GROWTH, OPTICAL AND MECHANICAL STUDIES OF L -THREONINE LITHIUM CHLORIDE SINGLE CRYSTAL

Submitted in partial fulfillment of the requirements for the award of

Master of Science Degree in Physics

By

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DEPARTMENT OF PHYSICS

SCHOOL OF SCIENCE AND HUMANITIES

SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)
Accredited with "A" grade by NAAC I 12B Status by
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BONAFIDE CERTIFICATE

This is to certify that this project report is the bonafide work of **R R SRIPRIYA (REG.NO 41590020)** who have carried out the project entitle **"GROWTH OPTICAL AND MECHANICAL STUDIES OF L- THEREOINE LITHIUM CHLORIDE SINGLE CRYSRAL"** under our supervision from August 2022-May 2023.

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Date:09-05-2023

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Place: Chennai **Signature of the candidate**

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LIST OF ABBREVIATION

E	_	Electric Field vector
C	_	Capacitance
D	_	Electric field displacement vector
ε0	_	Permittivity of free space
Er	_	Dielectric constant
χ(1)	_	Linear susceptibility
χ(2)	_	Nonlinear susceptibility
Mv	_	Micro volt
N	_	Work hardening coefficient
Hv	_	Vickers hardness number
P	_	Polarization
Nm	_	Nanometer
Mm	_	Micrometer
μ0	_	Permeability of free space
Ȧ	_	Angstrom
Ɵ	_	Theta
∆	_	Delta
Α	_	Alpha
Β	_	Beta
Ω	_	Omega
a, b, c	_	Unit cell parameter

Λ	_	Wavelength
NLO	_	Nonlinear optics
SHG	_	Second Harmonic Generation
UV	_	Ultra violet

ABSTRACT

The single crystal of L-Threonine Lithium Chloride (LTLC), an efficient Semiorganic nonlinear optical (NLO) material was grown successfully in slow evaporation method. Single crystal X-ray diffraction study reveals that LTLC crystallizes into orthorhombic system with the space group Pna21.The Optical absorption spectrum shows that LTLC has highly transparent in the entire visible region for large photon absorption. Vickers micro hardness measurement was performed to know the mechanical strength of the crystal. Dielectric constant and dielectric loss were calculated by varying frequency at different temperatures. The SHG efficiency of the crystal is also examined by Kurtz's powder test using Nd: YAG Laser.

CHAPTER -I

INTRODUCTION

1.1. INTRODUCTION TO NON LINEAR OPTICS

Non optics is given increases attention due to its wide application in the area of laser technology [1-2] a new effect in which light of one wavelength is transformed to light of another wavelength. The creation of light of new wavelength can be understood, as we think about the electrons in nonlinear crystal. Electrons in a nonlinear crystal are bound in potential Well, which acts like a spring (fig 1.1), holding the electrons to lattice point in the crystal. If an external force pulls an electron away from its equilibrium position the spring pulls it back with a force proportional to the displacement. The spring’s restoring force increases linearly with the electron away from its equilibrium position the spring pulls its back with a force proportional to the displacement. The electric field in a light wave passing through the crystal exerts a force optical material, the electrons oscillate about their equilibrium position. According to the fundamental law of physics an oscillation change will radiate at its frequency of oscillation, hence these electrons in the crystal “generate” light at the frequency of the original light wave.

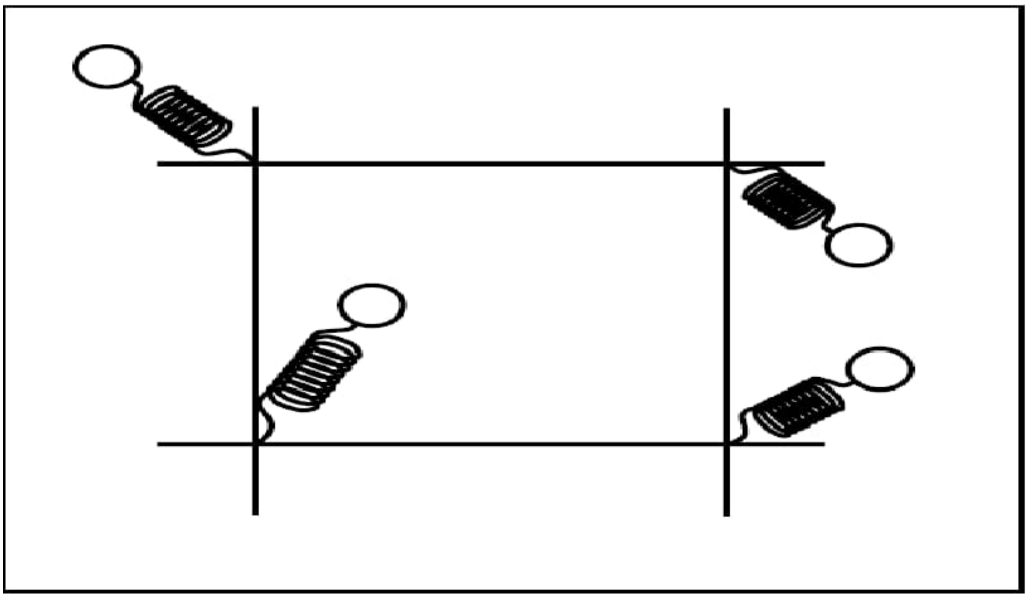


Fig 1.1 Electrons in a NLO are bound in a potential well, holding the electrons to lattice points

An NLO material is a compound in which a nonlinear polarization is invoked on application of an intense electric field. This electric field results from the external application of an intense laser source. The nonlinear material is different from the linear material in several aspects. A nonlinear material is one, whose electrons are bound by very short springs. If the light passing through the material is intense enough, its electric field can pull the electrons so Far that they reached the end of their springs. The restoring force is no longer proportional to the displacement and then it becomes nonlinear. The electrons are jerked back roughly rather than pulled back smoothly and they oscillate frequencies other than the driving frequencies of the light wave. These electrons radiate at the new frequencies, generating the new wavelength of light. The exact values of the new wavelengths are determined by conservation of energies. The energy of the new photon generated by the nonlinear interaction must be equal to the energy of the photons used.

Over the last three decades, the discovery of new crystals for optical applications has been an emerging area of research. Nonlinear optical crystals are significant in science and modern technology because of their technological importance in the areas of optical communication, optical modulators, laser spectroscopy, frequency conversion, optical bi-stable devices, electro-optical device applications in photonics technology, optoelectronics, information processing, sensors, laser technology, frequency doubling and color displays. Optical applications depend upon various physical features, such as refractive index, birefringence, thermal stability and physicochemical behaviors.

Materials with high second-order optical nonlinearity, high optical transmittance with low cut-off wavelength, high laser damage threshold value and easy growth with large dimensions are needed to understand many of these applications. The growth of the new kind of optical crystals with good physical and chemical properties are very important in optoelectronics, photonics laser processing and other applications. The search for high non-linear optical crystals for efficient signal processing has been stimulated by optoelectronics. [3-4]

They are usually used for doubling, tripling and quadrupling of a Nd: YAG laser under the room temperature. Most of the organic NLO crystals have poor thermal and mechanical properties and are susceptible damage during processing. Moreover, growth of large size bulk single crystal is difficult to grow for device fabrications. Crystals have excellent thermal and mechanical properties but possess relatively modest optical nonlinearity due to the lack of extended π-electron delocalization. For the above reasons interests have been made on semi organic NLO crystals, which have been combined the both properties of organic and inorganic crystals like chemical stability, high laser damage threshold, higher chemical strength and high transparency, which make them suitable for device fabrication. The semi organic crystals possess positive aspects of both organic and inorganic material hence it is important synthesis and growth of the novel semi organic NLO crystals.

Nonlinear optical (NLO) materials are essential for the development of advanced modern technologies ranging from telecommunication, signal processing, data storage, super resolution lithography, and microscopy to higher harmonic and terahertz (THz) generation. In particular, NLO materials with well-defined architectures on the (sub) wavelength length scales are regarded as key materials for the development of the next generation integrated photonic circuits. One of the most widely studied and applied second-order NLO effects is second harmonic generation, in which two photons of incident light combine and generate a photon with doubled frequency and energy. This effect emerges when an intense pulsed laser.

Harmonic generation is a non-linear optical process in which photons of intense incoming laser radiation interact with a non-linear material and radiation with corresponding harmonics frequencies is generated.

Nonlinear optics allows us to change the colour of a light beam, to change its shape in space and time, and to create the shortest events ever made by humans. Nonlinear optical phenomena are the basis of many components of optical communications systems, optical sensing, and materials research.

Nonlinear optics play a major role in many of the optical applications such as optical signal processing, optical computers, ultrafast switches, ultra-short pulsed lasers, sensors, laser amplifiers, and many others. Nonlinear optical (NLO) materials have long been known to interact with light, to produce a nonlinear response and the composition of these materials, generally falls into one of two classes, either inorganic or organic. [5]

Non-Linear Optical (NLO) materials are at the core of many optical electronic warfare (EW) systems and other next-generation defences technologies because they can be used to shift the wavelength and frequency of laser light, enabling operation in parts of the electromagnetic spectrum (EMS) that would normally be inaccessible.

