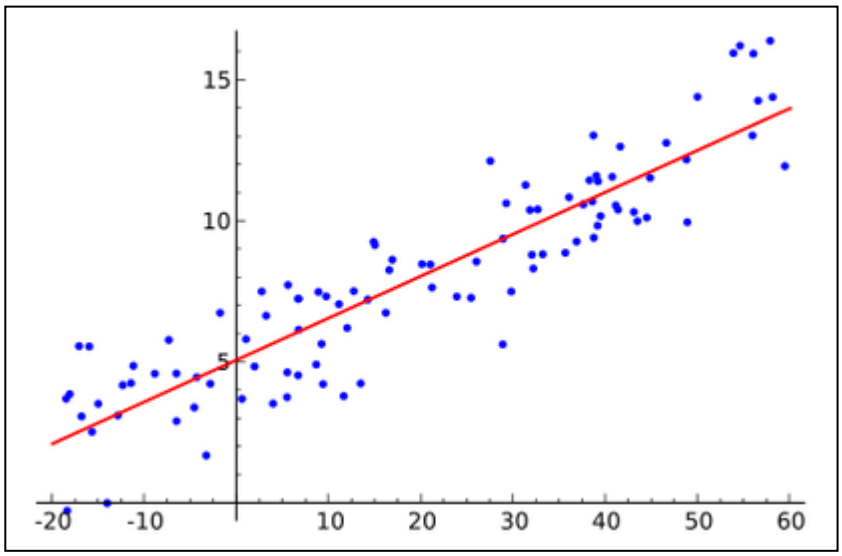
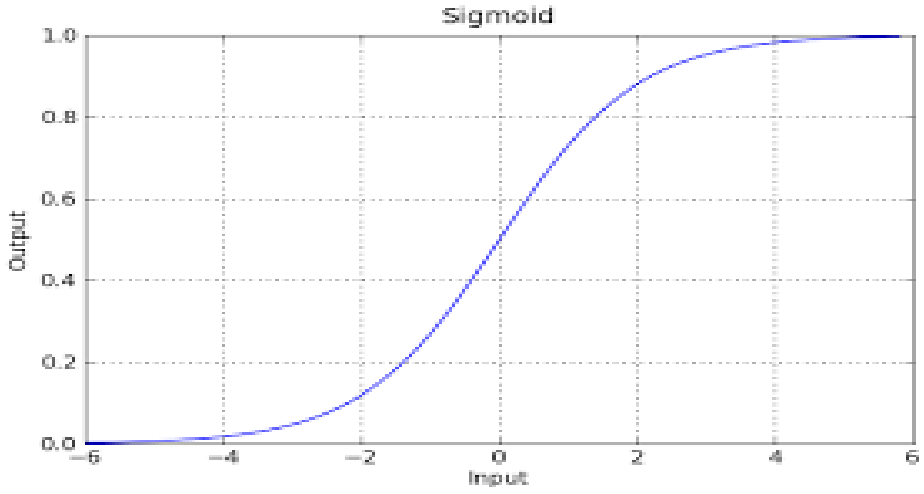


fig (5.II)Visual representation of the linear regression

- **Logistic Regression**

Logistic regression operates by extracting a set of weighted features from the input, taking their logarithm, and combining them linearly. This means that each feature is multiplied by a weight and then added together. It is a type of regression that predicts the probability of an event occurring by fitting the data to a logistic function. Similar to many forms of regression analysis, logistic regression utilizes a set of predictor variables that can be numerical or categorical[9].

