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Theme:

Prediction of some physical properties of metallic glasses using Machine Learning

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In front of the jury members:

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I thank the Lord Almighty, who enlightened us the path of wisdom and knowledge and pleased us to accomplish this humble work to be a reference for future generations and a gift I dedicate to all of them:

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To the wide chest and the pure heart, O you who do not complete righteousness without him: **Dear Father**.

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Kir Bilal

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General Introduction

General Introduction

The oldest synthetic, human-made materials are ceramics, copper, iron, and glasses. For more than 6,000 years, glass objects have been known and widely used. In the last two centuries, **vitreous** materials have been extensively explored; searches of the Scopus database and the Derwent Innovation Index reveal that over half a million scientific publications have been published, with a similar number of patents registered on vitreous materials. Over 400,000 inorganic glass compositions have previously been disclosed, according to the SciGlass database, whereas many others are still hidden in industrial laboratories. [1]

Optical fibers, ionic conducting materials, optically functional formulations, bioactive compositions, and mechanically robust glasses and glass-ceramics have all advanced significantly from domestic use to an expanding variety of high-tech applications. Glasses become so important to humanity that some authors coined the term "glass age" to describe the current period. [1]

By far, the majority of these hundreds of glass-making formulae were developed by empirical trial-and-error experimental methods guided mostly by experience and acquired knowledge. The glass community, however, is shifting to data analytic-based methodologies as a result of the introduction of computer simulation tools. Profiting from the abundance of accessible composition property datasets for data-driven modeling used Artificial Intelligence, namely machine learning (ML) techniques, would be one of the most efficient ways. The ML-based techniques' ultimate purpose is to describe a list of desirable attributes and discover suitable compositions. However, before this operation can be completed, ML algorithms must first create prediction models by extracting rich and innovative knowledge from thousands of glass composition-property values. [1]

Since Dreyfus pioneering work in 2003 to forecast the liquidus temperature for oxide glass-forming liquids, ML algorithms with reasonably big datasets have been applied in the context of oxide glasses, which is not a “glass property”, but critical for glass making.[1]

The exact and comprehensive physical understanding of the glass transition and glass natures is considered to be one of the most challenging problems in condensed matter physics and material science. Due to the random disordered structure, the characterization of the glasses are very difficult, and this leads to problems for understanding the formation, deformation, fracture, nature, and the structure–properties relationship of the glasses.[2]

Metallic glass, which is a newcomer in glassy family (discovered in 1959) and at the cutting edge of current metallic materials research, is of current interest and significance in condensed matter physics, materials science and engineering because of its unique structural features and outstanding mechanical, many novel, applicable physical and chemical properties.[2]

Chapter 1:

Glasses

and

Theory of elasticity

1. Introduction:

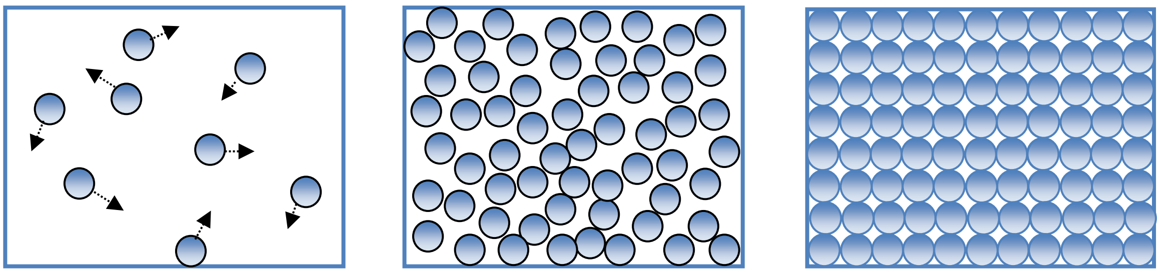
Glass is one of the oldest synthetic materials used by man and knowledge about the working and use of glass has been acquired over several centuries. The scientific study of glasses began at the beginning of the 19th century and is developing rapidly today, either with regard to the synthesis of new materials with specific properties or for the application of new techniques capable of improving our understanding. of the glass structure.

Glass is an isotropic and amorphous substance, theoretically presents an unlimited number of compositional possibilities [1]. That is why its properties are also very diverse, which has opened up many areas of use for it. As an example, glass is a hard and flexible material, when it subject to a mechanical stress it breaks, which leads us to study the content of the theory of elasticity.

In this chapter, we will present some basic notions about glass and its properties as well as briefly address the theory of elasticity in glass.

2. States of matter:

Matter is found in nature in three forms: gas, liquid and solid. The essential differences between the states of matter are shown in Figure (I-1).



(a) (b) (c)

Fig 1.1: The atomic arrangements in (a) a gas; (b) an amorphous solid; and (c) a crystalline solid

What distinguishes them is the arrangement of their constituent motifs:

- **Gases (**disorder): The particles forming matter, atoms, molecules, ions, have positions independent of the positions of neighboring particles (figure: I-1 (a)).

- **Molten liquids or solids (**short-range order): The position of a particle depends on the position of neighboring particles but not on that of more distant particles (figure: I-1(b)).

- **Crystals** (long-range order): The position of a particle depends on the positions of all the particles which surround it (figure: I-1(c)).

a. Crystal solid:

A crystal, also known as a crystalline solid, is a solid substance in which the components (such as atoms, molecules, or ions) are organized in a highly ordered microscopic structure to create a crystal lattice that extends in all directions. The word crystal comes from the Ancient Greek word “κρύσταλλος” (krustallos), which means both "ice" and "rock".

The most preferred (lowest potential energy) places occur at regular intervals in space in a solid composed of similar chemical units. If all of these positions are filled, the solid is known as a perfect crystal. A crystalline solid is defined by the fact that its structure is made up of repeated unit cells, each of which contains a tiny number of molecular units that have a definite geometric relationship to one another. The resulting long-range order forms a three-dimensional geometric structure known as a lattice. [2]

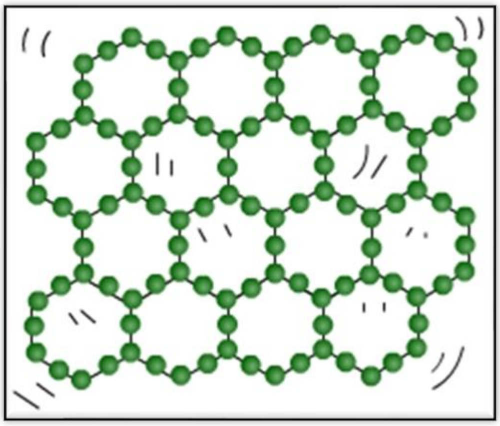


Fig 1.2: Crystal solid [3]

b. Non-crystalic solide:

An amorphous (from the Greek, *a* = "without" + *morphe* = "shape, form") or non-crystalline solid is a solid that lacks the long-range organization that characterizes crystals. Some earlier papers and books used the phrase synonymously with glass. Today, however, "glassy solid" or "amorphous solid" is regarded as the overarching idea, with glass seen as a specific case: glass is an amorphous solid kept below its glass transition temperature [4].

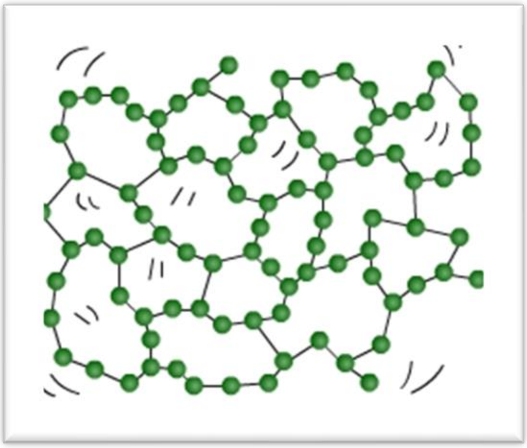


Fig I.3: Non-crystalic solide [3]

3. The Glassy State

3.1. Definition of glass

Glasses and other non-crystalline solids form a large family of non-crystalline materials that are typically produced by rapidly cooling a metastable liquid below its melting point or also via a wide range of other metastable synthesis routes [5]. During these routes, these materials acquire the properties of a solid without presenting a crystalline order at long distance and without periodicity in the arrangement of the atoms. In nature there are other non-crystalline solids obtained by freezing a liquid, but are not glasses, such as gels (for example). So, to determine the exact definition of glass, it is necessary to introduce the *notion of transition vitreous*, which characterizes *the vitreous state* [1].