Most NLO materials used for military and intelligence purposes are optical crystals. In these crystals, the electric field associated with light can interact with the crystal's internal structure – also known as its lattice – in non-linear (unexpected) ways. This nonlinear response usually only occurs under very intense irradiation, like that from a laser, and can be used to achieve frequency-converting processes that can shift the laser's wavelength into the spectral range needed for a particular use or application.

For efficient frequency conversion, a crystal must:

- Be non-centrosymmetric (have a non-zero nonlinearity)
- Have a nonlinear d-coefficient large enough to generate tuneable wavelengths over a broad range
- Be highly transparent at the required input and output wavelengths
- Be able to match different phases.

Nonlinear optics allows us to change the colour of a light beam, to change its shape in space and time, and to create the shortest events ever made by humans.

Nonlinear optical phenomena are the basis of many components of optical communications systems, optical sensing, and materials research.

An NLO material has crystal structure which is anisotropic with respect to electromagnetic radiation.

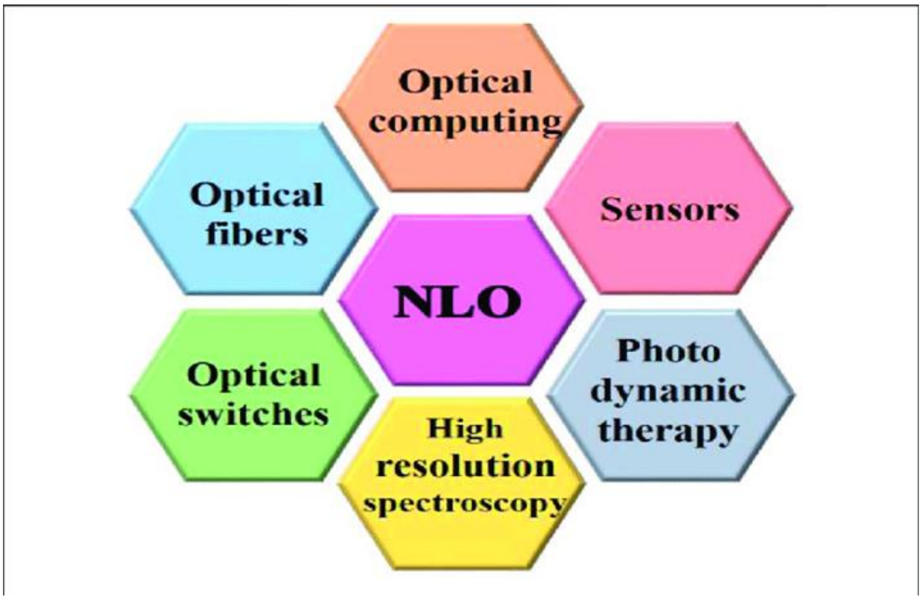


Fig 1.2 Types of NLO

1.2 INTRODUCTION TO SECOND HARMONIC GENERATIONS (SHG)

Harmonic generation is a non-linear optical process in which photons of intense incoming laser radiation interact with a non-linear material and radiation with corresponding harmonics frequencies is generated Second harmonic generation (SHG), also called frequency doubling, is a nonlinear optical process, in which photons interacting with a nonlinear material are effectively 'combined' to form new photons having twice the frequency of initial photons.

SHG was firstly demonstrated by Franken and his colleagues in 1961 [5]. In recent years, ferroelectric NLO powders with unexpected high efficiencies for frequency conversion and random lasers have attracted considerable attention. By embedding NLO nanocrystal in a transparent, deformable matrix, the fabrication of novel NLO device seems possible [6].

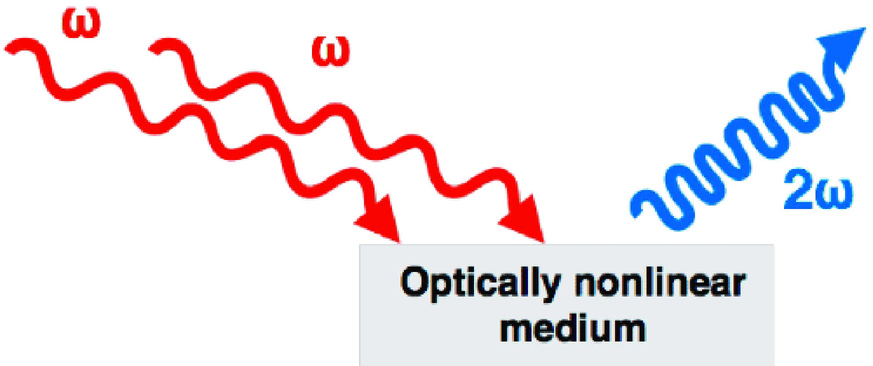
We mainly introduce the SHG behaviour The second-order nonlinear sub stability of a medium characterizes its tendency to cause SHG. Second-harmonic generation, like other even-order nonlinear optical phenomena, is not allowed in media with inversion symmetry. However, effects such as the Bloch – seigher shift (oscillation), found when two-level systems are driven at Rabi frequencies comparable to their transition frequencies, will give rise to second harmonic generation in Centro-symmetric systems.

In addition, in non centrosymmetric crystals belonging to crystallographic point group 432, if SBN nanocrystal/PC composites. The SHG is not possible and under Klein man's condition SHG in 422 and 622 point groups should vanish although some exceptions exist.

In biological and medical science, the effect of second-harmonic generation is used for high-resolution optical microscopy. Because of the non-zero second-harmonic coefficient, only non-centrosymmetric structures are capable of emitting SHG light.

1.2.1 OPTICAL SECOND HARMONIC GENERATION

Since media with inversion symmetry are forbidden from generating second-harmonic light via the leading-order electric dipole contribution surfaces and interfaces make interesting subjects for study with SHG. In fact, second-harmonic generation and sum frequency generation discriminate against signals from the bulk, implicitly labelling them as surface specific techniques. In 1982, *T. F. Heinz* and Y. R. Shen explicitly demonstrated for the first time that SHG could be used as a spectroscopic technique to probe molecular monolayers adsorbed to surfaces. Heinz and Shen adsorbed monolayers of laser dye Rhoda mine to a planar fused silica surface; the coated surface was then pumped by a nanosecond ultra-fast laser. SH light with characteristic spectra of the adsorbed molecule and its electronic transitions were measured as reflection from the surface and demonstrated a quadratic power dependence on the pump laser power.



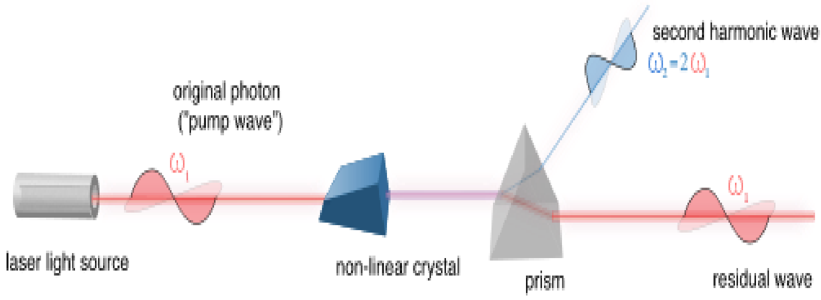


Fig 1.3 Second harmonic generation

1.3 INTRODUCTION TO CRYSTAL GROWTH

High heat, where crystals form, also determines the formation. Some crystals develop from vapour's. Others form in solid rock while it is in a fluid or plastic state. This allows molecules to slowly migrate toward each other and connect to form a crystal. Natural crystals often been formed at relatively low temperatures by crystallisation from solutions, sometimes in the course of hundreds and thousands years. Now a day's crystals are produced artificially to satisfy the need of science and technology [7-8]

Crystal growth from solution is the process of mass and heat transport from the environment to the crystal surface, followed by the integration of these molecules at the crystal surface. The rate constant of growth of a crystal is determined by two factors: the density of kinks on the interface with the growth medium, and the barriers, both entropic and enthalpy, for incorporation of a molecule into a kind. Crystals of inorganic materials can be used in radiation detection metal manufacturing, and in the creation of conductive surface production regenerative medicine, and industrial chemistry.

The growth of a crystal, which involves diffusion of the molecules of the crystalline substance to the surface of the crystal, diffusion of these molecules over the crystal surfaces at these sites on the surface in corporation of molecules into the surfaces at these sites and diffusion of heat away from the surface.