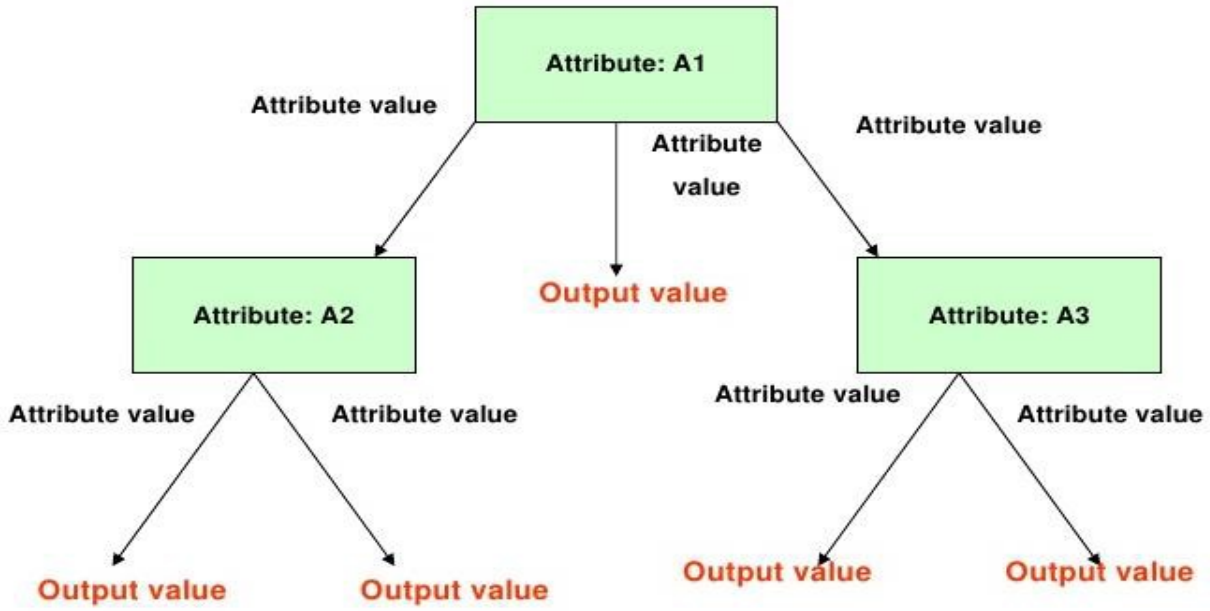


fig(6.II) Visual representation of the Logistic Function

5.2) Decision Tree

The decision tree is a decision support tool that uses a graphical representation similar to a tree or a model to display decisions and their possible outcomes, including the outcomes of chance events and utilities. Decision trees are commonly used in operations research and decision analysis to help determine strategies that are most likely to achieve the desired goal. They are also a common tool in machine learning. The decision tree can be easily converted into a set of rules by matching the path from the root to the leaves one by one. Relevant inferences can be obtained by following these rules[14].

The decision tree is a machine learning approach used to solve classification and regression problems by dividing the data based on specific attributes. Decisions are made at the leaves, and data is partitioned at the nodes. In a classification tree, the decision-representing variables are categorized as "yes/no," while in a regression tree, the decision-making variable is continuous. Decision trees have several advantages, including their ability to solve classification and regression problems, ease of result interpretation, handling of categorical and quantitative values, ability to fill in missing values with the most probable value, and high performance due to the efficiency of the algorithm's traversal in the tree, The problem of overfitting is a challenge that decision trees can face, and the solution to this problem is to use a random forest that relies on ensemble modeling[15].



fig(7.II) Decision tree example

5.3) Support Vector Machines

The Support Vector Machine (SVM) is a commonly used supervised machine learning algorithm. It aims to find a hyperplane that effectively separates different types of data. In a two-dimensional space, Support Vector Machines (SVMs) were initially introduced in statistical learning theory as binary classifiers that employ a linear separating hyperplane to classify data instances. The classification capabilities of traditional SVMs can be significantly improved by using the "kernel trick" to transform the original feature space into a higher-dimensional space. This enables SVMs to be applied to classification, regression, and clustering tasks , The appeal of SVMs lies in their ability to address overfitting issues commonly encountered in high-dimensional spaces through a global optimization approach. Some commonly used SVM algorithms include support vector regression, least squares support vector machine, and successive projection algorithm-support vector machine[16]

SVM are versatile and can be utilized for both classification and regression problems, making them supervised learning algorithms. The algorithm determines the margin, which represents the distance between the hyperplane and the nearest data points of different classes. Each data item is represented as a point in an n-dimensional space, where n corresponds to the number of features in the dataset. The value of each feature determines the coordinate value[17]. By finding the optimal hyperplane that maximizes the margin, SVMs effectively classify the data into distinct classes.

Many real-world problems involve data that cannot be separated by a hyperplane, which makes it impossible to classify positive and negative instances accurately in the training set. To tackle this issue, one approach is to map the data to a higher-dimensional space and define a separating hyperplane there. This higher-dimensional space is referred to as the feature space, in contrast to the input space occupied by the training instances.

By selecting an appropriate feature space with sufficient dimensionality, it becomes feasible to make any consistent training set separable. A linear separation in the feature space corresponds to a nonlinear separation in the original input space. This mapping of the data to another Hilbert space, possibly with infinite dimensions, denoted as $\Phi: Rd \rightarrow H$, allows the training algorithm to rely solely on dot products in H, specifically on functions of the form $\Phi(xi) \cdot \Phi(xj)$