The vitreous transition is a characteristic transformation observed on cooling, during the transition from a supercooled liquid phase to a vitreous phase, or, conversely, when the glass heats up to supercooled.

3.2. Formation of glass:

During cooling, such liquids crystallize on passing through fusion. Nevertheless, there are certain substances which, on melting, produce liquids endowed with high viscosity. If these liquids are cooled rapidly from a temperature above the melting point, crystallization can be avoided. The viscosity gradually increases as the temperature drops until it reaches a sufficient value which gives the liquid a solid character. When a liquid freezes without crystallizing, we say that it forms a glass, that it vitrifies or that it passes to the vitreous state. The glass transition is the term given to the physical phenomena which appear in a range of physical leads which appear in a range of viscosity between 10^{12} and 10^{14} poises, which corresponds to the glass transition temperature T_g [1, 6].

The formation of glass is best understood by looking at the most well-known diagram in glass science (Figure I-4), which plots the volume (or enthalpy) of a given mass of material vis temperature. The liquids only exist above the melting point (T_m). The liquid is in thermodynamic equilibrium and never crystallizes. Supercooled liquids exist between T_m and the glass transition temperature (T_g). They eventually crystallize (line BC) after a certain time. If the liquid is cooled quickly enough to avoid crystallization, the atoms do not have sufficient time to rearrange to the metastable equilibrium state (line BE). This cooling of the system occurs continuously and results in a non-equilibrium material known as “glass” [6]. The temperature at the intersection between the supercooled liquid line (BE) and glass line is the characteristic value of the T_g.

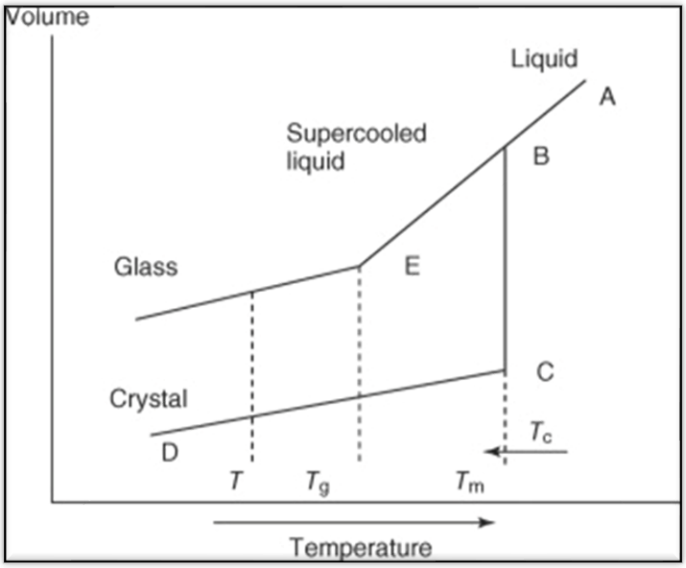


Fig 1.4: Volume change as a function of temperature during glass formation.

3.3. Types of glass

2.3.1. Oxide glass

The main oxides forming oxide glasses are SiO_2 , B_2O_3 , GeO_2 and P_2O_5 . They all come from a particular region of the periodic table (columns 13, 14 and 15): oxides of elements with intermediate electronegativity whose bonds with oxygen have an iono-covalent character. The resulting structures can be viewed as three-dimensional polymeric structures. These oxides can vitrify alone.

Heavy oxide glasses such as GeO_2 , As_2O_3 , Sb_2O_3 , TeO_2 have remarkable properties. They have high refractive indices and wide transmission in the infrared down to 6-7 µm. They are used as a waveguide for signal transmission. When doped with rare earths, these oxides are used as a laser source or as an optical amplifier [1].

2.3.2. Halide glass

The term "halide glass" refers to glasses, in which the anions are among the elements of group VIIA of the periodic table, namely, F, Cl, Br and I. Although halide glasses on beryllium fluoride (BeF_2) and zinc chloride ($ZnCl_2$) are well known, the glass-forming ability of ZrF4, AlF3, HfF4, and PbF2 have also been demonstrated. Halide are multicomponent (multi-component: halogens such as fluorine, in combination with heavy metals, such as zirconium, barium, or hafnium). Practical interest in halide glasses has been generated almost entirely by their optical properties, which cannot be reproduced in conventional oxide glass. The obstacles to the practical implementation of halide glasses have their origin in the properties of the materials in which they can be significantly inferior to metal halide glasses. oxides, for example, mechanical strength, resistance of the melt to crystallization, chemical durability, etc. [8].

2.3.3. Chalcogenide glasses

Chalcogen elements S, Se, and Te are used to make chalcogenide glasses. Other elements such as Ge, As, Sb, Ga, and others are used to create these glasses. They are low-phonon-energy materials that are usually transparent from visible to infrared wavelengths. Because chalcogenide glasses may be doped with rare-earth elements like Er, Nd, Pr, and so on, several applications of active optical devices have been proposed. [9]. Chalcogenide glasses have been used as optical materials. They have a wide transparency range, minimal optical losses within a 2–12 µm range, and are resistant to ambient moisture. Using chalcogenide glass fibers, a variety of technical challenges in optics and optoelectronics may be efficiently handled. [10]

3.4. Properties of glasses

There are different types of glass that have distinct properties. Choosing the best type of glass for a particular application requires knowing the different physical features that each form of glass has.

There are 5 main properties of glass to be considered: Optical properties, Thermal properties, Chemical resistance, Electrical properties and Mechanical properties.

3.4.1. Optical properties

Glass, a homogeneous and isotropic material, has unique intrinsic properties in the field of optics. These properties are based on the interaction of medium with the energy of electromagnetic waves.

3.4.1.1. Refractive index

Light travels in a straight line in dielectric media (glass) at a given speed. This speed, characteristic of the medium crossed, determines the refractive index $n(\lambda)$ at a given wavelength and defined by the ratio of the speed ***c*** of light in vacuum to that ***v*** the speed in the material:

$$n(\lambda) = \frac{c}{v} \tag{1.1}$$

To characterize the glasses, we use the refractive indices corresponding to three determined wavelengths [1]:

n_c For $\lambda = 6563 A^\circ$ (H_α hydrogen line)

n_D For $\lambda = 5893 \overset{\circ}{A}$ (yellow sodium stripe)

n_F For $\lambda = 4861 \overset{\circ}{A}$ (H_β hydrogen line)

Sometimes instead of n_D we use n_d which corresponds to the yellow line of hydrogen D_3 for $\lambda = 5876 \overset{\circ}{A}$. The difference $(n_F - n_c)$ is called *dispersion average* and the ratio $\left(\frac{n_F - n_c}{n_D - 1}\right)$ is called *relative dispersion*[1].

The inverse of the relative dispersion constitutes the *Abbe number,* which is frequently used to characterize optical glasses:

$$\nu = \frac{n_D - 1}{n_F - n_c} \tag{1.2}$$

3.4.1.2. Optical transmission

Optical transmission is one of the essential and best-known properties of glasses. It depends entirely on the chemical composition and the elements present in the glass. The transmission range of a material is limited to short wavelengths by the ultraviolet-visible barrier and to long wavelengths by the infrared barrier. Figure (1.5) show the transmission spectra of some types of glasses [11] .