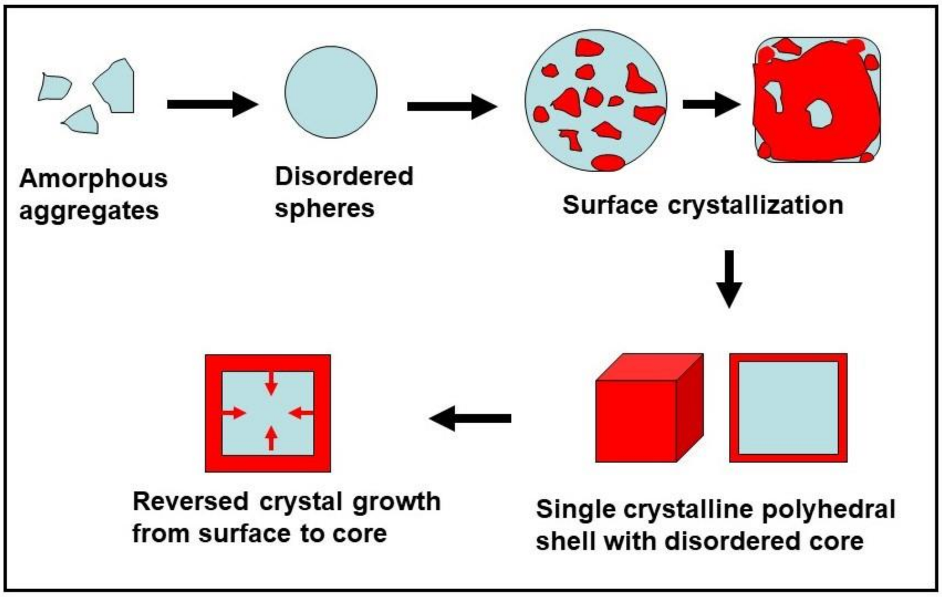


Fig 1.4 Crystal growth

Crystals are important for a variety of reasons, both practical and scientific. Here is some of the key importance of crystals:

MATERIALS SCIENCE: Crystals play an important role in materials science as they are the building blocks of many materials such as metals, semiconductors**,** ceramics and polymers. The properties of their materials depend on the arrangement of atoms or molecules in their crystal structures.

TECHNOLOGY: Many technologies such as electronics, optoelectronics and photonics rely on the unique properties of crystals. For example, the use of single crystals in semiconductors and transistors has revolutionized the field of electronics.

RESEARCH: Crystals are also important in scientific research as they can be used to study the behaviour of atoms and molecules in a solid state. This can provide insights into the fundamental properties of matter and help to develop new materials with unique properties.

HEALTH: Crystals are used in medicine for a variety of purposes such as drug delivery, imaging and diagnosis. For example, X-ray crystallography is a powerful tool used to determine the three-dimension structure of proteins, which is important for drug design.

AESTHETIC: Crystals are also valued for their beauty and used in jewellery, decoration and art. Many people find crystals to aesthetically pleasing and believe that they have healing properties.

1.3.1. IMPORATANCE OF CRYSTAL GROWTH

The driving force, on super saturation the ambient phase, (i.e.) whether the crystal is grown from a melt or a solution. The solute –solvent interaction energy (i.e.) the nature of the solvent in which the crystal is grown impurities, which modify the edge free energy by absorbing onto growth steps.

Crystal growth refers to the artificial synthesis of crystals and can be roughly -classified into three groups, i.e. solid-solid, liquid-solid and gas-solid processes, depending on which phase transition is involved in the crystal formation. Crystals act as a power hold for healing as they allow positive, fruitful energy to flow into the body and do away with the negative, toxic energy. Like other forms of alternative therapy, crystals work by channelizing your energy levels, thereby, focus on healing your body from the inside.

The atoms in a crystalline solid are arranged in a three-dimensional, geometric pattern called a crystal lattice. This lattice is incredibly strong and gives the solid its rigidity. One of the most important properties of crystalline solids is their melting point.

Crystalline solids have well-defined edges and faces, diffract x-rays, and tend to have sharp melting points. In contrast, amorphous solids have irregular or curved surfaces, do not give well-resolved x-ray diffraction patterns, and melt over a wide range of temperature.

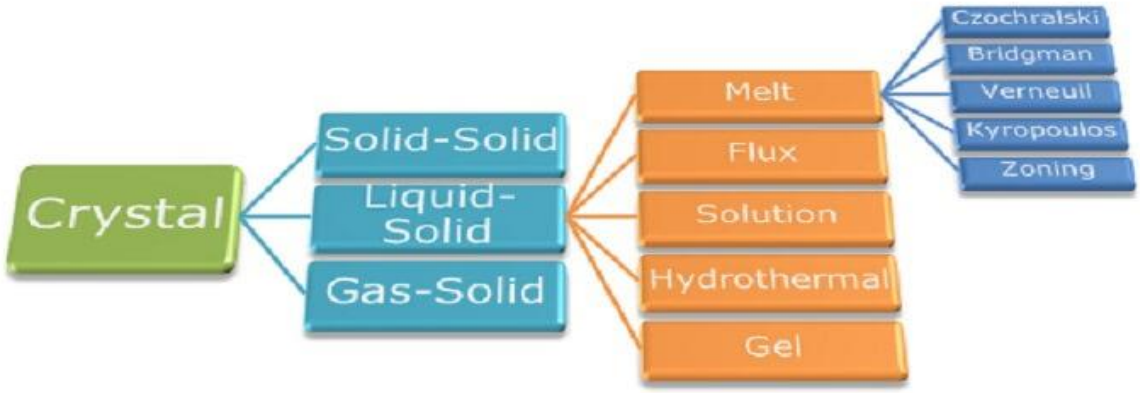


Fig 1.5 various types of Crystal

1.3.2 INDUSTRIAL USES FOR CRYSTALS

Crystals have a wide range of industrial application due to their unique physical and chemical properties. Some common industrial us of crystals are:

SEMICONDUCTORS: Crystals are used in the production of semiconductors, which are used in electronic devices such as computers, Smartphone and television. Silicon is the most commonly used semiconductor material and its crystal structure plays a key role in determining its electronic properties.

OPTICS: Crystals are used in the production of optical components such as lenses, mirrors and prisms. Certain crystals have unique optical properties that make them useful for specific applications such as the use of sapphire in laser technology.

PHARMACEUTICALS: Crystals are used in the pharmaceutical industry to produce drugs in a crystalline form, which can improve their stability, bioavailability and effectiveness, Crystal engineering techniques are used to optimize the crystal structure of drugs for specific applications.

CHEMICALS: Crystals are used in the production of a variety of chemicals such as fertilizers, pigments and catalysts. For example, zeolites are crystalline materials with a porous structure that make them useful as catalysts in the chemical industry.

ENERGY: Crystals are used in the production of solar cell, which convert sunlight into electricity. Certain crystal such as silicon and cadmium telluride has the unique properties required to efficiently convert solar energy into electricity.

Overall, crystals have a wide range of industrial applications, from electronics to pharmaceuticals to energy production. The unique physical and chemical properties of crystals make them versatile materials for a variety of industrial processes.

1.3.3 VARIOUS METHODS OF CRYSTAL GROWTH

There are several methods for crystal growth each of which is suited to different types of materials and application. Here are the most common methods:

SOLUTION GROWTH: In solution growth crystals are grown from a solution by controlling the temperature, pressure and concentration of the solvent and solute. This method is commonly used for growing single crystals of inorganic salt and organic compounds.

VAPOUR DEPOSITION: Vapour deposition involves depositing a vaporized material onto a substrate, where it condenses into a crystal. This method is used for growing thin films of materials such as metals, semiconductors and ceramics.

BRIDGMAN-STOCKBARGER METHODS: The Bridgman-stock Barger method involves slowly cooling a melt of the material to be grown, which creates a gradient of temperature and concentration. This method is used for growing large single crystals of oxides.

CZOCHRALSKI METHODS: The Czochralski method involves melting the material in a crucible and then slowly pulling a seed crystal through the melt, which causes the crystal to grow on the end of the seed. This method is used for growing large, high-quality single crystals of semiconductors such as silicon.

HYDROTHERMAL SYNTHESIS: Hydrothermal synthesis involves growing crystals from a superheated water solution under high pressure. This method is commonly used for growing crystal of minerals and synthetic materials.

FLAME FUSION METHODS: In flame fusion method, a powdered material is melted in a flame and then rapidly cooled to form a crystal. This method is commonly used for growing synthetic gemstones such as ruby and sapphire.

