Ultra Scientist Vol. 28(4)B, 110-113 (2016). ISSN 2231-3478 (Print)
www.ultrascientist.org 2319-8052 (Online)

Growth, Micro hardness and Dielectric Studies on the NLO Material Tristhiourea potassium chloride crystals

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(Acceptance Date 2nd August, 2016, Online Publication date 2nd Sep. 2016)

Abstract

Metal organic compounds as NLO materials have attracted much more attention for the high NLO efficiency, stable, physicochemical properties and better mechanical intentionTristhiourea potassium chloride single crystals (TTPC) were grown by slow evaporation method under room temperature. The grown crystals were subjected to single crystal XRD analysis and confirm its structure and lattice parameters. The SHG efficiency of grown crystal could enhance nonlinearity behavior. Inaddition the electrical parameters such as dielectric constant confirms the NLO property.

Key words: Crystal growth, SXRD, NLO, Dielectric constant.

Introduction

Non Linear Optical (NLO) materials find a variety of applications such as frequency conversion, light modulation, optical switching, optical memory devices and optical second harmonic Generation (SHG)[1-5]. A strong need continues to exist for NLO materials especially for lower cost, more efficient, higher average power materials in the field of optical parametric amplifier operation and second harmonic generation throughout the blue-near-UV spectral region. Much attention has been paid to metal organic compounds as nonlinear optical (NLO) materials for their high NLO efficiency.The search for new and efficient NLO materials has resulted in the development of a new class of materials called semiorganics. These materials have the potential for combining the high optical nonlinearity and chemical flexibility of organic materials with the thermal stability and mechanicalrobustness of inorganic NLO materials[6]. Thiourea is a centro-symmetric material when it is incorporated into inorganic material. It yields excellent non-centro-symmetric material. It is also an interesting inorganic matrix modifier due to its large dipole moment. Recently researches are focusing on growing metal complexes of thiourea related crystals[7]. Metals like zinc, cadmium, mercury readily combine with thiourea resulting in stable compounds with high optical nonlinearity and good physiochemical behavior because of their closed shells. Thiourea based organo metallic optical crystals like thiourea doped triglycine zinc chloride (TGZC)[8], Urea thiourea zinc chloride (UTZC), Cadmium chloride doped Zinc Tristhioureasulphate (CZTS), Semi-organic Zinc Tristhiourea chloride (ZTC)[9] have gained significant attention in the last few years, because of both organic and inorganic components in them contribute specifically to the process of second harmonic generation. In the present investigation, an attempt has been made to grow a semiorganic metallic mixed optical crystal of TrisThiourea Potassiumchloride and its effect in mechanical and optical studies were also made.

Experiment

Tristhiourea potassium chloride was prepared by mixing potassium chloride and thiourea in the stochiometric ratio 1:3 in deionized water in room temperature. To prepare TTPC, 20ml of deionized water is taken in a beaker. To this, first add the amount of thiourea and completely stir it. When thiourea is completely dissolved, add potassium chloride to it and stir well. After complete dissolution of solutes in solvent, the mixture was heated with constant stirring followed by slow evaporation of solution at room temperature for getting good and homogeneous yield of Tristhiourea potassium chloride.The product was further purified by repeated crystallization. Growth was carried out by low temperature solution growth technique by slow evaporation. The solution is then kept in room temperature. The solution containing beaker is covered with perforated filter paper to promote slow evaporation.The obtained TTPCcrystal is shown below.