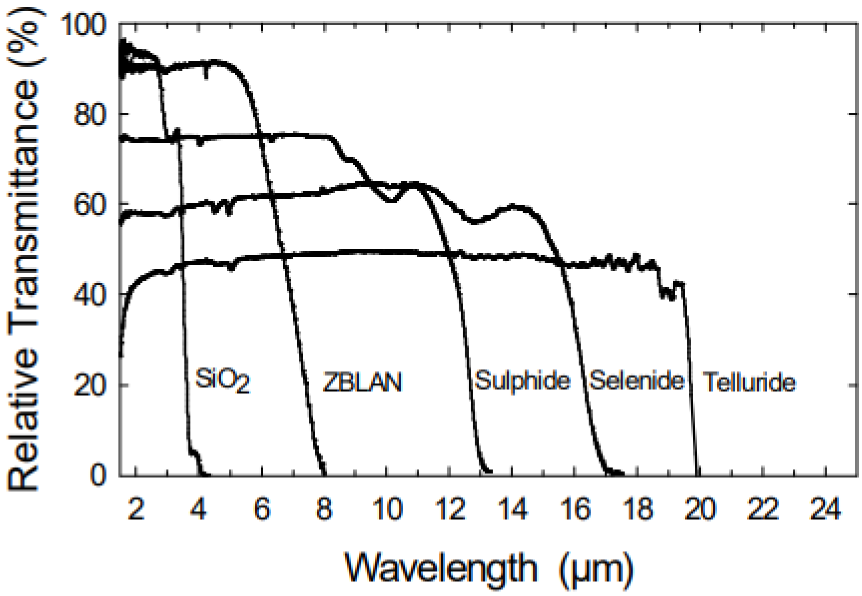


Fig 1.5: Transmission spectra for several glasses (thickness of about 2-3 mm) [11]

The optical transmission of glasses defined by *BERR-LAMBERT's law*:

$$\frac{I}{I_0} = \exp(-\alpha x) \tag{1.3}$$

I_0 : Incident intensity entering the glass of thickness x.

I : Intensity of light transmitted

x : Glass thickness in cm.

α : Absorption coefficient.

3.4.2. Thermal properties

The thermal properties are very important for the solidification and heat treatment of glass. among these properties, we can cite viscosity and thermal expansion.

- **Viscosity**

Viscosity is not only an essential property for the production and manufacture of glasses, it also is closely connected with the nature and structure of the glass melt. Viscosity is the industrially most important property for shaping glass objects. Viscosity evolves continuously from stable liquid to glass at room temperature. Figure (1.6) shows the variation of viscosity with temperature [12].

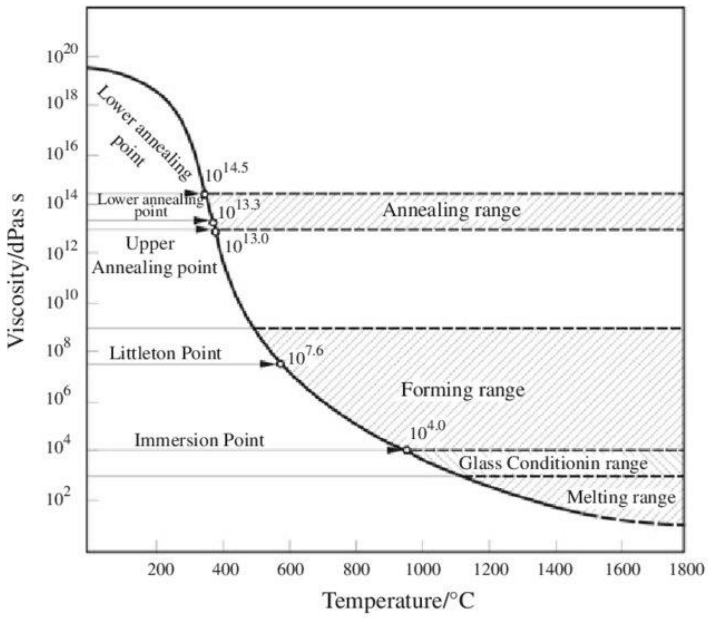


Fig 1.6: Variation of the viscosity of a glass as a function of temperature [12].

Viscosity variation as a function of temperature can be given by the *Vogel-Fulcher-Tammann (VFT) relationship* [13].

$$\eta = \eta_0 \exp\left[\frac{D_f T_0}{T - T_0}\right] \tag{1.4}$$

Where η_0 is the pre-exponential constant, D_f the fragility parameter, and T_0 is the VFT temperature.

- **Thermal expansion**

During glass melting, viscosity is one of the decisive properties. In the production process, annealing follows melting and forming. There another property becomes important which has already been involved in determining the transformation temperature: thermal expansion. Thermal expansion is produced by the increase in temperature which increases the distance between two atoms bound by (non-harmonic) forces. Each particle of a substance vibrates, as a result of the ever - present thermal energy. With increasing temperature, the thermal energy becomes greater, which results in an increase in the vibration amplitude. That is, as the temperature increases an expansion takes place [14,15].

The evolution of the dilation according to the temperature is represented in the figure (1.7) [16], it is seen that the point of inflection of the curve corresponds to the glass transformation temperature T_g .

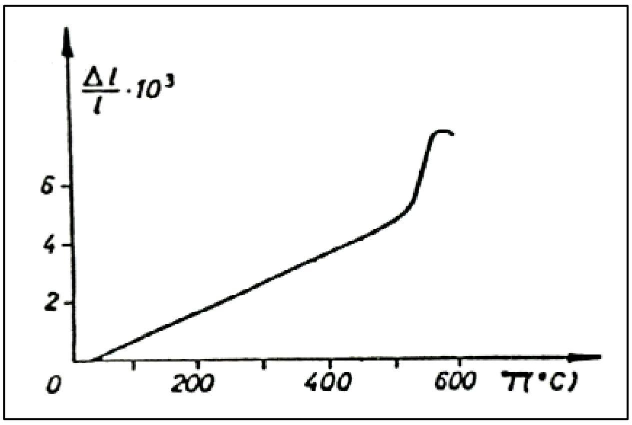


Fig 1.6: Evolution of thermal expansion as a function of temperature [16]

The value of the slope is called *the coefficient of expansion*, and can be expressed by:

$$\alpha = \frac{1}{l_0} \times \frac{\Delta l}{\Delta T} \tag{1.5}$$

$\frac{\Delta l}{l_0}$: Relative elongation of a sample of initial length l_0 .

ΔT : Temperature interval considered.

3.4.3. Chemical resistance

In addition to the transparency to light, glass is also distinguished, among other properties, by its great resistance with respect to almost all chemicals at usual temperatures. Without this property, the wide range of applications of glass would be unthinkable.

Chemical durability is the expression of the material's resistance to an environment. For a glass, it expresses its resistance to degradation in aqueous solutions. This quantity is generally related to the unit area of matter per unit time. Of the better-known reagents, it is only hydrofluoric acid which makes an immediately noticeable attack on glass; it brings the chief components of glass into solution [1,16,17].

3.4.4. Electrical properties

The many and various areas of application of glass also include electronics. To base temperature, glass is insulating. When heated enough, it becomes a conductor of electricity. The mobility of divalent and higher valence ions is generally very low compared to that of alkali ions. So, the conductivity of the glass increases with the increase in alkaline content [1,17] (figure (1.7))

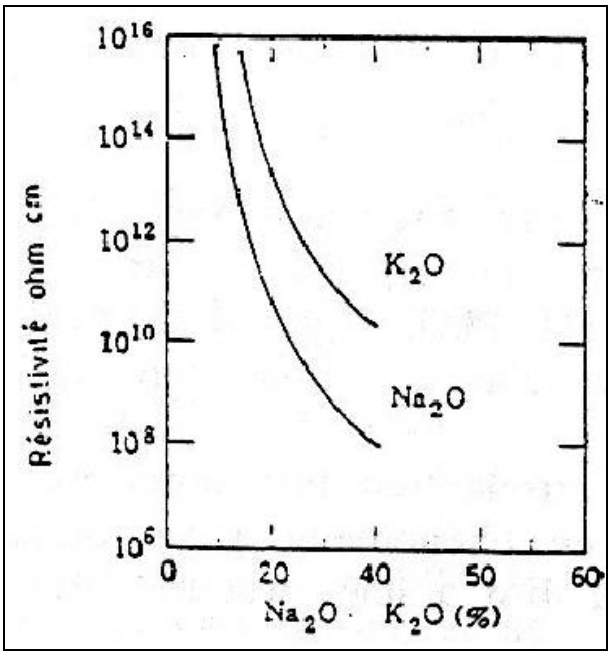


Fig 1.7: Partial replacement effect of SiO_2 by K_2O and Na_2O on electrical conductivity [1]

3.4.5. Mechanical properties

Glasses are fragile materials. However, the quantity as well as the variety of glasses available are constantly growing. At each period of the life of the glass, specific mechanical properties are sought. These properties must allow the development and shaping by industrial processes and guarantee good performance in service [18]. In the mechanical properties of glass emphasis is placed on its strength, hardness and elasticity:

- **Strength:**

The strength of materials is associated with the influence of forces and the interpretation of the deformations caused by such forces [19].In the use of glass, its resistance to breakage is very important. For a long time, attempts have been made to understand better the causes of its proverbial susceptibility to breakage in order to be able to produce stronger glasses in a more systematic way [20].