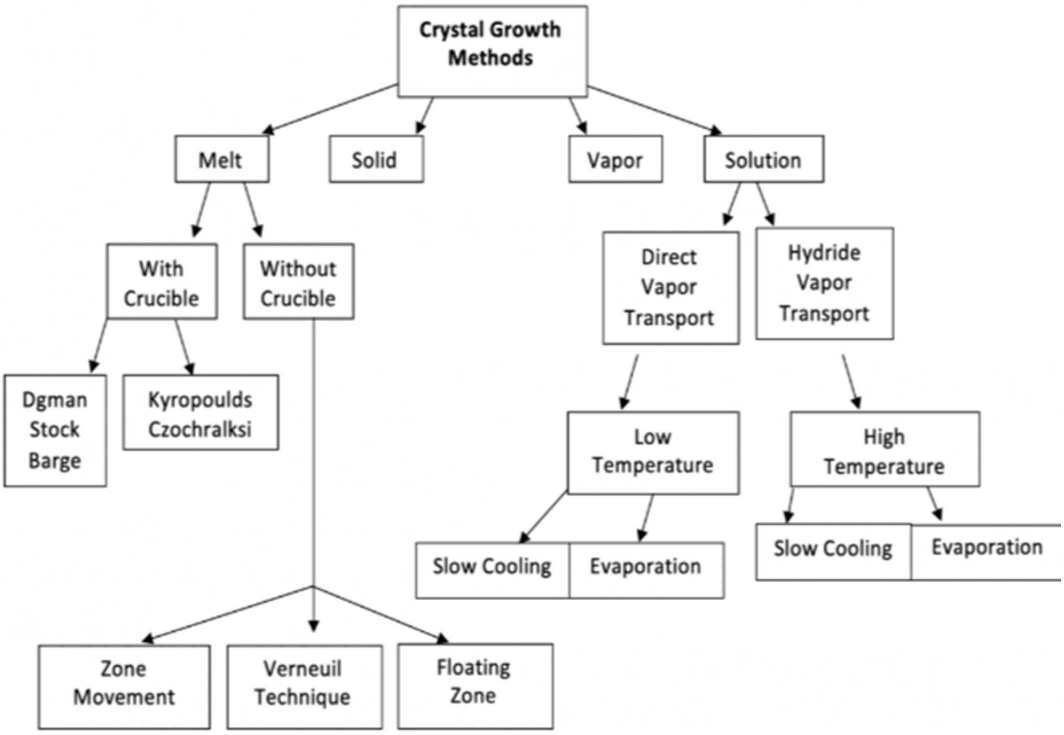


Fig 1.6 Types of crystal growth

1.4. SLOW EVAPORATION METHOD:

The slow evaporation method is a common technique used to grow crystals from a solution. It involves dissolving a solid solute in a solvent to create a supersaturated solution, which is then allowed to slowly evaporated under controlled conditions. As the solvent evaporates, the solute evaporates, the solute concentration in the solution increases until it reaches a point where crystals start to form.

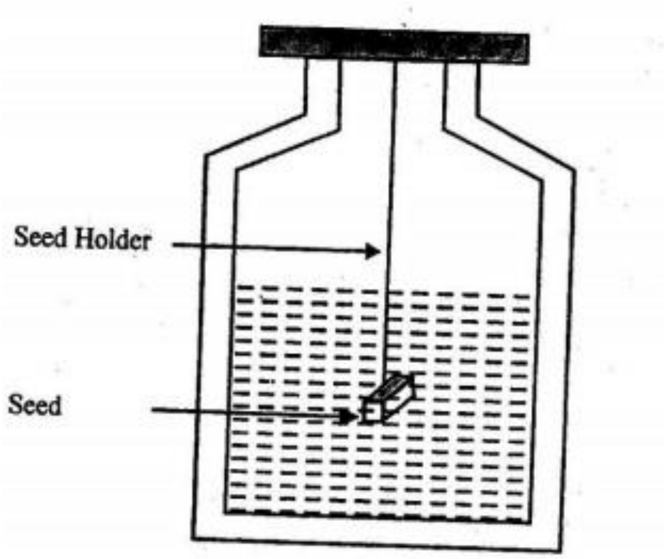


Fig 1.7 Formation of bulk crystal

The process of slow evaporation typically involves the following steps:

PREPARATION OF THE SOLUTION: The solute is dissolved in a suitable solvent to create a supersaturated solution. The solubility of the solute in the solute in the solvent must be carefully controlled to achieve the desired level of super saturation.

SELECTION OF THE CONTAINER: The contain used to hole the solution must be clean, smooth and free from any impurities that could interfere with crystal growth.

CONTROLLED EVAPORATION: The container is left open to the air and the solvent is allowed to slowly evaporate under controlled conditions. This can be achieved by covering the container with a lid that has small holes or using a desiccators to regulate the humidity and temperature of the environment surrounding the solution.

CRYSTAL GROWTH: As the solvent evaporates, the solute concentration in the solution increases, reaching a point where crystal start to form. The crystal will continue to grow until the solute concentration in the remaining solution falls below the saturation point.

HARVESTING THE CRYSTALS: Once the crystals have reached the desired size, they can be harvested by carefully removing them from the solution using a spatula or a filter paper.

The slow evaporation method is often used to grow small to medium sized crystal of various compounds, including salt, organic compounds and proteins. The size and morphology of the crystals depend on factors such as the solute concentration; the solvent used the rate of evaporation and the environment condition during crystal growth. Carefully control of these parameters is essential to achieve high quality crystals with uniform size and shape.

The evaporation of the solvent causes the molecules of the soluble compound to separate out as crystals due to the higher concentration exceeding the chemical compound's solubility. This is the most popular method of crystallization, especially when working with common compounds such as inorganic salts and sucrose.

Solvent-evaporation synthesis produces crystals by slowly increasing the concentration of the mother liquor. Crystals can slowly grow as the solution becomes saturated by either cooling of the solution or by evaporation of excess solvent.

Method of crystalline – low temperature solution growth. There are three types of growth slow cooling method, slow evaporation method, temperature gradient method. Prepare a solution of the compound in a suitable solvent filter the solution through a clean glass fir into a clean vessel and cover but not tightly gently put the container in a quiet, out of the way place and allow the solvent to evaporate slowly. This method works best when there is sample material to allow for at least a few mile liters of solvent.

The next method being slow cooling (from high temperature to Room Temperature or Low temperature, slowly). The Method: The compound can be dissolved in a single solvent or mixture of two solvents and left for Slow

Evaporation. It can be done either under atmospheric conditions or under inert atmosphere.

Evaporation is also used to concentrate liquid foods such as noodles and make condensed milk, the product of a process that removes water from milk. Similarly, pharmaceutical companies use evaporators to remove excess moisture from drugs, thus improving product stability.

The general disadvantages are:

- Generally, only purifies one component.
- Yield is limited by phase equilibria.
- Process kinetics are more complex and less well-understood than some alternatives; obtaining detailed kinetic parameters involves complex experimental procedures.
- One disadvantage of evaporation to dryness is that any soluble impurity present will be deposited together with the required solid. Evaporation to dryness is also not suitable for all substances as many substances decompose when heated strongly.
- Evaporation method is only used for separating homogeneous mixtures when solid is dissolved completely in liquid. It is not useful for separating heterogeneous mixtures. They can be separation.

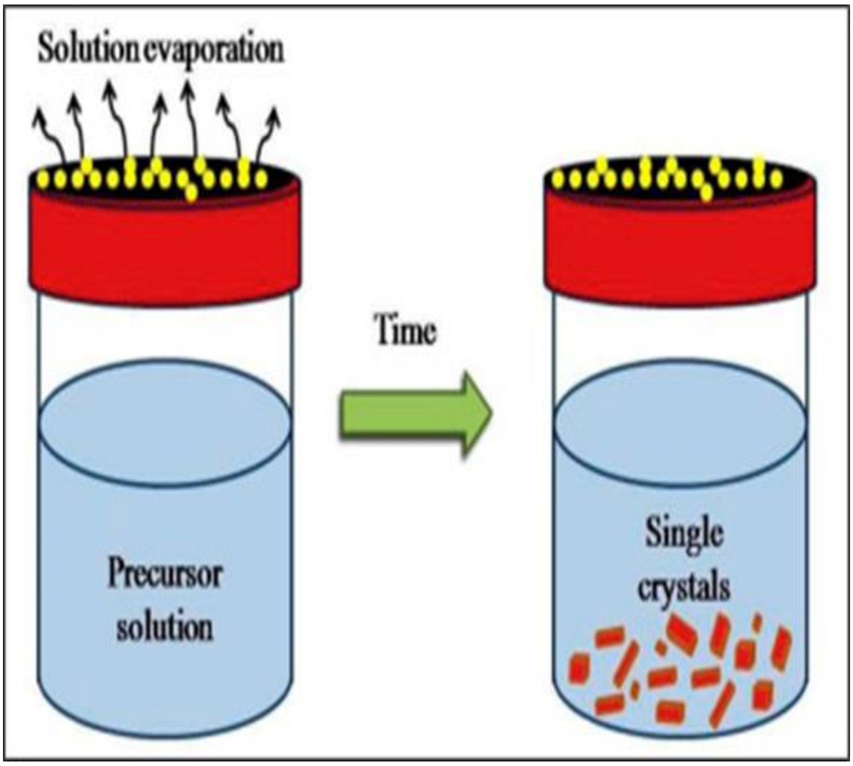


Fig 1. 7 Solution growth

CHAPTER-2

INSTRUMENTATION FOR CHARACTERIZATION

2.1 XRD ANALYSIS

X-Ray diffraction (XRD) replies on the dual wave/particle nature of X-rays to obtain information about the structure of crystalline materials. A primary use of the technique is the identification and characterization of compounds based on their diffraction pattern.