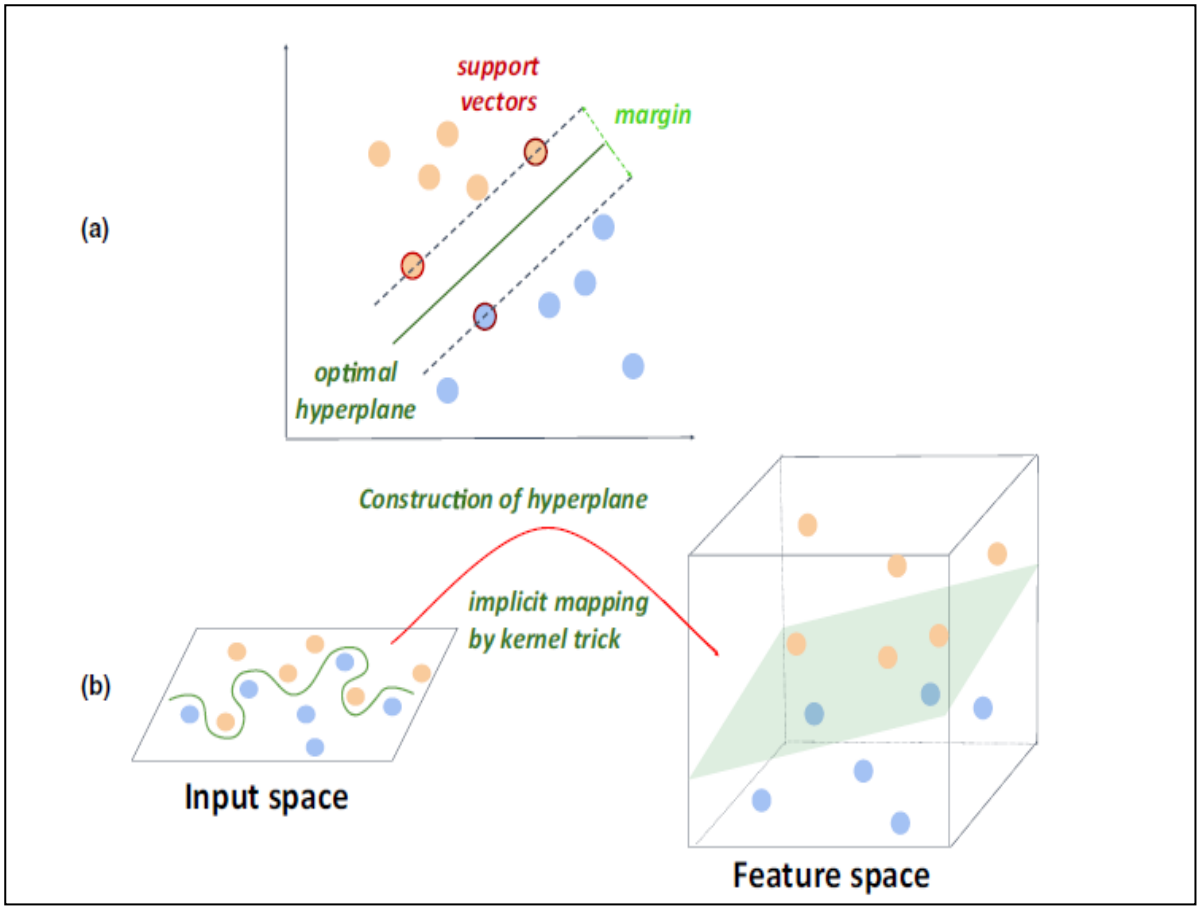
If a "kernel function" K exists such that $K(xi, xj) = \Phi(xi) \cdot \Phi(xj)$, then it is only necessary to use K in the training algorithm, without explicitly determining Φ. Kernels belong to a special class of functions that facilitate the calculation of inner products directly in the feature space[18],

eliminating the need for the aforementioned mapping process Once a hyperplane is established, the kernel function is employed to map new points into the feature space for classification

SVMs are versatile for regression tasks, offering linear and non-linear modeling options through different kernel functions. Training both a linear SVM and an SVM with an RBF kernel is a recommended strategy to evaluate the benefits of non-linear modeling while considering interpretability challenges[19].

- Support Vector Regression

In Support Vector Regression (SVR), kernel functions play a critical role in transforming the input data into a higher-dimensional space. These kernel functions capture the similarity or distance between pairs of data points, enabling SVR to discover non-linear relationships between the input variables and the target values. The Radial Basis Function (RBF) kernel is a widely used kernel function in SVR. It is also known as the Gaussian kernel. The RBF kernel measures the similarity between data points based on their Euclidean distance. It assigns higher weights to nearby data points and lower weights to distant data points. The RBF kernel is characterized by a smooth and continuous function, allowing SVR to capture complex non-linear patterns in the data.Support Vector Regression (SVR) with the Radial Basis Function (RBF) is a kernel-primarily based totally set of rules belonging to the Support Vector Machine (SVM) family. It is widely used for predicting continuous values in various domains.. RBF represents the relationship between independent variables and the dependent variable within the SVR process. RBF relies on the concept of radial basis, where the center of the radial basis represents the point around which the highest values of the expected regression concentrate, gradually decreasing with distance from the center[20]. The center of the radial basis is determined based on the available data and specific problem requirements. In the context of SVR with RBF, the radial basis function is used to estimate the expected values of the dependent variable (the predicted output) at specific points in the space. The expected regression value is determined by calculating the radial basis for points near the target point and using it to estimate the expected value.



fig(8.II): llustration of support vector machine (SVM) principles. (a) Illustration of a simple case (b) Illustration of performing nonlinear classification

6)The Generic Model of ML

The general principle for model selection and assessment is to choose the best model and evaluate its performance. This involves the following steps:

I).Collection and Preparation of Data: The number one mission of withinside the gadget mastering method is tocollect and prepare data in a format that can be given as input to the algorithm. A large amount may be available for any problem. Web data is usually unstructured and contains a lot of noise, i.e., irrelevant data as well as redundant data. Hence the data needs to be cleaned and pre-processed to a structured format[2].

II). Feature Selection: The data obtained from the above step may contain numerous features, not all of which would be relevant to the learning process. These features need to be removed and a subset of the most important features needs to be obtained[21]

III).Choice of Algorithm: Not all system getting to know algorithms are supposed for all problems. Certain

algorithms are more suited to a particular class problem as explained in the previous section.