- **Hardness:**

In glass technology, the concept of hardness has several meanings. Hardness is the ability of a body to resist permanent deformation [21].

- **Elasticity:**

Glass is an elastic solid material, which means that when subjected to mechanical stress, it will break completely. The mechanics of solids represents the content of the theory of elasticity, which is known as the response of materials to stresses applied to them, which describes the method of solid deformations when external stresses are applied. A solid body undergoes a strain through a deforming force. If after the removal of the force this strain completely reverses, the body is called ideally elastic.

4. Theory of elasticity

4.1.Theory of elastic properties of solids:

The mechanical properties are not determined by the energies of the interatomic bonds alone, but depend on the coordination, the degree of interconnection (or polymerization), and the topology of piling (rings, chains, sheets) at a supramolecular scale where small domains could be observed [18]. The theory of elasticity treats the relationship between forces applied to an object and the resulting deformations. In practice, the analysis of the elastic behavior of a material is reduced to the study of simple deformations and the determination of the corresponding elastic constants [22].

The macroscopic behavior of a solid material is described by the continuous field theory, which is the theory of elasticity, which describes the process of solid deformations when external stresses are applied, and the ability of the material to restore its original shape after removing the deforming force. Under the action of applied stress, solid body exhibits shape and volume changes to some extent, and every point in the solid body is in general displaced. Let the position vector before the deformation be **r**, and after the deformation has a value **r'** with component $\mathbf{x_i}$. The displacement of this point due to deformation then given by the displacement vector $u = r - r'$or$u_i = x_I' - x_i$. If $u_{ij}(x_1, x_2, x_3)$ is the jth component of the displacement at point(x_1, x_2, x_3), the strain tensor for small deformations is [23,24]:

$$u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_i}{\partial X_i}\right) \tag{1.6}$$

When deformation occurs, the body will not be in its original state of equilibrium, and therefore forces called internal stresses arise that tend to return the body to its state of equilibrium. If the deformation of the body is rather small, it returns to its original state when the influence of external forces ceases, and these deformations are known as elastic deformations. As for major deformations, when external forces are removed, the body cannot return to its full shape after deformation, and these deformations are plastic. There are different types of moduli, where the type of modulus depends on the type of deformation that the material is subjected to, such as elongation, bending, and others. All coefficients are represented by finding the stress-strain ratio within the limits of elasticity [25].

Stress is a quantity that describes the magnitude of forces that cause deformation. It is defined as force per unit area (unit Newton/m^2). Stress types including [26]:

- ***Tensile stress***: resulting in an increase in length, when forces pull on an object and cause its elongation, like the stretching of an elastic band.
- ***Compressive stress***: results in a decrease in length or a change in volume, when forces cause a compression of an object.
- ***Shear stress*** (tangential stress): change in the shape of the geometric body, when an object is being squeezed from all sides.

Strain is defined as the deformation of material. It is also defined as the relative change caused by stress to the dimensions, shape or size of the body.

4.2. Elastic moduli [23,27]:

A solid deforms under the action of a deforming force. If by removing this force, the deformation disappears, the body is said to be: elastic or fragile.

Hooke's law expresses that the deformation *D* is proportional to the stress σ applied:

$$\sigma = M\,D \tag{1.7}$$

The proportionality constant *M* is called the elastic modulus. Depending on the type of deformation, there are different moduli (E, G, K or μ).

• **Young's modulus E**

Under tensile stress, an elongation appears which is characterized by the modulus of elasticity E (or Young's modulus), this modulus defines the resistance of the material before rupture.

• **Shear modulus G and K**

A shear stress leads to a shear process characterized by the shear modulus G . In the case of a pressure exerted on all the faces, the modulus of compression K is used.

• **Poisson's ratio ν**

During dilation, a transverse contraction occurs in the direction perpendicular to the elongation. If we take the relative elongation Δd/l and the relative transverse contraction Δd/d we then define the fish coefficient μ by the ratio:

$$\mu = \frac{\left(\dfrac{\Delta d}{l}\right)}{\left(\dfrac{\Delta d}{d}\right)} \tag{1.8}$$

The measurement of the moduli of elasticity E, G, K and the Poisson's ratio ν is carried out by ultrasonic echography. The principle of the method is based on the measurement of the longitudinal v_L and transverse v_T propagation velocity of the ultrasonic wave generated from a potential difference in a piezoelectric transducer. The latter, which plays the role of transmitter and receiver at the same time, transmits a mechanical impulse through a gel. The wave propagating in the glass is reflected on the opposite side of the sample. The speed of propagation of the wave directly depends on the rigidity of the bonds of the material. The time interval between two successive echoes is measured and allows us to calculate the propagation speed of the longitudinal and transverse waves (figure 1.8)

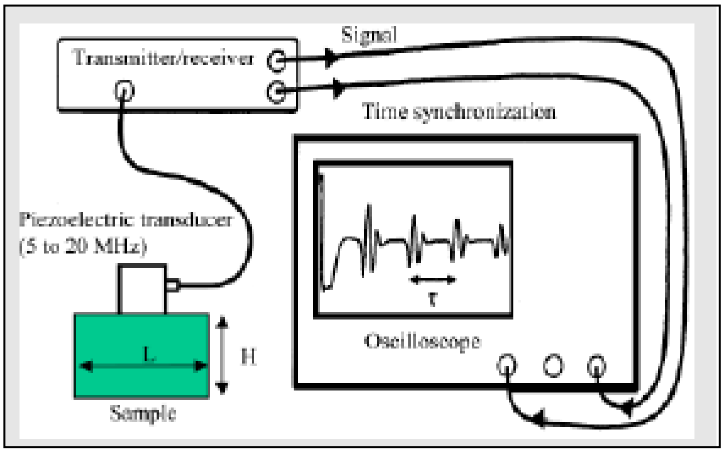


Fig 1.8: Dchematic illustrations for ultrasonic method.

Wave is independent of its frequency and the dimension of the material. In isotropic and homogeneous solids such as glassy materials, the one-dimensional acoustic wave equations are expressed as [12]:

$$\frac{d^2u}{dt^2} = \frac{Ld^2u}{\rho dx^2} \quad \text{(Longitudinal mode or compressional wave)} \tag{1.9}$$

$$\frac{d^2u}{dt^2} = \frac{Gd^2u}{\rho dx^2} \quad \text{(Shear mode or transverse mode)} \tag{1.10}$$

Where u is displacement, L is longitudinal modulus. From above equations, one obtains:

$$G = \rho v_s^2 \tag{1.11}$$

$$L = \rho v_l^2 \tag{1.12}$$

Where $v_l$and $v_s$are longitudinal and transverse sound velocities, respectively.