2.1.1 PRINCIPLE

Consider two parallel monochromatic X-ray beams with the wavelength falling on the successive planes of the crystal at an angle, Constructive interference of the reflected rays from two successive plane occurs, only the path difference between the two rays fulfils the inter planar distance.

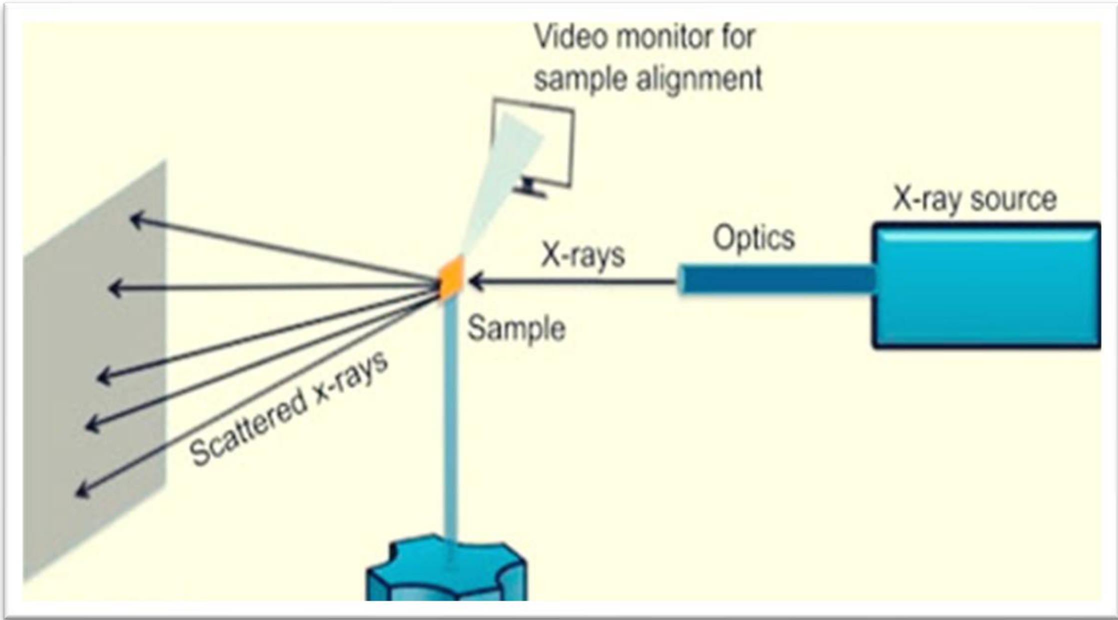


Fig 2.1 Experimental arrangement of XRD analysis

2.1.2 WORKING

The domain effect that occurs when an incident beam of monochromatic X-ray interacts with a target material is scattering of those X-ray from atom within the target material. In material with regular structure, the scattered X-rays undergo constructive and destructive interference. This is the process of diffraction. The direction of possible diffractions depends on the size and shape of the unit cell of the material. The intensities of the diffracted waves depend on the kind and arrangements of atoms in the crystal structure. However, most materials are not the single crystals, but are composed of many tiny crystallites in all possible orientations called polycrystalline aggregate. When a powder with random oriented crystalline is placed in an X-ray beam, the beam will see all possible inter atomic planes. If the experimental angle is systematically changed, all possible diffraction peaks from the crystal will be detected.

Fig .2.2 Instrumental setup of BRUKER KAPPA APEX 2 CCD diffractometer

2.1.3 WORKING

Single crystal X-ray diffraction is an analytical technique in which X-rays are employed to determine the actual arrangement of atoms within a crystalline specimen. The single crystal structure of compounds, which can be grown as single crystals. In the present study, the single crystal X-ray diffraction analysis was performed using BRUKER kappa 2.CCD single crystal X-ray diffractometer. A single crystal is mounted on a thin glass fiber fixed on the goniometer head. The unit cell dimensions and orientation matrix are determined using multiple reflections and then the intensity data of a given set reflections are collected automatically by the compute. The instrumental setup of BRUKER kappa Apex 2CCD diffractometer is shown in fig .2.2.

2.1.4 CALCULATION OF CRYSTAL SIZE

The crystal structure is found using **BRAGG'S LAW** in order to find its length, distance etc.

According to Bragg Equation:

$$n\lambda = 2d \sin\Theta \qquad (1)$$

According to the equation of Bragg's Law:

The equation explains why the faces of crystals reflect X-ray beams at particular angles of incidence (Θ, λ).

The variable d indicates the distance between the atomic layers, and the variable The variable d indicates the distance between the atomic layers, and the variable λ specifies the wavelength of the incident X-ray beam and n as an integer**.**

2.1.5 XRD APPLICATION

To measure both the physical and chemical properties of crystalline powders, thin films, epitaxial films, and bulk solid materials. The atomic planes of a crystal cause an incident beam of X-rays to interfere with one another.

2.2 ULTRAVIOLET –VISIBLE SPECTROSCOPY (UV –VISIBLE)

UV-Vis spectroscopy is an analytical technique that measures the amount of discrete wavelengths of UV or visible light that are absorbed by or transmitted through a sample in comparison to a reference or blank sample. This property is influenced by the sample composition, potentially providing information on what is in the sample and at what concentration. The good transmission of the crystal in the entire visible region is important for NLO devices. [9]

UV detector employs a deuterium discharge lamp as a light source, with the wavelength of its light ranging from 190 to 380 nm. If components are to be detected at wavelength longer than this, a UV-VIS detector is used, which employs an additional tungsten lamp.

2.2.1 PRINCIPLE

Measuring in UV /visible region covers the wavelength of 200nm to 800nm. The absorption of UV or visible radiation by a molecule leads to transitions among the electronic energy levels of the molecule. It is ideal for characterizing the optical and electronic properties of various materials such as: films, powders, solids and liquids.

Infrared region of the electromagnetic spectrum utilizes wavelength from about 700-1000nm.The transitions measured in this region are generally related to overtone and combination band.

Fig 2.3 5E VARIAN CARY UV –VIS SPECTROPHOTOMETER

2.2.2 WORKING

The experimental arrangement of **Varian Cary 5E UV–VIS-IR spectrophotometer is shown in fig 2.3.** UV -VIS –IR when incident light strikes matter it can be absorbed, reflected, or transmitted. The absorbance of radiation in the UV-Vis range causes atomic excitation, which refers to the transition of molecules from a low-energy ground state to an excited state.

Light is focused into the entrance slit of the monochromatic from the source. Monochromatic uses dispersing elements, namely optical grating to separate the light by wavelength. The light is passed into a charged coupled device (CCD), which is made up of individual tiny detectors; hence the intensity of light at each wavelength will be measured. CCD is read-off to a computer and the result obtained is a spectrum, which shows the intensity of each wavelength of light. Strengths and limitations of UV-Vis spectroscopy

2.2.3 APPLICATIONS

No single technique is perfect and UV Vis spectroscopy is no exception. The technique does, however, have a few main strengths listed below that make it popular.

- The technique is non destructive, allowing the sample to be reused or proceed to further processing or analyses.
- Measurements can be made quickly, allowing easy integration into experimental protocols.
- Instruments are easy to use, requiring little user training prior to use.
- Data analysis generally requires minimal processing; again meaning little user training is required.
- The instrument is generally inexpensive to acquire and operate, making it accessible for many laboratories.

2.3 MICRO HARDNESS TEST – VICKERS HARDNESS

2.3.1 INTRODUCTION

Micro hardness Testing is a method of determining a material's hardness or resistance to penetration when test samples are very small or thin, or when small regions in a composite sample or plating are to be measured. It can provide precise and detailed information about surface features of materials that have a fine microstructure, are multi-phase, non-homogeneous or prone to cracking.

2.3.2. PRINCIPLE

The micro hardness test can measure surface to core hardness on carburized or case-hardened parts (case depths), as well as surface conditions such as grinding burns, carburization or decarburization. It is based on the principle of creating an indentation on the surface of the material using a diamond indenter, and then measuring the size of the indentation. The Vickers hardness test is widely used in industry and research because it can provide accurate and reproducible results. The decrease in hardness number with increase load provides information about the formation of cracks due to release of internal stress generated by local indentation. From the results, it is also concluded that the crystal has reverse indentation size effect due to increasing hardness number with respect load. [10]

Fig 2.4 Arrangement of hardness test

2.3.3 Experimental setup of Vickers hardness test

The experimental setup for the Vickers hardness test typically involves the following steps:

- **Sample preparation:** The sample material is prepared by cutting and polishing it to a flat surface with a smooth finish. The surface must be free from any debris or contaminants that could affect the hardness measurements.
- **Mounting:** The sample is then mounted onto a sample holder or stage, which allows it to be securely held in place during the test.