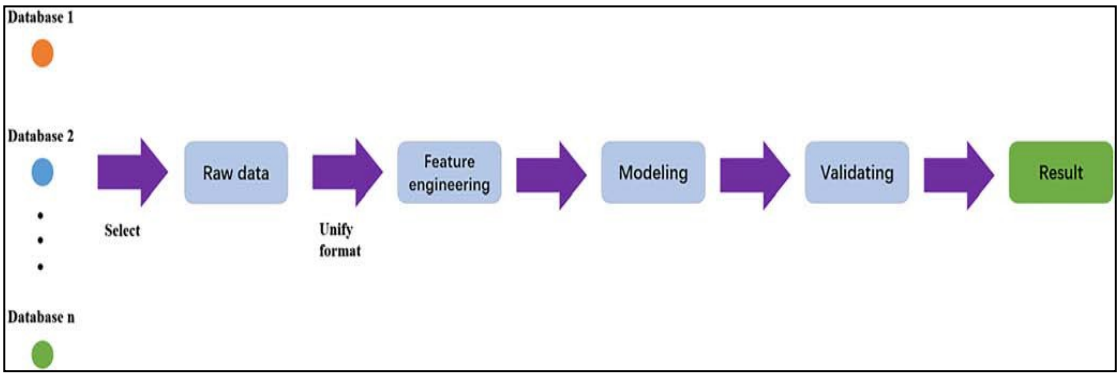
Selecting the best machine learning algorithm for the problem at hand is imperative in getting the

best possible results[22]

IV) Selection of Models and Parameters: Most of machine learning algorithms require some initial manual intervention for setting the most appropriate values of various parameters[4].

v).Training: After deciding on the ideal set of policies and suitable parameter values, the model needsto be trained using a part of the dataset as training data[23]

vi). Performance Evaluation: Before real-time implementation of the system, the model must be tested against unseen data to evaluate how much has been learnt using various performance parameters like accuracy, precision and recall[7]



fig(9.II) Workflow of machine learning

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7)Applications of Machine Learning

Table enlists some popular real-life applications of ML

Application	Description
Playing Checkers Game	A computer program learns to play checkers game, improvises its performance as determined by its ability to win at various class of tasks involving the game, through experience obtained by playing games against itself.
Medical Field	TRISS: Trauma & Injury Severity Score, which is widely used to predict mortality in injured patients, become initially advanced via way of means of Boyd et al. the usage of logistic regression.Many different clinical scales used toverify severity of a affected person had been advanced the use of logistic regression
Autonomous Vehicles	Machine learning models are these days being applied to drive autonomous vehicles like Cars, Drones etc. Example: Google Driver Less Cars, Tesla Cars. Machine learning techniques are also highly effective in controlling sensor-based applications

Table(2.II): enlists some popular real-life applications of ML

8)Conclusion

Machine studying strategies offer interesting new approaches to exploitThe to be had computational strength and information in a whole lot of scientific domains.They can examine big quantities of facts in a relativelyshort time that is not possible by manual labor. This provides opportunities for scientists to develop new experimental procedures And to channel their efforts at the maximum promising questions in their trouble domain.However, computerized answers aren't a alternative for good medical judgment.Like every other tool, a gadget getting to know techniqueneeds to be utilized in a careful manner to make the most out of its use. It is better to start with the simpler methods to judge problem difficulty and to gain more insight about algorithm behavior.It is likewise vital to attempt some unique algorithms and compare their performances**.**

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References

[1] C. M. Bishop and N. M. Nasrabadi, *Pattern recognition and machine learning*, vol. 4, no. 4. Springer, 2006.

[2] T. Hastie, R. Tibshirani, J. H. Friedman, and J. H. Friedman, *The elements of statistical learning: data mining, inference, and prediction*, vol. 2. Springer, 2009.

[3] J. Alzubi, A. Nayyar, and A. Kumar, 'Machine learning from theory to algorithms: an overview', presented at the Journal of physics: conference series, IOP Publishing, 2018, p. 012012.

[4] I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT press, 2016.

[5] S. Minton and M. Zweben, 'Learning, planning, and scheduling: An overview', *Machine Learning Methods for Planning*, pp. 1–29, 1993.

[6] G. Carleo *et al.*, 'Machine learning and the physical sciences', *Reviews of Modern Physics*, vol. 91, no. 4, p. 045002, 2019.

[7] Y. Baştanlar and M. Özuysal, 'Introduction to machine learning', *miRNomics: MicroRNA biology and computational analysis*, pp. 105–128, 2014.

[8] D. Sharma and N. Kumar, 'A review on machine learning algorithms, tasks and applications', *International Journal of Advanced Research in Computer Engineering & Technology (IJARCET)*, vol. 6, no. 10, pp. 2278–1323, 2017.

[9] V. Nasteski, 'An overview of the supervised machine learning methods', *Horizons. b*, vol. 4, pp. 51–62, 2017.

[10] J. G. Greener, S. M. Kandathil, L. Moffat, and D. T. Jones, 'A guide to machine learning for biologists', *Nature Reviews Molecular Cell Biology*, vol. 23, no. 1, pp. 40–55, 2022.

[11] R. Muhamedyev, 'Machine learning methods: An overview', *Computer modelling & new technologies*, vol. 19, no. 6, pp. 14–29, 2015.

[12] S. Badillo *et al.*, 'An introduction to machine learning', *Clinical pharmacology & therapeutics*, vol. 107, no. 4, pp. 871–885, 2020.

[13] T. H. D. Ngo and C. La Puente, 'The steps to follow in a multiple regression analysis', presented at the Proceedings of the SAS Global forum, Citeseer, 2012, pp. 22–25.

[14] P. E. Utgoff, N. C. Berkman, and J. A. Clouse, 'Decision tree induction based on efficient tree restructuring', *Machine Learning*, vol. 29, pp. 5–44, 1997.

[15] S. Ray, 'A quick review of machine learning algorithms', presented at the 2019 International conference on machine learning, big data, cloud and parallel computing (COMITCon), IEEE, 2019, pp. 35–39.

[16] K. G. Liakos, P. Busato, D. Moshou, S. Pearson, and D. Bochtis, 'Machine learning in agriculture: A review', *Sensors*, vol. 18, no. 8, p. 2674, 2018.