Based on the E, K, and v of the isotropic solids such as glasses can be given in terms of v_l, v_s and density as:

$$K = \rho(v_l^2 - \frac{4}{3}v_s^2) \tag{1.13}$$

$$v = \frac{v_l^2 - v_s^2}{2(v_l^2 - v_s^2)} \tag{1.14}$$

$$E = \rho v_s^2 \, \frac{3v_l^2 - 4v_s^2}{v_l^2 - v_s^2} \tag{1.15}$$

5. Conclusion

In this chapter we have covered two parts:

The first part revolves around the history of glass and some of its concepts. We also find that glass is an amorphous body and there are different types of it, including oxide, halogen, and chalcogenic. We find that the different types of glass lead to a difference in its composition, and we also mentioned the properties of glass, which are optical, thermal, chemical, electrical, and mechanical.

As for the second part, we have explained the theory of elasticity and described the elastic properties of the solid, and we also learned about the elastic coefficients, which are the longitudinal modulus, bulk modulus, shear modulus, Young's modulus, and Poisson’s ratio.

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Chapter 2:

Machine Learning

1. Introduction:

In context of solving problems, a major difference between human and computer is that the first can automatically improve his way of solving a problem, humans learn from their previous mistakes and try to solve them by correcting them or look for a new approach to tackle the problem, whereas traditional computer programs cannot learn from their outcome and hence they are unable of improving their performance. The field of machine learning addresses this problem to simulate humans and tries to create computer programs that are able to learn and therefore improve their performance by collecting data and try to make inferences.

Machine learning is defined as a sub-domain of artificial intelligence focuses on the development of models capable of representing certain characteristics, learn and detect some statistical pattern from data in order to accomplish various tasks, there are many techniques in machine learning we will discuss some of them in the below sections [1].

2. Unsupervised learning:

Unsupervised Learning (UL) is an elusive branch of Machine Learning (ML), including problems such as clustering and manifold learning, which seeks to identify structure among unlabeled data. UL is notoriously hard to evaluate and inherently indefinable.

The term "unsupervised learning" is generically associated with the idea of using a collection of observation $X_1. . ., X_n$ sampled from a distribution p(X)to describe properties of p(X) [2].

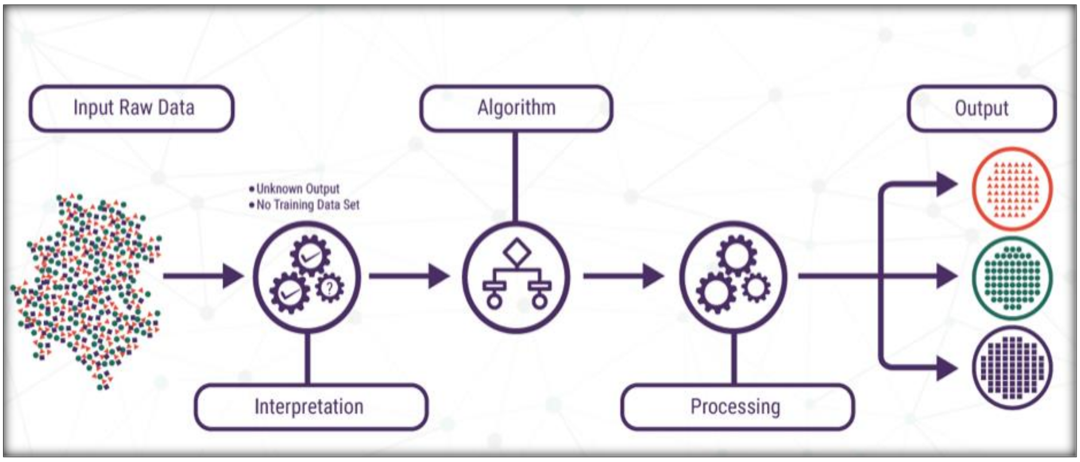

Fig 2.1: Unsupervised learning process.

3. Supervised learning:

Supervised learning refers to the problem where the data is on the form $\{x_i, y_i\}_{i=1}^{n}$, where $x_i$denotes inputs and $y_i$denotes outputs. In other words,in supervised learning we have labeled data in the sense that each data point has an input $x_i$and anoutput $y_i$which explicitly explains "what we see in the data" [3].

Supervised learning is categorized into two type classification and regression depending on whether the output of a problem is quantitative or qualitative; in this chapter we will cover regression since classification is beyond the scope our work.

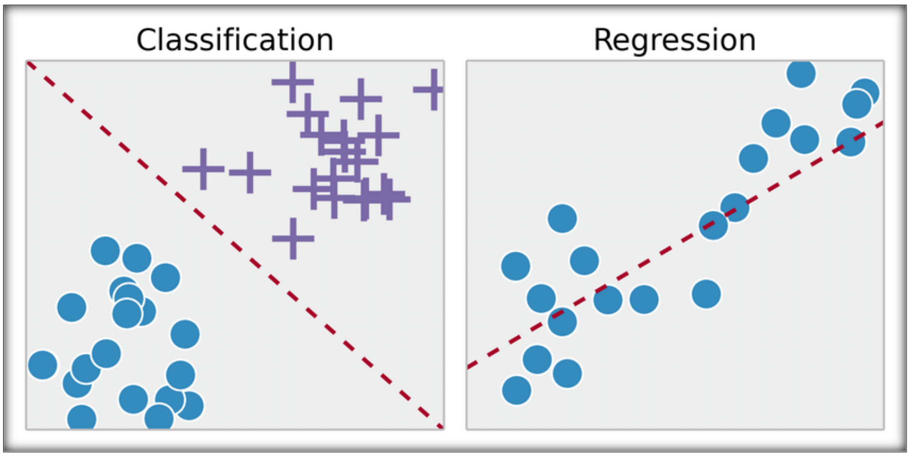

Fig2.2 : Difference between classification and regression **[4]**

3.1.Regression:

Regression is to map an input data to a numerical value. In another words for an input $Xi \in \mathbb{R}^d$ that represents d dimensional features vector and continues output space$Y \subset \mathbb{R}$, the learning algorithm is asked to produce a function $f : \mathbb{R}^d \to \mathbb{R}^n$ that maps any given input X_i to a corresponding value $y \in Y$. Examples Neural Networks, Support Vector Regression, Linear Regression, Polynomial Regression .. [1]

- **Linear regression:**

The simple linear regression model for n observations can be written as:

$$y_i = \beta_0 + \beta_1 \mathrm{X}_i + e_i \tag{2.1}$$

The designation simple indicates that there is only one predictor variable x, and linear means that the model is linear in β_0 and β_1. The intercept β_0 and the slope β_1 are unknown constants, they are both called regression coefficients; e_i'sare random errors.

To estimate β and β_1 we use the method of least squares, it consists of calculating the difference between the observations y_i and the regression line and minimize the following expression [4]:

$$\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 X_i)^2 \tag{2.2}$$

And the solution is:

$$\beta_1 = \frac{\sum_{i=1}^{n} x_i y_i + \frac{1}{n}\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i^2 - \frac{1}{n}\left(\sum_{i=1}^{m} x_i\right)^2} \tag{2.3}$$

$$\beta_0 = y - \beta_1 x \tag{2.4}$$

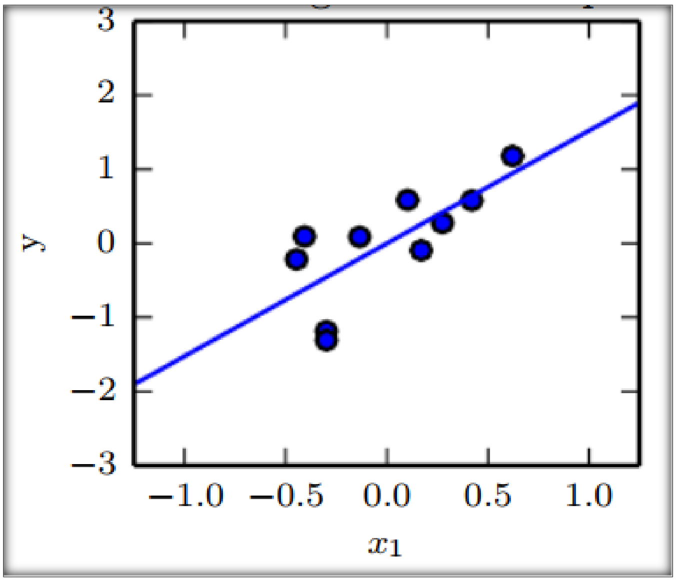

Fig 2.3: A linear regression problem, with a training set consisting of ten data points.