- **Calibration:** The Vickers indenter is calibrated to ensure that it is accurately measuring the indentation size. This is typically done by using a standard reference material with a known hardness value.
- **Indentation:** The Vickers indenter is placed on the surface of the sample, and a load is applied for a set period of time. The load typically ranges from a few grams to several kilograms, depending on the material being tested.
- **Measurement:** The size of the indentation is measured using a microscope, which can be either manual or automat ed. The indentation size is typically measured in micrometers or millimeters.
- **Calculation:** The Vickers hardness number (HV) is calculated using the formula HV = 1.8544 P/d^2, where P is the applied load in kilograms and d is the average diagonal length of the indentation in millimeters.
- **Data analysis**: The results of the Vickers hardness test can be used to compare the hardness of different materials or to factors such as heat treatment or deformation.

Overall the Vickers hardness test is a versatile and widely used method for measuring the hardness of materials, and its experimental setup is relatively straight forward and well- established. The experimental setup for Vickers hardness test is shown in fig 2.5

Fig 2.5 Experimental setup of Vickers hardness test

2.4 DIELECTRICS

Dielectric, insulating material or a very poor conductor of electric current. When dielectrics are placed in an electric field, practically no current flows in them because, unlike metals, they have no loosely bound, or free, electrons that may drift through the material. Instead, electric polarization occurs. The positive charges within the dielectric are displaced minutely in the direction of the electric field, and the negative charges are displaced minutely in the direction opposite to the electric field.

This slight separation of charge, or polarization, reduces the electric field within the dielectric. The presence of dielectric material affects other electrical phenomena. The force between two electric charges in a dielectric medium is less than it would be in a vacuum, while the quantity of energy stored in an electric field per unit volume of a dielectric medium is greater.

2.4.1 PRINCIPLE

In which it consists of two types' dielectric constant and dielectric loss. One of the useful methods of characterization of electrical response is dielectric studies. A study on the dielectric properties of solids gives an electric field distribution within solid. The frequency dependence of these properties gives great insight into the materials applications. The range of measurement depends upon the properties and the material of interest. From the study of dielectric constant as a function of frequency, temperature…etc., the different polarization mechanisms in solids such as atomic such as atomic polarization of the dipoles, space –charge polarization etc. can be understood. the dielectric study provides information regarding the dielectric constant arises from the contribution of different polarizations mechanism, namely electronic, ionic, atomic, space charge, etc., developed in the material subjected to the electric field variations. The frequency may be due to the loss of significance of these polarizations [11] arising at the grain boundary interface.

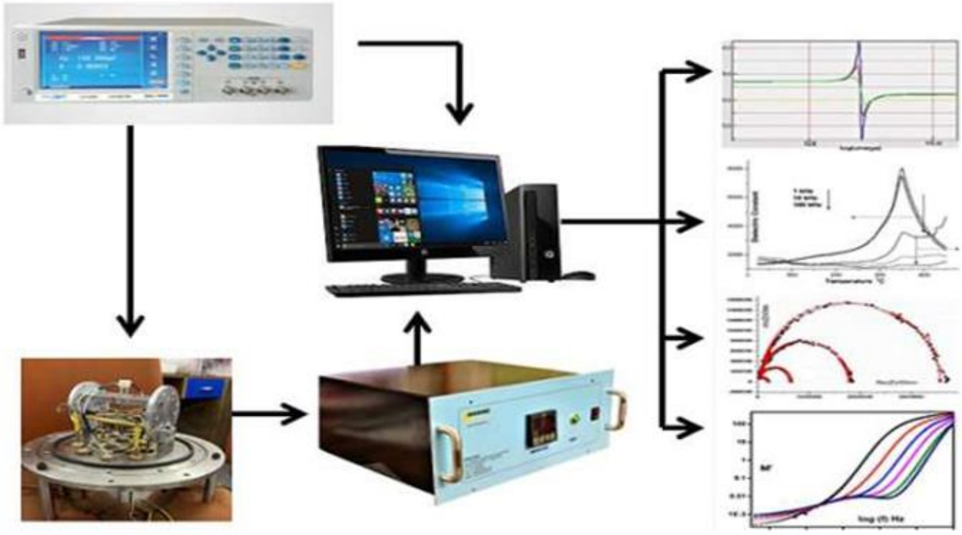


Fig 2.6 Instrumental setup dielectrics

2.4.2 WORKING

The suitably cut and polished samples (with known dimensions) of grown crystals subjected to dielectric studies by using HIOKI 3532-50 HITESTER LCR meter (fig 2.7) with a conventional four terminal sample holder for investigations involving temperature variations and a conventional two terminal sample holder(westpal) for only ambient conditions. The sample are prepared and mounted between copper platforms and electrodes. In order to ensure good electrical contact, the crystal faces are coated with the silver paint. The capacitance and the electrode having the sample as a dielectric medium are measured. The measurements are made at frequencies ranges from 50HZ to 5MHZ at different temperature. The low value of dielectric loss at high frequencies reveal the high optical quality of the crystal with lesser defects, and this parameter is of vital importance for nonlinear optical applications [12].

Fig 2.7   HIOKI 3532-50 HITESTER LCR METER

2.4.3 APPLICATIONS

- Dielectrics are used as a capacitor for storing energy.
- The dielectric material in a transformer is used as an insulator and as a cooling agent.
- To enhance the performance of a semiconductor device, high permittivity dielectric materials are used.

2.5 NLO TEST – KURTZ POWDER SHG METHOD

2.5.1 INTRODUCTION

Recent interest is focused on to find the materials which have suitable nonlinear optical properties for use as the active media in efficient second harmonic generators, tunable parametric oscillators and broadband electro-optic modulators.

KURTZ and PERRY (1968) proposed a powder SHG method for comprehensive analysis of the second order nonlinearity. Employing this technique, Kurtz (1968) surveyed a very large number of compounds. Can be used in great impact on information technology and industrial applications [13].

2.5.2 EXPERIMENTAL SETUP

Nonlinear optical (NLO) materials play a major role in nonlinear optics and in particular they have a great impact on information technology and industrial applications. The nonlinear optical property of the single crystals can be tested by passing the output of Nd: YAG Quanta ray laser, where two photons of the same frequency are converted into a single photon with twice the frequency. The experimental setup for SHG typically involves the following components:

Laser: A high - power laser is used as the light source. Typically, a pulsed laser is used, since provides higher peak powers and shorter pulse durations, which increases the efficiency of SHG.

Nonlinear crystal: A nonlinear crystal is used as the medium for SHG. The crystal must have a non-centrosymmetric structure, which allows the generation of a second harmonic wave. The crystal should also have a high nonlinear coefficient to ensure efficient conversion of the incident light into the second harmonic wave. Popular nonlinear crystals for SHG include potassium dehydrogenate phosphate (KDP).

Optics: A series of lenses and mirrors are used to focus and direct the laser beam onto the nonlinear crystal. The optics is carefully aligned to ensure that the laser beam is properly focused and that the polarization of the incident beam is properly aligned with the crystal axis.

Filters: Filters are used to remove any residual fundamental light can interfere with the detection of the second harmonic signal.

Detector: A photo detector is used to measure the second harmonic signal. The detector must be sensitive to the second harmonic wavelength and have a high signal-to-noise ratio to detect the weak second harmonic signal.

Overall, the experimental setup for SHG is a complex and delicate process that requires careful alignment of laser, crystal and optics to ensure efficient conversion of the incident light into the second harmonic wave.

Fig 2.8 Experimental setup of SHG method

2.5.3 APPLICATION

They are also excellent electro-optic crystals with high electro-optic coefficients, widely used as electro-optical modulators, such as Q-switches, Pockets Cells, etc.

CHAPTER - 3

AIM AND SCOPES

3.1 OBJECTIVE AND SCOPE

Crystal growth is an important field of materials science which has got scientific as well as technological important. Scientific importance of the subject is mainly related to the growth of single crystals and its characterization while the technological importance deals with the growth of large single crystals and its application on the device fabrication.

The present investigation deals with,

- Synthesizing the chosen materials for the growth of single crystals
- Determining the solubility of the materials
- Growth of single crystal
- Identifying the crystal structure by single crystal X-ray analysis
- Characterization of the grown crystals by UV-VIS-NIR, Vickers Micro hardness test, Dielectric studies and NLO.

The future scope of the work is also mention for further research. It is possible to grow bulk size crystals with improved optical quality by carefully adapting either the slow evaporation methods or by some innovations techniques with modified apparatus. Attempts can be made to identify suitable which could provide better optical properties and enhance the NLO property of the crystals.