[17] S. B. Kotsiantis, I. D. Zaharakis, and P. E. Pintelas, 'Machine learning: a review of classification and combining techniques', *Artificial Intelligence Review*, vol. 26, no. 3, pp. 159–190, 2006.

[18] B. Schölkopf, A. J. Smola, and F. Bach, *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2002.

[19] D. Bzdok, M. Krzywinski, and N. Altman, 'Machine learning: supervised methods', *Nature methods*, vol. 15, no. 1, p. 5, 2018.

[20] D. Boswell, 'Introduction to support vector machines', *Departement of Computer Science and Engineering University of California San Diego*, vol. 11, 2002.

[21] I. Guyon and A. Elisseeff, 'An introduction to variable and feature selection', *Journal of machine learning research*, vol. 3, no. Mar, pp. 1157–1182, 2003.

[22] S. Raschka and V. Mirjalili, *Python machine learning: Machine learning and deep learning with Python, scikit-learn, and TensorFlow 2*. Packt Publishing Ltd, 2019.

[23] C. C. Aggarwal, 'Neural networks and deep learning', *Springer*, vol. 10, no. 978, p. 3, 2018.

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CHAPTER III

Results and discussion

1)Introduction

Accurately predicting glass transition temperature (Tg) is crucial in materials science for designing and customizing materials with specific properties. This study aims to forecast Tg using Support Vector Regression (SVR) and sparse Principal Component Analysis (PCA). By combining these methods, a predictive model can estimate Tg values with high precision. The significance lies in its potential implications for the advancement of glass materials. Precise Tg prediction enables informed decisions regarding material selection and optimization. It facilitates designing and synthesizing new materials with desired Tg values and tailoring properties for thermal stability, processing conditions, and mechanical performance. Tg prediction assists in optimizing processing parameters, ensuring the reliability and performance of the final product. It also aids in assessing material durability and reliability, guiding selection for specific operating conditions. Tg prediction serves as a tool for quality control, allowing manufacturers to evaluate product consistency and detect anomalies. The findings of this study have the potential to significantly impact the development and optimization of glass materials, improving performance and applicability across industries

2) Data Collection and Preprocessing

The data collection process for this study involved leveraging the SciGlass database, which is a comprehensive repository of glass compositions and their associated properties. The database contains a wide range of glass systems, including oxide, non-oxide, and mixed compositions. The data in SciGlass is curated from various sources, including scientific literature, patents, and experimental measurements we focus of this study on tellurate oxide glasses, which are a particular category of glasses consisting of tellurium dioxide (TeO2) and other oxides. These glasses possess unique properties and have potential applications in fields like optical devices, telecommunications, and sensors. To select the appropriate tellurate oxide glasses from the SciGlass database, certain criteria were considered, including specific composition ranges, availability of Tg data (glass transition temperature), and data quality. The selected glasses needed to have Tg values available as the target variable for training and testing the predictive model.

Application of Sparse Principal Component Analysis (PCA): Sparse Principal Component Analysis (PCA) is employed in this study to address data sparsity and reduce the dimensionality of the input matrix. Data sparsity refers to situations where many of the input

variables have zero or negligible values, resulting in a high-dimensional dataset with a large number of irrelevant features. Sparse PCA tackles this issue by promoting sparsity in the principal components. It identifies a small subset of the most important variables that contribute significantly to the variance in the data, while setting the remaining variables to zero or near-zero weights. This feature selection process helps in reducing the dimensionality of the dataset and removing redundant or irrelevant information. In the context of Tg prediction, sparse PCA is applied to the glass composition dataset. It identifies the composition descriptors that have the most significant impact on Tg and discards less relevant descriptors. By reducing the dimensionality of the input matrix, sparse PCA aids in building a more efficient and interpretable predictive model. The application of sparse PCA in this study we focus on the key composition features that contribute to the glass transition temperature. It improves the efficiency of the predictive model by reducing computational complexity and enhances the interpretability of the selected features' influence on Tg prediction.

Overall, the combination of SVR and sparse PCA provides a powerful approach for Tg prediction by leveraging the strengths of machine learning and dimensionality reduction techniques. By employing these methods, the study aims to develop a robust and accurate model for estimating Tg values based on input variables, thereby advancing material design and development.

3) Methodology

The SVR (Support Vector Regression) algorithm is used in this study for Tg prediction. SVR is an extension of the Support Vector Machines (SVM) algorithm, which is primarily used for classification tasks. However, SVR is specifically designed for regression analysis. Its objective is to find the best regression function that maximizes the margin between the predicted output and the actual output, while allowing for a specified error tolerance.

SVR utilizes a kernel function to map the input data into a higher-dimensional feature space, where a hyperplane is constructed to separate the data points. This allows SVR to capture complex non-linear relationships between the input features and the target variable. By maximizing the margin, SVR aims to generalize well to unseen data and provide accurate predictions.

One of the key advantages of SVR is its ability to handle non-linear relationships and make accurate predictions even with a small number of training samples. It is particularly suitable for

problems where the underlying data distribution is non-linear and where the relationship between the features and the target variable is complex

3-1)Implementation of SVR for Tg Prediction:

Data Split: The dataset is divided into a training set and a testing set. The training set is used to train the SVR model, and the testing set is used to evaluate the model's performance. in this study we trained with 80% and testing with 20% of the available data , We narrowed down our inquiry to focus on tellurate oxide glasses. As a result, we excluded any samples that had less than 0% tellurium and a molar fraction of oxygen below 30%. The dataset consists of 62 input features representing oxide glass compositions, with the target variable being the Tg value. We had a total of 4561 samples, To address the data sparsity issue (many zero values) and reduce the dimensionality of the input matrix from 62 to 30, we employed sparse Principal Component Analysis (PCA).