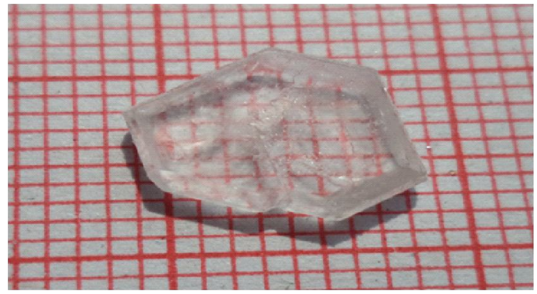

Figure. 1 photograph of grown TTPCcrystal

Results and Discussions

Single crystal X-ray diffraction analysis :

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. With the set of X-ray diffraction data collected, it is possible to get unit cell parameter, space groups, molecular structure of the crystalline solids and Miller indexing. The single crystal of TTPC was subjected to single crystal XRD using a computer controlled EnrafNonius – CAD4 X-ray diffractometer with Mo K_α radiation (λ = 0.71073 Å). The lattice parameters of tristhioureapotassium chloride are a=7.561Ap, b=7.250Ap, c=6.69Ap, $\alpha=\beta=\gamma=90°$ which shows the orthorhombic crystal structure.

Microhardness studies :

In the present study to understand the mechanical property of the grown crystals the microhardness measurements were made using a Leitzmicrohardness tester fitted with a diamond pyramidal indentor. A plot between the load and the hardness number is shown in Figure 2, which shows that the micro hardness number increases with increasing load. In the present study the work hardening coefficient of the grown crystal is greater than 1.6, and hence it was concluded that the TTPC crystal belong to the category of soft material.

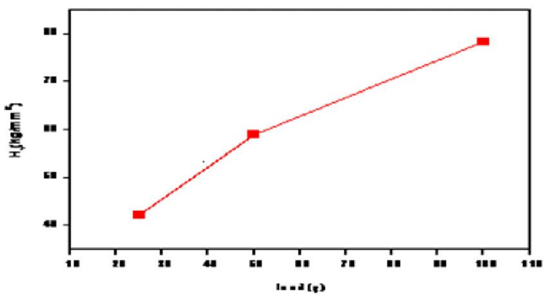

Figure 2. Variation of hardness number with applied load for TTPC crystal.

Second harmonic generation :

The powder Second Harmonic Generation (SHG) measurement for the the grown crystal was performed using the Kurtz and Perry powder technique and hence the SHG efficiency is compared with KDP. TTPC crystals possess 1.7 times the SHG of KDP crystal. The high value of second harmonic generation efficiency proved that the grown crystal can be used as an efficient frequency conversion material[10].

Dielectric studies :

An important property of a dielectric is its ability to supportan electrostatic field while dissipating minimal energyin the form of heat. Dielectric constant of a material can be measured by determining the change in the specially designed capacitor when the crystals are inserted between the plates of the capacitor. The capacitance (C_{crys}) and dielectric loss factor (tan δ) measurements were carried out to an accuracy of $\pm$2% using an LCRmeter (Agilent 4284 A)[11].

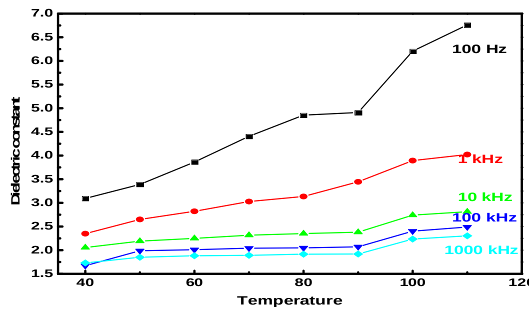

Fig. 3 The dielectric constant for $CdCl_2$ doped KHP crystal

The high dielectric constant value of the crystals at low frequency enumerates from fig.3 the contribution from all the four known sources of polarization namely electronic, ionic, oriental and space charge polarization. Space charge polarization is generally active at lower frequencies[12]. Again it was observed that the dielectric constant increases with increase of temperature. This is attributed to the presence of space charge polarization near the grain boundary interfaces which depends on the purity and perfection of the sample[13] which enhances NLO property.

Conclusion

The tristhiourea potassium chloride crystals are grown which are transparent and colourless.The Lattice parameters were confirmed by Single crystal X- ray studies.

The work hardening coefficient (n) was calculated which inferred that the grown crystal is a soft type material. The SHG efficiency of grown crystal could enhance nonlinearity behavior. In addition the electrical parameters such as dielectric constant confirms the NLO property and hence it can be used as an efficient frequency conversion material.

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