3.2 GROWTH AND CHARACTERIZATION OF L THREOINE LITHIUM CHLORIDE

Amino acids are currently the focus of significant research regarding the hunt for newer nonlinear optical materials since they may have a wide range of possible applications

Amino acid complexes with inorganic salts frequently combine the benefits of an organic amino acid and an inorganic salt, making them suitable building blocks for SHG properties. [15–16].

As a result, different inorganic acids were utilized to examine the production of salt utilizing L-arginine, L-histidine, L-threonium, L-alanine, and L-valine. [17-18].

Among which**, L - THREONINE LITHIUM CHLORIDE (LTLC)**, is a desirable candidate for electro optic and second harmonic generation devices, in view of its low angular sensitivity and high molecular interaction with intense light.

Recently, there is considerable interest in the synthesis of new materials with large second order optical nonlinearities because of their potential use in applications including telecommunications; optical computing, optical data storage, and optical information processing such applications require materials. LTLC is one of the semi organic crystals that have been put to practical uses. It has larger nonlinear optical coefficients, a high degree of relatively.

L-threonine is the smallest molecule among the amino acids, its growth aspects and characterizations are very important because L-threonine can be considered as the fundamental building block for the formation of complex amino acids with improved NLO properties. The importance of amino acid for NLO application lies on the fact that almost all amino acids contain an asymmetric carbon atom and crystallize in non-Centro symmetric space group.

Uses of Lithium Chloride Licl:

Lithium Metal by Electrolysis Lithium chloride is primarily used at 450 ° C (842 ° F) for the preparation of lithium metal by electrolysis of a LiCl / KCl. As Brazing Flux Lithium chloride is also used as a brazing flux for aluminum in automobile parts.

As desiccant in drying air streams. lithium chloride is use determine the space group and crystal

Biochemical Applications:

LiCl is used to precipitate RNA from cellular extracts as a flame colorant, Lithium chloride is used to produce dark red flames.

L-Threonine uses as follows:

In Food

L-Threonine can be used as nutrition supplements, flavor enhancer in food such as in cottage cheese, poultry, fish, meat, lentils, black turtle bean and sesame seeds.

In Pharmaceutical

L-Threonine is used to treat various nervous system disorders including spinal spasticity, multiple sclerosis, familial spastic paraphrases, and amyotrophic lateral sclerosis in Pharmaceutical.

In Health and Personal care

L-Threonine may be used in cosmetics and personal care products such as in baby products, bath products, cleansing products, eye makeup, shaving preparations and hair and skin care products. Threonine is an amino acid used in cosmetics and personal care products because of its ability to promote growth though protein balance maintenance. According to the Cosmetics Database, it is a fragrance ingredient, skin and hair conditioning agent, and anti-static agent. It is often seen in hair straightness because of its protein promotion.

3.3 EXPERIMENTAL PROCEDURE

3.3.1 Synthesis

The title compound (LTLC) was synthesized by mixing purified L-THREOINE LITHIUM CHLORIDE in de-ionized water in the stoichiometric ratio 1:1.

CH3-CH (OH)-CH (NH2)-COOH+LiCl $\longrightarrow$ Li CH3-CH (OH)-CH (NH2)-COOH Cl

- In the double-distilled water, salt is left to dissolve.
- After that, the salt is set to dissolve in a magnetic stirrer until it gets fully dissolved.

• Then the salt is filtered using filter paper, and the beaker top is covered with a butter sheet,

• The saturated sample is kept at room temperature until a seed crystal form.

• The salt is kept again for the recrystallization process for a bulk crystal.

3.3.2 FORMATION OF SEED CRYSTAL

Crystal formation in solution is a self-assembly process in which the crystal seed formed in liquid, known as homogeneous nucleation. If the seed of crystal is formed on the interface of liquid and solid, it is known as heterogeneous nucleation. Finally, a well-defined single crystal was obtained. Photographic of grown crystal is shown in fig.3.1

Fig 3.1 Photograph of Seed crystal

CHAPTER -4

RESULTS AND DISCUSSION

4.1. SINGLE CRYSTAL X-RAY DIFFRACTION

The created LTLC crystal is put through single crystal X-ray diffraction experiments using a Bruker Kappa APEX-2 diffractometer with Mo K (A=0.71073) radiation in order to evaluate cell properties and crystal structure. The results show that LTLC crystallises into an orthorhombic system with space group Pna21. The values previously published for the lattice parameters, a=5.792, b=7.822, and c=13.02, are well-matched by the values found in this work. [19]. The single crystal data were analysed and depicted in table (4.1)

Table 4.1 Crystallographic data of LTLC single crystal

LTLC	Crystal Data
Empirical formula	Li CH3-CH (OH)-CH (NH2)-COOH Cl
Crystal system	orthorhombic system
Space group	Pna21
Lattice Parameter	a=5.792 Å, b=7.822Å, and c=13.02Å,

4.2. OPTICAL ABSORPTION STUDIES

The optical absorption spectra of LTLC, single crystal were acquired in the 200-2000 nm range using a VARIAN CARRY 5E MODEL spectrometer, which covers the entire UV-vis and near-infrared ranges. The collected spectra in Fig.1 show that neither the visible nor the IR spectrums exhibit much absorption. This is the characteristic of materials with NLO activity that is most in demand. The delocalization of the electron cloud available for charge transfer is what causes the low absorption value in the area. The crystal's cut off wavelength was discovered to be 260 nm. Due to its decreased absorption, the material may be suitable for photonic and optoelectronic devices. [20]

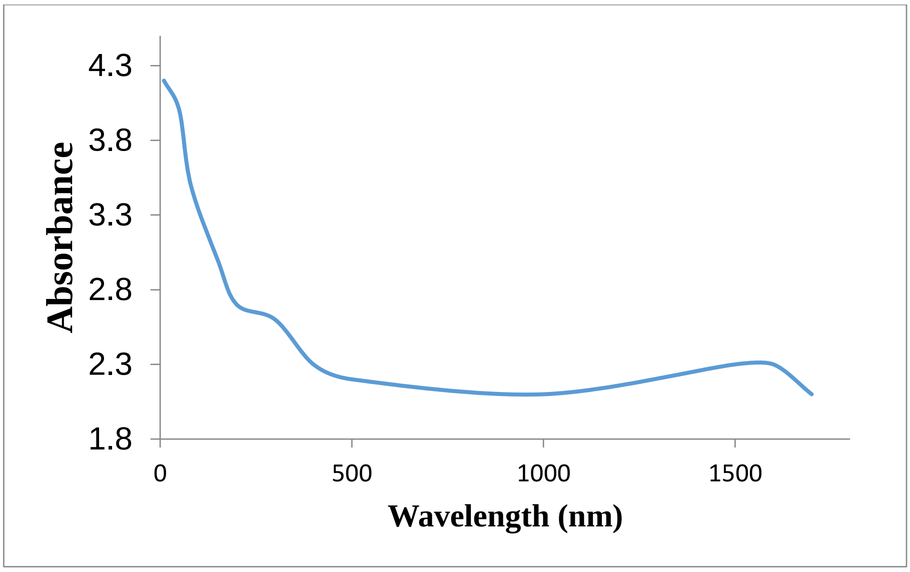


Fig. 4.1 Optical absorption spectrum of LTLC crystal

4.3. Vickers micro hardness test

Using a Vickers micro hardness tester at room temperature, a static indentation test was performed on the cut and well-polished LTLC crystal. Using loads ranging from 50 to 200 g with an average indentation time of 10 seconds, impressions were formed on the sample's plane. The distance between succeeding indentations was preserved at more than five times the diagonal length of the indentation to prevent surface effects. Using the connection, the Vickers hardness number (Hv) for various loads was computed [21].

$$Hv = 1.8544 \frac{p}{d^2} kg/mm^2 \qquad (2)$$

Where P is the applied stress in kilograms, d is the indentation diagonal's length in millimetres, and 1.854 is the diamond pyramid's geometric constant. Figure 8 depicts how the micro hardness profile changes with applied load. According to the profile, the hardness rises with increasing load and reaches a maximum hardness number of 76 kg/mm2 at 95 g. Additionally, the load variation demonstrates that, above 95 g, the hardness value drops as the weight rises. A crack's development due to the release of internal stress caused by local indentation is indicated by the hardness number decreasing as the load is increased**.** The findings also suggest that the crystal's increasing hardness number with regard to loading has the opposite effect on indentation size [22].