Feature Selection: Sparse PCA is applied to the training dataset to reduce the dimensionality by selecting the most informative features related to glass composition. This step helps in improving the efficiency and interpretability of the SVR model.

SVR Model Training: The training dataset, after feature selection, is used to train the SVR model. The SVR algorithm learns the relationship between the input features (selected composition descriptors) and the corresponding Tg values. The model aims to find the optimal hyperplane in the high-dimensional feature space that best fits the training data.

3-2) Kernel Function Selection

A kernel function is selected to transform the input data into a higher-dimensional feature space, where a linear hyperplane can be used to separate the data points. The choice of the kernel function is crucial in capturing the non-linear relationships between the input features and Tg

in this study, different kernel functions, including the Radial Basis Function (RBF), polynomial, sigmoid, and linear kernels, are experimented with to evaluate their performance in predicting Tg values

Polynomial Kernel:

- The polynomial kernel allows modeling non-linear relationships by applying polynomial transformations to the input data.
- It is useful when the relationship between variables is expected to be polynomial in nature.

- The polynomial kernel is controlled by hyperparameters such as gamma, coef0, and degree.
- The degree parameter determines the degree of the polynomial transformation, while gamma and coef0 control the scaling and shifting of the polynomial.

Sigmoid Kernel:

- The sigmoid kernel applies a sigmoid function to the dot product of the input vectors, which maps the data into a non-linear feature space.
- It can capture non-linear relationships between variables, but it is less commonly used compared to the RBF and polynomial kernels.
- The sigmoid kernel is controlled by hyperparameters gamma and coef0, which affect the shape and scaling of the sigmoid function**.**

. Linear Kernel:

- The linear kernel represents a linear relationship between the input variables and the target variable.
- It is the simplest kernel function in SVR and assumes a linear decision boundary.
- The linear kernel is suitable when the relationship between variables is expected to be linear.
- It does not require any additional hyperparameters.

When selecting a kernel for SVR, it is important to consider the underlying data distribution and the type of relationships expected between the features and the target variable

Model Evaluation: Therefore, we experiment with different kernel functions, evaluate their performance, and compare them using appropriate evaluation metrics to help determine the best choice for predicting the value of Tg.

Root Mean Square Error (RMSE): It measures the square root of the average squared difference between the predicted Tg values and the actual Tg values. RMSE provides a measure of the model's overall prediction error.

R-squared (R^2) Score: It represents the proportion of variance in the Tg values that can be explained by the SVR model. R^2 score ranges from 0 to 1, with higher values indicating a better fit of the model to the data. These evaluation metrics provide quantitative measures of the SVR

model's accuracy, precision, and goodness-of-fit. They help assess the model's ability to predict Tg values and compare the performance of different models or parameter

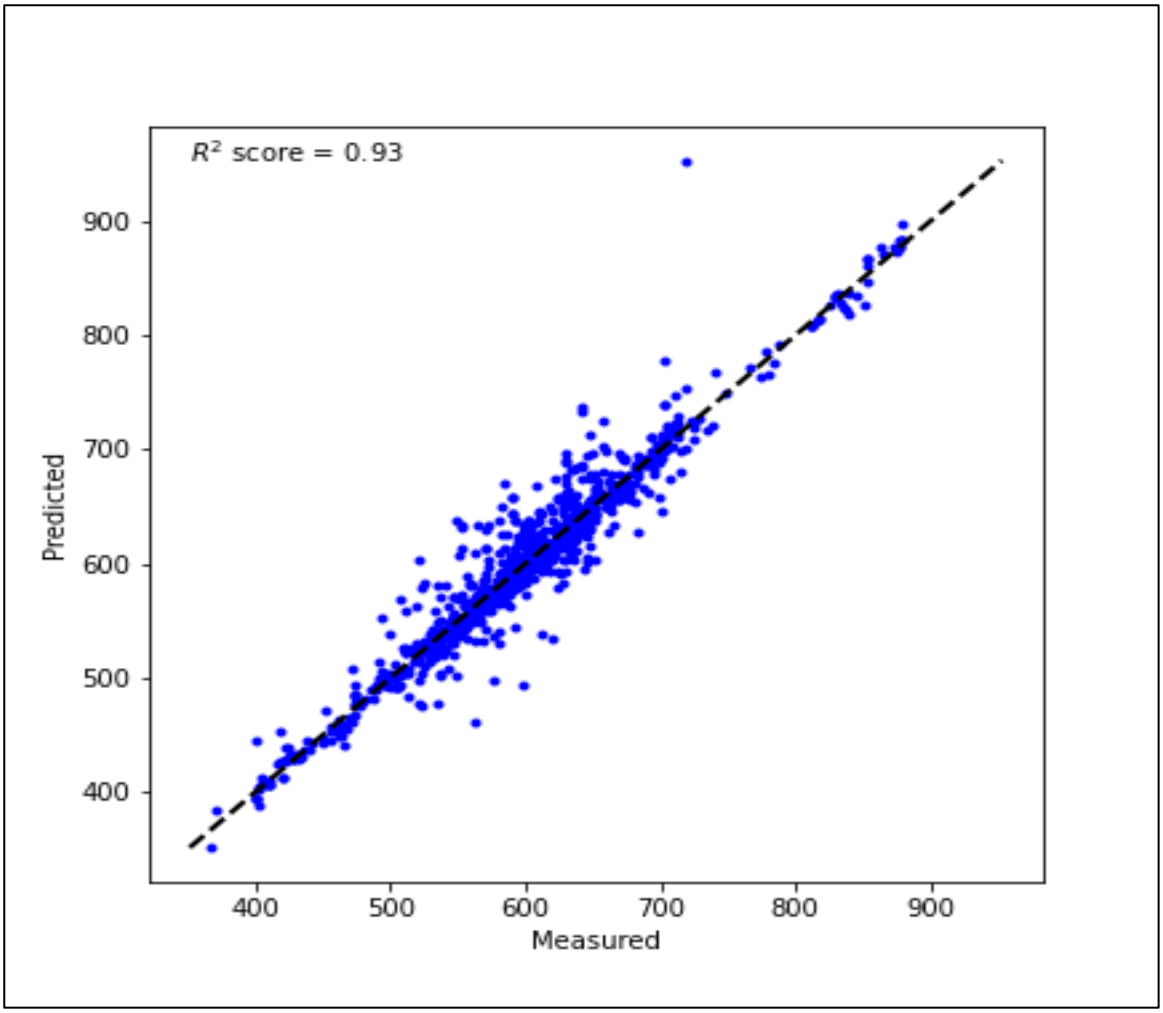
In this study, different kernel functions, including the ones mentioned earlier, were experimented with to evaluate their performance in predicting Tg values. Evaluation metrics such as R2 and RMSE were used, which provide quantitative measures to compare the performance of different kernel functions in SVR. These metrics help in selecting the best choice for predicting Tg values.