- **Nonlinear regression:**

The nonlinear regression model is a generalization of the linear regression model which does not depend only on a weighted sum of vector as mentioned in the previous subsection.

The nonlinear model is of the form:

$$Y_i = f\left(x_i, \gamma\right) + e_i \tag{2.5}$$

Where f is a nonlinear function of the parameters γ and

$$\underset{q\times 1}{x_i} = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{iq} \end{bmatrix}, \underset{p\times 1}{\gamma_i} = \begin{bmatrix} \gamma_0 \\ \vdots \\ \gamma_{p-1} \end{bmatrix} \tag{2.6}$$

In both the linear and nonlinear cases, the error terms ε_i are often (but not always) independent normal random variables with constant variance [5].

4. Support vector machine :

One of the most influential approaches to supervised learning is the support vector machine (Boser et al., 1992; Cortes and Vapnik, 1995). This model is similar to logistic regression in that it is driven by a linear function $w^T x + b$. Unlike logistic regression, the support vector machine does not provide probabilities, but only outputs a class identity. The SVM predicts that the positive class is present when.

$W^T x + b$ is positive. Likewise, it predicts that the negative class is present when.

$W^T x + b$ is negative.

One key innovation associated with support vector machines is the kernelrick. The kernel trick consists of observing that many machine learning algorithms can be written exclusively in terms of dot products between examples. For example it can be shown that the linear function used by the support vector machine can be re-written as:

$$\omega^T x + b = b + \sum_{i=1}^{m} \alpha_i x^T x^{(i)} \tag{2.7}$$

This function is nonlinear with respect to x, but the relationship between φ(x) and f (x) is linear. Also, the relationship between α and f(x) is linear [6].

- **SVM kernels:**

The kernel-based function is exactly equivalent to preprocessing the data by applyingφ(x) to all inputs, then learning a linear model in the new transformed space. The kernel trick is powerful for two reasons. First, it allows us to learn models that are nonlinear as a function of x using convex optimization techniques that are guaranteed to converge efficiently.

The most commonly used kernel is the Gaussian kernel.

$$k\left(u,v\right)=N\left(u-v;0,\delta^2 I\right) \tag{2.8}$$

Where N(x; μ, Σ) is the standard normal density. This kernel is also known as the radial basis function (RBF) kernel, because its value decreases along lines in v space radiating outward from u. The Gaussian kernel corresponds to a dot product in an infinite-dimensional space[24].

In the following table we give other kernel functions [7]:

No	Kernel function	Formulas
1	Linear	k(x_i, x)=$x_j^T x$
2	Polynomial	k(x_i, x)=$\left(x_j^T x + 1\right)^d$ d=1,2,….
3	Gaussian radial basis function	k(x_i, x)=exp(-$\gamma \|\|x - x_i\|\|)^2$ k(x_i, x)=exp(-$\frac{1}{2\delta^2} \|\|x - {x_i}^T\|\|)^2$
4	Splines	k(x_i, x)=$\prod_{m=1}^{n} k_m(x_m, x_{im})$

Table 1: SVM kernels.

5. Support vector regression:

The SVR method purpose is to improve generalized performance by selecting the appropriate use of kernel functions. Therefore, the kernels election is very important for a particular application. SVR was first introduced and developed from the concept of SVM theory.

SVM can approach the regression function by using the ε-insensitive loss function concept. The concept of ε-insensitive loss function is used to evaluate how well the regression function is used. The application of SVM in regression cases is called SVR-Regression.

The basic objective of the SVR is to find the function f (x) which has the most ε deviation from the actual target obtained from all training data, and at the same time the function must be as flat as possible. In other words, the error does not matter, as long as the error is less than epsilon ε. In SVR it is known as support vector, support vector is training data used in testing.

$$f(x) = w^T \varphi(x) + b \tag{2.9}$$

Φ(x) is the mapping result of the T function in the input space, w is weighting vector dimension 1andb is bias or deviate. The w and b coefficients are estimated by minimizing the risk function defined in the previous equation.

The coefficients w, b minimizes the risk function of the following equation:

$$R=\min\frac{1}{2}\|w\|^2 + c\,\frac{1}{l}\left(\sum_{i=1}^{l}(L_\varepsilon(y_i), f(x_i))\right) \tag{2.10}$$

SVR will find a function f(x_i) which has the greatest deviation ε from the actual target $y_i$for alltraining data. Then with SVR, when ε is equal to 0, a perfect regression will be obtained. Conversely, a high ε value is associated with a small slack variable value and low accuracy. The addition of this slack variable is to solve the problem of infeasible margin limiter in the optimization problem [8]

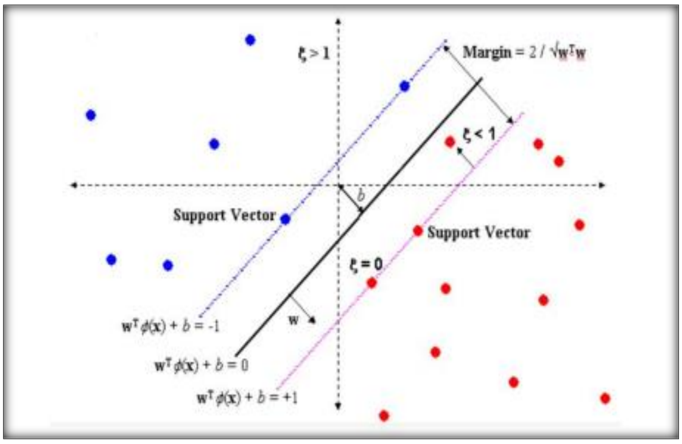

Fig2.4: Support Vector.[23]

6. Training process:

The central challenge in machine learning is that we must perform well on new, previously unseen inputs, not just those on which our model was trained. The ability to perform well on previously unobserved inputs is called generalization. Typically, when training a machine learning model, we have access to a training set, we can compute some error measure on the training set called the training error, and we reduce this training error

For example in a linear model we train the model by minimizing the following error

$$\frac{1}{m^{(train)}}\left\|x^{(train)}\omega - y^{(train)}\right\|_2^2 \qquad (2.11)$$

- **Underfitting:** Is when a machine learning model can not properly learn from the training data (have low accuracy). Some of the reasons why underfitting happens in neural networks is to have a small model or using a linear model with none linear dataset (features in the dataset are complex). Another reason is the noisy data (containing wrong labels) [1].
- **Over-fitting:** is when a machine learning model gives a high prediction accuracy on the training data, but the prediction accuracy gets low if the model tested on previously unseen data (a data that was not present during the training),another term for describing overfitting is “high generalization error”. Overfitting occurs when the model gets closely fit to the training data, this is because the training data is not all the possibilities of input data. A good model should have a good accuracy on the training data and the other. In other word, (it should be able to generalize) [1].

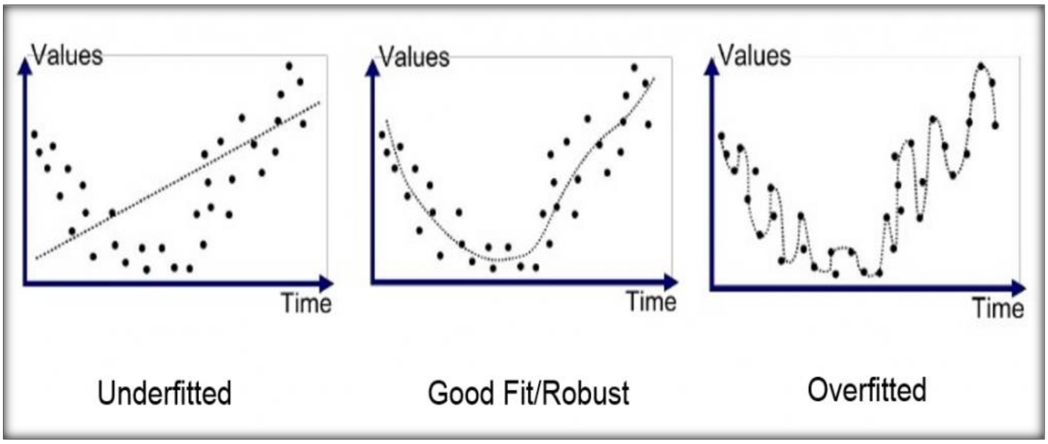

Fig2.5: The difference between overfitting, underfitting [1].