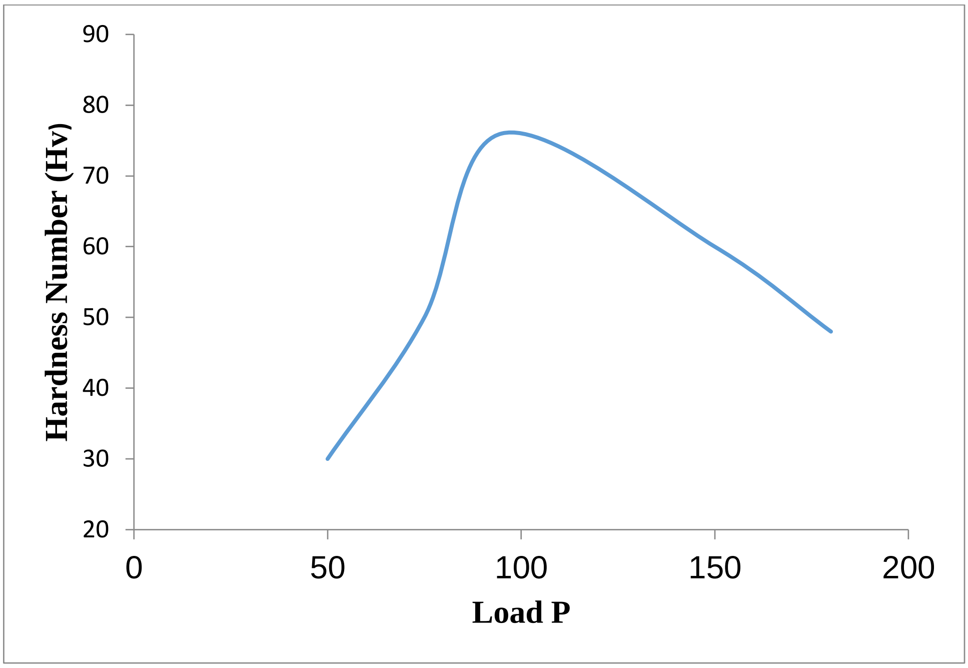


Fig .4.2 Plot of P versus Hv for LTLC crystal

4.4. Dielectric studies

Dielectric measurements for the LTLC single crystal in the frequency range of 50 Hz to 5 MHz at various temperatures are carried out using an HIOKI 3532-50 LCR HITESTER. The selected sample is cut with a diamond saw and polished using paraffin oil and fine alumina powder to produce an exceptional surface quality. To improve ohmic contact, the sample has been coated with silver paste on both sides. The relationship is used to compute the dielectric constant.

$$\varepsilon = \frac{cd}{A\varepsilon_0} \qquad (3)$$

A is the cross-sectional area, c is capacitance, d is thickness, and 0 is the absolute permittivity of open space, with a value of 8.854x10-12 F/m. Using the relation, the dielectric loss is also determined.

$$\varepsilon' = \varepsilon \tan\delta \qquad (4)$$

The fluctuations in dielectric constant and dielectric loss with frequency are depicted in Figures 4.3 and 4.4. The graph shows that both the dielectric constant and the dielectric loss decrease with increasing frequency as temperature rises. Dielectric materials are useful in understanding the interactions of a substance with different polarisations, such as electronic, ionic, atomic, and space charge polarisations that develop when the electric field varies. When the dielectric constant is high at low frequencies, there is space charge polarisation that develops [23] at the grain boundary contact. The low amount of dielectric losses at high frequencies suggests that the crystal has good optical quality and few faults for nonlinear optical applications. [24**]**

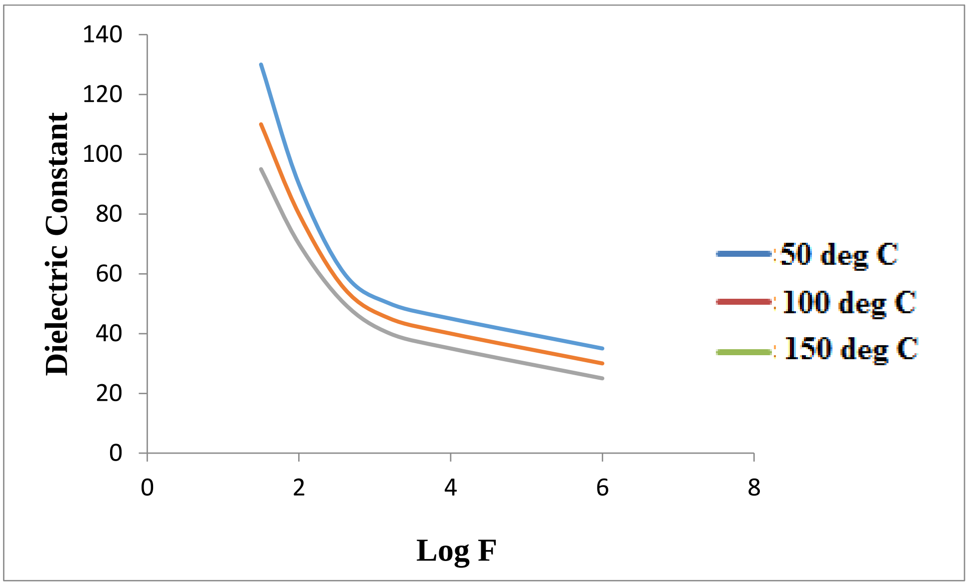


Fig. 4.3 Variation of dielectric constant with log F of LTLC crystal

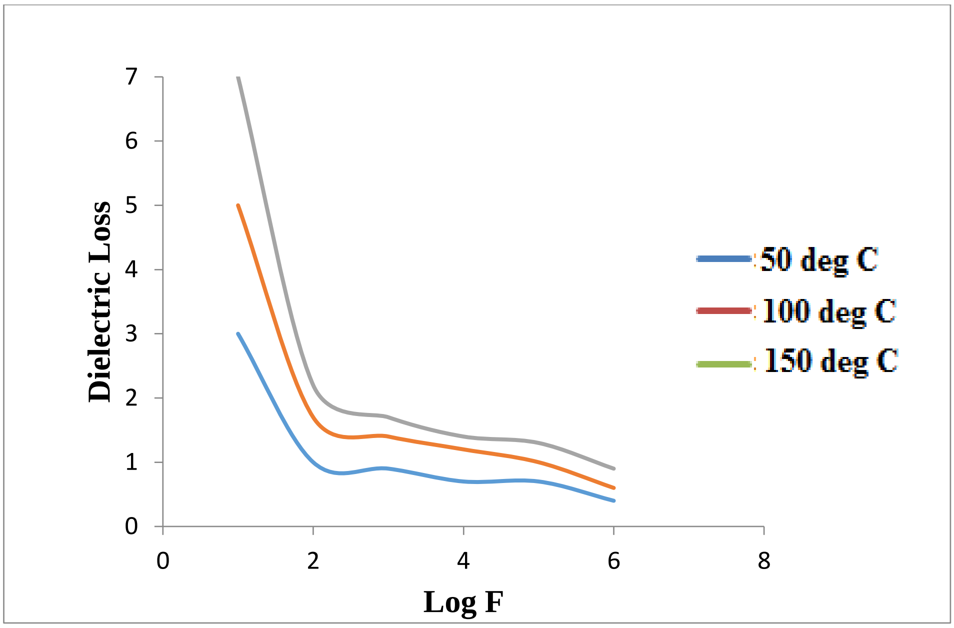


Fig. 4.4 Variation of dielectric loss with log F of LTLC crystal

4.5 Second harmonic generation (SHG) study

The Kurtz and Perry powder test [25] verified the developing crystal's nonlinear optical (NLO) characteristic. A uniformly sized powder made from the LTLC single crystal was tightly packed between two sheets of transparent glass. The KDP crystal was ground into a powder of the same size and used as a standard for the SHG measurement. The sample was pushed to come into contact with a Nd: YAG laser beam that had a wavelength of 1064 nm, an 8-ns pulse length, and a 10-Hz pulse repetition rate. The output of green light serves as confirmation that the second harmonic is being produced in the crystal.

The output power was determined to be 17.56 mV for LTLC and 9 mV for KDP for a constant input energy of 1.9 mJ/pulse given for both crystals. As a result, it was discovered that the developing crystal's SHG efficiency was 1.95 times greater than that of the KDP. The outcome suggests that optical and photonic device applications for the LTLC crystal are viable**.**

Table 4.2 SHG signal output of LTLC compared with KDP

Input Power (mJ/pulse)	KDP (Mv)	TLC (mv)
1.9	9	17.56

CONCLUSION

Slow evaporation technique has been employed for the growth of semi organic L-Threonine Lithium Chloride (LTLC) single crystal. Single crystal XRD confirms that the crystal belongs to orthorhombic system with the space group Pna21.UV-VIS spectrum shows that the crystal possesses high transparency in the entire visible and IR region. Micro hardness measurement reveals that Vickers' hardness number increases as the load increases and then decreases for higher loads, satisfying reverse indentation size effect. The low dielectric constant and dielectric loss at high frequencies suggest that the sample possesses enhanced optical quality with lesser defects. Kurtz powder test shows that the SHG sufficiency of LTLC is nearly 1.95 times of standard KDP crystal. The detailed characterization and the nonlinear optical properties confirm that the grown crystal is suitable for the fabrication of various optoelectronic and photonic devices.

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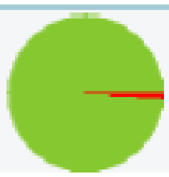

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CHAPTER -4

RESULTS AND DISCUSSION

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