4) Results and Analysis

Our findings revealed that the SVR model utilizing the RBF kernel function achieved the highest R^2 score of 0.93, surpassing the performance of the other three models. Specifically, the linear, polynomial, and sigmoid models obtained R^2 scores of 0.80, 0.93, and -196, respectively. The study emphasized the superior predictive capability of the SVR model with the RBF kernel function in estimating the glass transition temperature (Tg). The RBF kernel, being a non-linear function, effectively captured the intricate relationships between the descriptors of glass composition and Tg values, surpassing the linear or polynomial kernels in this regard. Consequently, the SVR model with the RBF kernel function can be considered the optimal choice for predicting the Tg of tellurite oxide glasses in this study.

tapel (1.III): Results and discussion

	Kernels			
Metric	Polynomial	RBF	Sigmoid	**Linear**
R2	0.93	0.93	-196	**0.80**
RMSE (K)	23	22	83	**35**



fig(1.III): Results and discussion

the study focused on predicting the glass transition temperature (Tg) of tellurate oxide glasses using a support vector regression (SVR) model with a radial basis function (RBF) kernel. The main findings of the study can be summarized as follows:

1-The SVR model with the RBF kernel outperformed other kernel functions in terms of predictive accuracy and goodness-of-fit for Tg prediction in tellurate oxide glasses.

2-The strong correlation between Tg and the composition of tellurate oxide glasses was demonstrated, indicating that the selected composition descriptors have a significant impact on determining Tg values.

3-The SVR model successfully captured the complex relationships between the composition descriptors and Tg, highlighting the importance of machine learning techniques in predicting glass properties.

The significance of this study lies in its contributions to the field of Tg prediction for tellurate oxide glasses. By accurately predicting Tg based on composition descriptors, the study provides valuable insights for the design and development of glass materials. It offers a data-driven approach that can accelerate materials design and reduce the trial-and-error process.

The research also demonstrates the advantages of using SVR coupled with sparse principal component analysis (PCA) for predicting properties of glasses. This approach not only improves predictive accuracy but also provides insights into the key features influencing Tg. It has the potential to be applied to other types of glasses and predict various properties beyond Tg.

5)Potential Areas for Future Research

There are several potential areas for future research in this domain Exploration of Different Machine Learning Models and Techniques: While SVR has shown promising results, other machine learning algorithms, such as random forests, neural networks, or deep learning models, can be investigated for glass property prediction. Comparing and evaluating the performance of different models can provide insights into the most suitable algorithms for specific glass property predictions. Collecting More Data: Increasing the size and diversity of the training dataset can enhance the model's generalization ability and predictive accuracy. Obtaining experimental data for a wide range of glass compositions and properties will contribute to the development of more robust machine learning models. Incorporating Physics-Based Features: Integrating physics-based features, such as atomic configurations, bond energies, or structural parameters, into the machine learning models can further enhance their predictive capabilities. This hybrid approach, combining physics-based knowledge with data-driven techniques, can improve the interpretability and accuracy of the models. Incorporating Time-Temperature Superposition: Glass properties, including Tg, can be influenced by the time-temperature history. Incorporating time-temperature superposition principles into machine learning models can enable predictions of glass behavior under various temperature and time conditions, providing valuable insights for practical applications. Exploring Other Glass Systems: Extending the study to other glass systems, such as borosilicates, aluminosilicates, or chalcogenide glasses, can validate the effectiveness and

applicability of the proposed SVR and sparse PCA approach in different material systems. It can also uncover unique composition-property relationships specific to those glass systems.