7. Conclusion:

In this chapter we have discussed several technique we need to construct our SVR predictive model, the way to incorporate the data set to train the machine learning model, In the next chapter we will present the different experiments we done in this framework and discuss the obtained results as well.

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Chapter 3:

Results and discussion

Result and discussion:

In this chapter we will begin by presenting the data-set and data prepossessing we proceeded after that we are going to present the SVR model we established to predict our shear modulus and poison ratio {G, υ}, finally we will discuss the result we obtained.

1. Method:

- The data has been collected from the articale of W.H.Wang et al (The elastic properties, elastic perspectives of metallic glasses.
- It consist of more than 150 glass samples with their corresponding elastic properties.
- In our work we will focalize on predicting shear modulus and poisson ratio using support vector regression model.

2. Data analysis:

The data consist of 150 × 52 matrix, 150 glasses sample, the first 45 features are the glasses compositions percentage, and the rest are glasses physical properties however in this work we will focus on glasses elastic properties.

	Zr	Ti	Cu	Ni	Be	Al	C	Y	Fe	Mg	...	Lu	DENSITY	Vl	Vs	K	G	E	V	THETAD
s1	41.00	14.00	12.50	10.0	22.50	0.0	0.0	0.0	0.0	0.0	...	0.0	6.125	5.174	2.472	114.1	37.4	101.2	0.352	326.8
s2	46.75	8.25	7.50	10.0	27.50	0.0	0.0	0.0	0.0	0.0	...	0.0	6.014	5.182	2.487	111.9	37.2	100.5	0.350	327.1
s3	45.40	9.60	10.15	8.6	26.25	0.0	0.0	0.0	0.0	0.0	...	0.0	6.048	5.163	2.473	111.9	37.0	99.9	0.350	325.6
s4	52.50	0.00	15.00	10.0	12.50	10.0	0.0	0.0	0.0	0.0	...	0.0	6.295	5.033	2.384	112.0	35.9	97.2	0.355	306.6
s5	50.00	0.00	15.00	10.0	15.00	10.0	0.0	0.0	0.0	0.0	...	0.0	6.311	5.075	2.478	110.9	38.8	104.1	0.343	321.5

Fig 3.1: Dataset head.

Furthermore, we observe a problem with the data, namely the design matrix of inputs is very sparse (many zeros) as shown in the following figure.

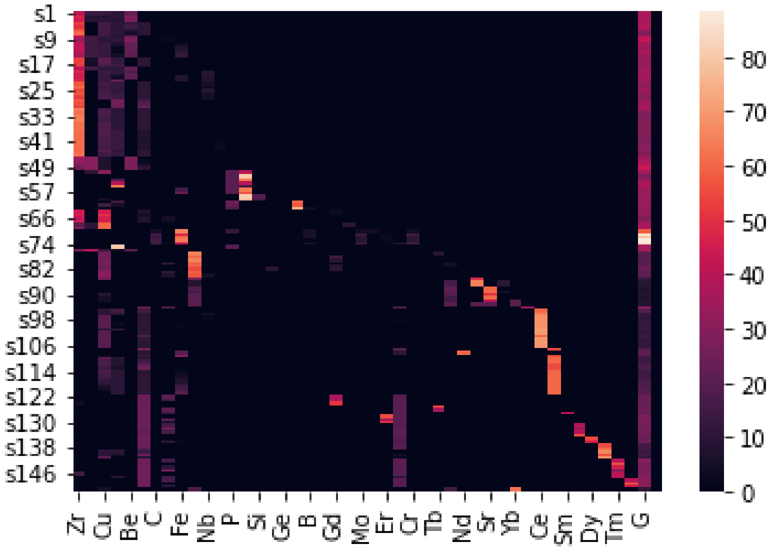

Fig 3.2: Data heat map.

Next we investigated the density distribution of our parameter of interest, and we observe that the distribution of G is skewed (left or right side), asymmetric and discontinued between [60-80], whereas for the distribution of υ is less asymmetric with no discontinuity.

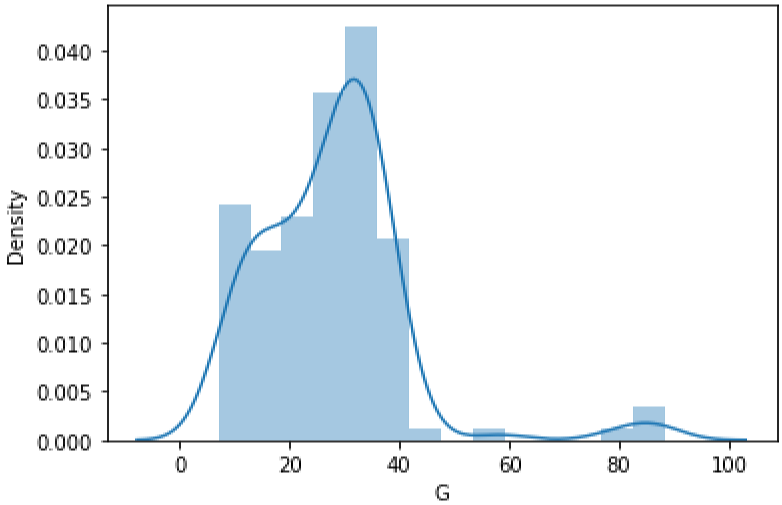

Fig 3.3: Density distribution of G.

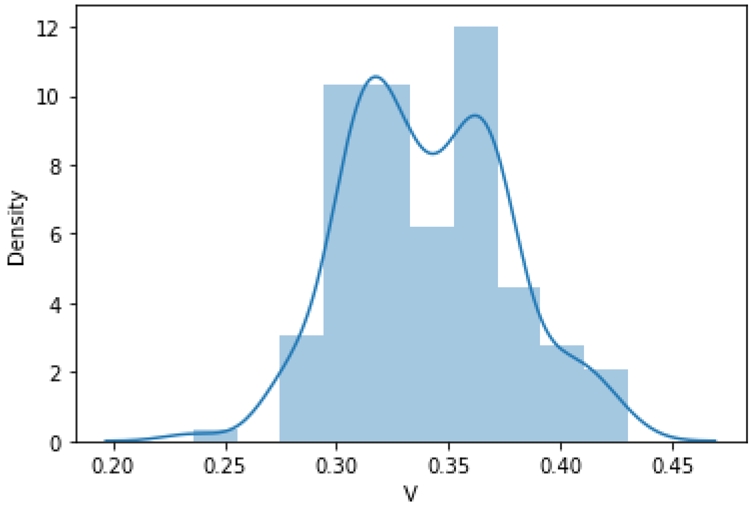

Fig 3.4: Density distribution of υ.

The below figure depicts the correlation matrix of the glass compositions in the design matrix. White indicates a positive correlation of p-value 1(strong statistical evidence of correlation), and violet indicates a negative correlation of p-value -0.4. The closer to 1, the more evidence there is of correlation. We observe that there are many instances of positively or negatively correlated features

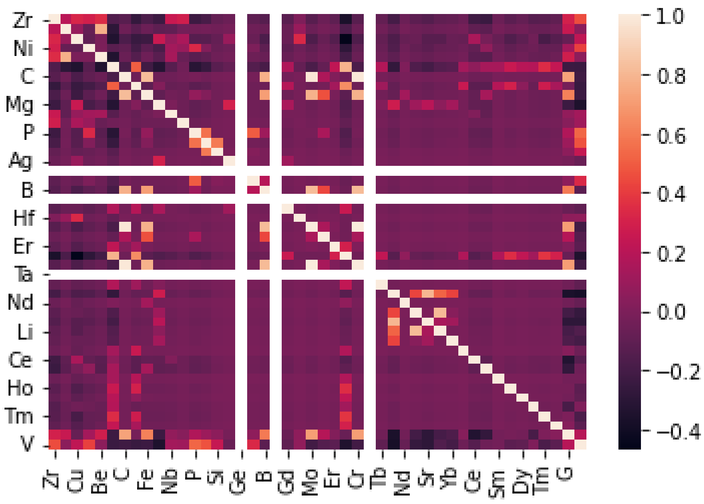

Fig 3.5: The correlation matrix between the target and input features.