6)conclusion

The potential impact of this research is significant. It enables researchers and engineers to optimize glass formulations for specific applications by tailoring the composition to achieve desired Tg values. This has implications for various industries, such as electronics, optics, and materials science, where controlling Tg is crucial for achieving desired material properties.

Further investigations are essential to advance the field of Tg prediction for glasses. Exploring different machine learning models and techniques, expanding the dataset, and incorporating physics-based features can enhance predictive capabilities. Additionally, extending the study to other glass systems and exploring the effects of time and temperature variations would provide more comprehensive insights into glass behavior and further improve the accuracy of predictions.

In conclusion, this study contributes to the understanding of Tg prediction for tellurate oxide glasses and offers a valuable framework for predicting properties of other types of glasses. The research has the potential to revolutionize glass design and development processes and open new avenues for innovation in materials science

General conclusion

General conclusion

In this study, we examined the performance of the Support Vector Regression (SVR) algorithm in predicting the glass transition temperature using different kernel functions, namely the Radial Basis Function (RBF), sigmoid, and linear kernels. We collected data from the SciGlass database, focusing specifically on tellurate oxide glasses. The performance of these models was assessed using the R^2 and RMSE metrics.

Among the various kernel functions tested, the RBF kernel exhibited the highest R2 score of 0.93, surpassing the performance of the other three models. The linear, polynomial, and sigmoid models achieved R^2 scores of 0.80, 0.93, and -196, respectively.

These results indicate that the RBF kernel function demonstrated superior predictive capability for the glass transition temperature compared to the other models. The polynomial kernel also showed promising performance with a high R^2 score. However, the sigmoid kernel exhibited poor performance with a negative R^2 score.

In conclusion, our findings highlight the effectiveness of SVR with appropriate kernel functions for accurately predicting the glass transition temperature in tellurate oxide glasses. Overall, this study contributes to the advancement of predictive modeling in glass science and provides valuable insights into the relationship between the bulk composition and the glass transition temperature, paving the way for enhanced materials design and development in the future.

Abstract

This study aims to predict the glass transition temperature (Tg) using Support Vector Regression (SVR) and sparse Principal Component Analysis (PCA) for designing and customizing materials with specific properties. The data was collected using the comprehensive SciGlass database, which contains glass compositions and their associated properties. SVR algorithm was utilized for Tg prediction, and the RBF kernel function demonstrated superior performance compared to other kernel functions in terms of predictive accuracy and goodness-of-fit for Tg prediction in tellurate oxide glasses. The study provides valuable insights into the design and development of glass materials and offers a data-driven approach that can expedite the materials design process and reduce trial-and-error efforts. Future research can explore different machine learning models and techniques, expand the dataset, and incorporate physics-based features to enhance predictive capabilities.

Keywords: Glass, glass transition temperature, machine learning, support vector regression, kernel function .

Résumé

Cette étude vise à prédire la température de transition vitreuse (Tg) en utilisant la régression par vecteurs de support (SVR) et l'analyse en composantes principales (PCA) pour la conception des matériaux présentant des propriétés spécifiques. Les données ont été collectées à partir de la base de données exhaustive SciGlass, qui contient des compositions de verre et leurs propriétés associées. L'algorithme SVR a été utilisé pour la prédiction de Tg, et la fonction de noyau RBF a démontré une performance supérieure par rapport aux autres fonctions de noyau en termes de précision prédictive et d'adéquation pour la prédiction de Tg dans les verres à base d'oxyde tellurique. Cette étude offre un aperçu précieux sur la conception et le développement des matériaux en verre, et propose une approche basée sur les données qui peut accélérer le processus de conception des matériaux et réduire les essais et erreurs. Les recherches futures peuvent explorer différents modèles et techniques d'apprentissage automatique, élargir l'ensemble de données et incorporer des caractéristiques basées sur la physique pour améliorer les capacités prédictives.

Mots-clés: Verre, température de transition vitreuse, régression par vecteurs de support, fonction de noyau, apprentissage automatique.

الملخص

تهدف هذه الدراسة إلى التنبؤ بدرجة حرارة التزجج (Tg) باستخدام انحدار المتجه الداعم (SVR) والتحليل عبر المركبات الرئيسية (PCA) لتصميم المواد وفق خصائص محددة. تم جمع البيانات باستخدام قاعدة بيانات SciGlass الشاملة، والتي تحتوي على التراكيب الزجاجية والخصائص المرتبطة بها. تم استخدام خوارزمية SVR للتنبؤ بـ Tg، وأظهرت وظيفة نواة RBF أداءً فائقًا مقارنة بوظائف الأنوية الأخرى من حيث الدقة التنبؤية وملاءمة التهيئة لتنبؤ Tg في زجاج أكسيد التيللوريت. توفر الدراسة رؤى قيمة في تصميم وتطوير المواد الزجاجية وتقدم نهجًا قائمًا على البيانات يمكنه تسريع عملية تصميم المواد وتقليل جهود التجربة والخطأ. يمكن للبحث المستقبلي استكشاف نماذج وتقنيات مختلفة للتعلم الآلي، وتوسيع مجموعة البيانات، ودمج الميزات القائمة على الفيزياء لتعزيز القدرات التنبؤية.

الكلمات المفتاحية: الزجاج، درجة حرارة التزجج، انحدار المتجه الداعم، وظيفة النواة، التعلم الآلي