3. Data preprocessing:

As discussed above, sparsity of the input matrix is problematic for several reasons and the SVR model may not be robust to solve our task of interest, as a result we have applied sparse principle component analysis (PCA) for better data representation.

The sparse PCA was conducted using predefined function from SKlearn package in python with 33 principle component and as default for the other sparsepca parameters in details:

1) Controlling parameter of 1 (default),
2) Ridge shrinkage parameter of 0.01 (default),
3) Max iterations of 1000(default)
4) Tolerance of 10^8 (default).

Moreover we scaled the element of the input matrix using standard scaler which follows the next formula:

$$z = (x - u) / s \tag{3.1}$$

Where u is the mean of the training samples or zero if with_mean=False, and s is the standard deviation of the training samples or one if with_std=False.

4. Result:

After doing data cleaning and preprocessing, we have applied our support vector regression model using python SVR function from SKlearn package with radial basis function as kernel function.

Moreover, we followed leave one out as cross-validation procedure, where the number of folds equals the number of instances in the data set. Thus, the learning algorithm is applied once for each instance, using all other instances as a training set and using the selected instance as a single-item test set.

We introduce in the table below some of our result of predicting shear modulus G and poison ratio υ :

	G		υ	
Glasses samples	Predicted values	Actual values	Predicted values	Actual values
41Zr14Ti12.5Cu10Ni22.5Be	37.52912821	37.4	0.35225629	0.352
53Zr5Ti20Cu12Ni10Al	31.09800532	31.3	0.37052505	0.37
45Zr13Cu4Ni22Be8Fe8Nb	35.34571098	35.1	0.35484361	0.361
14.3Cu5.7Ni25Al55Pr	26.1724204	26.19	0.31782908	0.319
24Al20Y36Gd20Co	26.73940947	26.58	0.32111764	0.317
25Al10Y20Co45Tm	27.76600377	27.3	0.30681106	0.309
25Al20Co55Tm	30.12648252	30.6	0.31367097	0.307
57Zr15.4Cu12.6Ni10Al5Nb	31.65590991	32	0.36986171	0.365
60Zr14Cu13Ni10Al3Nb	31.65590991	32	0.36986171	0.365

5. Discussion:

In this work, we proposed an alternative framework to predict glasses elastic properties namely shear modulus G and poisson's ratio using the bulk composition of a given material. Based on SVM regression, it is clear that the relationship between the bulk composition and the corresponding parameters of interest of a sample does in fact exist, with significant low root mean squared error (RMSE) of poisson's ratio around 0.01 and a relatively high RMSE of 1.67 for the shear modulus, for the reason that the distribution of the shear modulus in the collected data is skewed and discontinued as we pointed before. However, we have demonstrated that having the bulk composition and the corresponding elastic parameters of a relatively small number of materials is enough to estimate the elastic properties of similar compositions with a reasonable bound on the error.

6. Conclusion:

The estimation of the elastic parameters within the traditional paradigm is mathematically and experimentally involved, which certainly poses a substantial barrier for subsequent innovation, for these reasons we have tested an alternative framework to directly predict glasses elastic properties using bulk composition in order to reduce the computation, physical and time cost.

Our SVR model is at first effective in detecting the correlation between quantity of interest (G, υ) and glasses compositions, nevertheless, it can be more tested with more data and more physical properties included thus we can say that this result is not final and can be further improved.

General conclusion

General Conclusion

In this work, we investigated the predictive performance of a machine learning algorithm, SVM, for two glass elastic properties: shear modulus G and poisson's ratio υ, using the bulk composition. For such, we used a dataset of about 150 metallic glasses.

Based on SVM regression, relationship between the bulk composition and the corresponding parameters of interest of a sample does exist. A significant low root mean squared error (RMSE) of poisson's ratio was founed to be around 0.01. Nevertheless, a relatively high RMSE of 1.67 for the shear modulus, this can be interpreted according to the skewed and discontinued of the distribution of the shear modulus in the collected data. We have demonstrated that having the bulk composition and the corresponding elastic parameters of a relatively small number of materials is enough to estimate the elastic properties of similar compositions with a reasonable bound on the error.

These results can be further improved to help bulk compositional tuning and computer - aided inverse design of glasses.

Abstract:

In this work, we proposed an alternative framework to predict two glasses elastic properties: shear modulus G and poisson's ratio using the bulk composition. Based on SVM regression, relationship between the bulk composition and the corresponding parameters of interest of a sample does exist. A significant low root mean squared error (RMSE) of Poisson's ratio was obtained to be around 0.01. However, the RMSE of the shear modulus is relatively high and is about 1.67, this can be interpreted according to the skewed and discontinued of the distribution of the shear modulus in the collected data. We have demonstrated that having the bulk composition and the corresponding elastic parameters of a relatively small number of glasses is enough to estimate the elastic properties with a reasonable bound on the error. These results can be further improved to help bulk compositional adjustment and computer aided inverse design of glasses.

Keywords: Glass, Machine Learning, SVM regression, Shear modulus, Poisson's ratio.

الملخص:

في هذا العمل ، اقترحنا إطارا بديلاً للتنبؤ بخاصيتين مرونيتين للزجاج : معامل القص ونسبة بواسون وذلك باستخدام التركيب الكتلي . استنادا إلى انحدار SVM، فإنه توجد علاقة بين التركيب الكتلي والمعاملات الموافقة له للعينة. ثم الحصول على خطأ تربيعي متوسط (RMSE) منخفض لنسبة بواسون ليكون حوالي 0.01. ومع ذلك، فإن RMSE لمعامل القص مرتفع نسبيا ويبلغ 1.67، ويمكن تفسير ذلك وفقا لانحراف وتقطع توزيع معامل القص في البيانات المجمعة . لقد أوضحنا أن وجود التركيب الكتلي ومعاملات المرونة المقابلة لعدد صغير نسبيا من التركيبات الزجاجية كاف لتقدير الخصائص المرونية بحد معقول للخطا . يمكن تحسين هذه النتائج بشكل أكبر للمساعدة في الضبط التركيبي والتصميم العكسي للزجاج بمساعدة الكمبيوتر .

الكلمات المفتاحية: الزجاج ، تعلم الآلة انحدار SVM، معامل القص، نسبة بواسون.

Résumé:

Dans ce travail, nous avons proposé un cadre alternatif pour prédire deux propriétés élastiques des verres le module de cisaillement G et le coefficient de Poisson en utilisant la composition massique. Sur la base de la régression SVM, il existe une relation entre la composition et les paramètres d'intérêt correspondants d'un échantillon. Une faible erreur quadratique moyenne significative (RMSE) du coefficient de poisson a été obtenue à environ 0,01. Cependant, le RMSE du module de cisaillement est relativement élevé et est d'environ 1,67, cela peut être interprété en fonction de la distribution asymétrique et discontinue du module de cisaillement dans les données collectées. Nous avons démontré qu'il suffit d'avoir la composition massique et les paramètres élastiques correspondants d'un nombre relativement petit de verres pour estimer les propriétés élastiques avec une borne raisonnable sur l'erreur. Ces résultats peuvent être encore améliorés pour faciliter l'ajustement de la composition en masse et la conception inverse assistée par ordinateur des verres.

Mots-clés: Verre, Apprentissage automatique, régression SVM, module de cisaillement, coefficient de poisson.