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An Optical Transmittance Study Used UV—Vis Spectra

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ABSTRACT

Single crystals of 2-Aminothiazole 3,5-Dinitrobenzoic acid has been synthesized and good quality optical crystals were grown by slow evaporation technique at room temperature. The crystallinity nature of the grown crystal was confirmed from X-ray diffraction technique. An optical transmittance study was also carried out by UV – Vis spectra. FTIR spectra confirm the presence of functional groups in the grown crystal. The dielectric measurements were carried out in the range of 50Hz to 2MHz. The dielectric constant was seen to increase exponentially at lower frequencies. The microhardness studies were carried out using Vickers hardness indenter. Photoluminescence study shows that maximum emission occurs at 435nm.

KEYWORDS

2AT 3; 5DNB; Microhardness; XRD; Band gap; Photoluminescence.

1. Introduction

With rapid advancement of the microelectronic and the optoelectronic industry in the country, the demand for crystals has increased dramatically during the past two decades. The requirement for better and well characterized single crystals has been a driving force behind extensive research and development in crystal growth[1,2]. Organic materials have very high optical non–linearity and great possibilities for twisting the molecular structure using molecular engineering and chemical synthesis. Also they have attracted much attention because of their application in frequency shifting, optical modulation optical switching, optical logic and optical memory for the emerging technologies in areas such as optical interconnections, telecommunications and signal processing[3,4].

Hassan A. Mohamed et al [5] reported the structural and optical studies of this crystal but to best of our knowledge there is no detailed studies are available on this material. So, in the present paper we report the powder XRD, Dielectric, Microhardness and Photoluminescence studies of 2AT 3, 5DNB crystals.

2. Materials and Methods

In the present investigation the title compound was synthesized by dissolving 2-Aminothiazole and 3,5Dinitrobenzoic acid in equimolar ratio using THF/Methanol Mixed solvents. The product was stirred well and filtered twice using whatmann filter paper to remove the impurities and covered with thick paper with perforated lid in order to control evaporation rate. Slow evaporation technique was employed to grow the single crystals. After 15 days good quality of crystals were harvested from the mother solution. The grown crystal is shown in Fig.1.

3. Results And Discussion

3.1 Powder X-Ray Diffraction Analysis

Powder X-ray diffraction study was carried out for the grown crystal by employing SEIFERT JSO DEBYEFLEX diffractometer with Ni filtered CuKα (Wavelength λ=1.5405 Å) radiation.

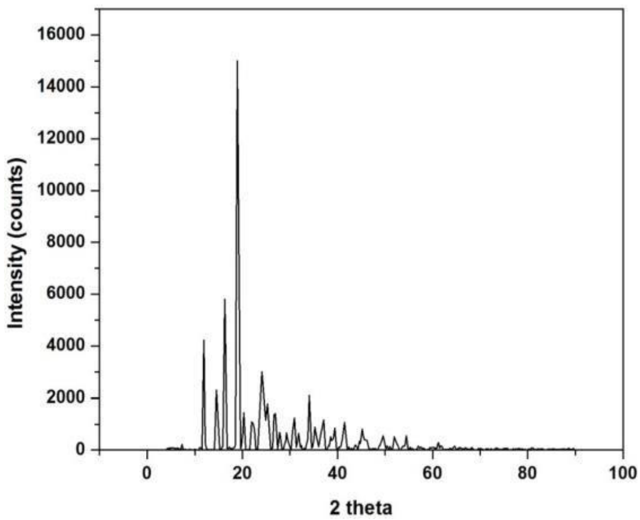

Figure 2. Power XRD Spectrum of 2 AT-3, 5 DNB Crystal

The powdered sample was scanned over the range 20–70° at a rate of 1°/min. The powder X-ray diffraction spectrum is displayed in Fig. 2. The sharp intense peaks on the pattern reveal that the crystallites are pure and dislocation free.

3.2 UV – Visible Transmittance Studies

The transmittance spectra of the grown crystals were recorded in the wavelength region from 200-1100 nm using PerkinElmer Lambda 35 UV-Vis spectrometer. The scanned spectrum is displayed in Fig. 3 and the spectrum shows the crystal is transparent in the entire visible region. This makes the crystal a potential candidate for optical applications.

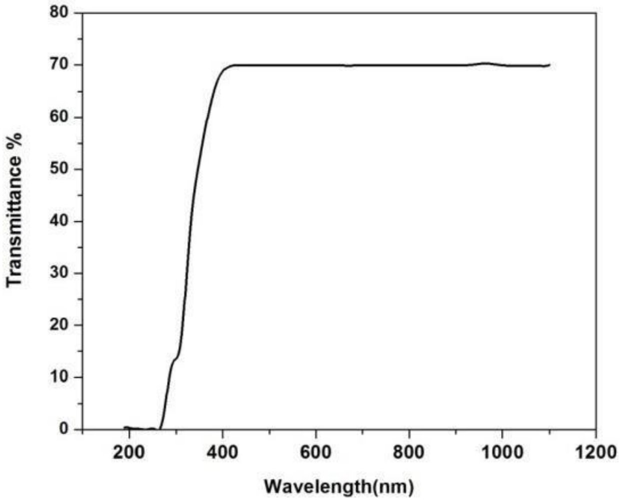

Figure 3. UV-Vis transmission Spectrum

3.3 FT-IR Analysis

The FT-IR spectra of 2-AT 3,5-DNB crystal were recorded in the wave number range of 4000 to 450 cm-1 using the KBR pellet technique.

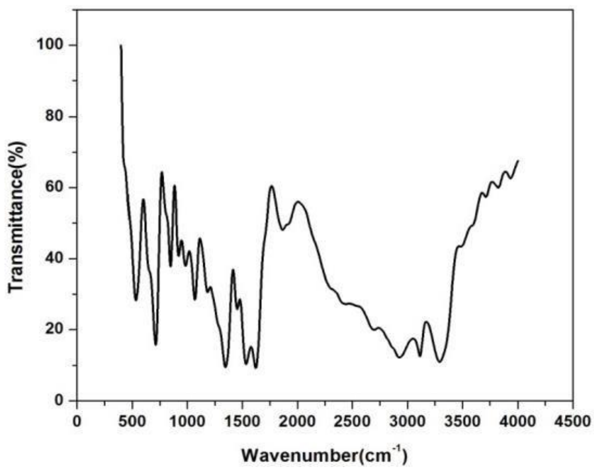

Figure 4. FTIR Spectrum of 2 AT - 3, 5 DNB Crystal

The observed peak at 3292.19 cm-1 is assigned to OH stretching vibration. The peak broadening in this region is assigned to the intermolecular hydrogen bonding. The NH stretching vibration is observed at 3112 cm-1. C=O stretching vibrations are observed in the range of 1866.01 and 1620 cm-1 respectively. NO stretching vibration occurs at 1420 and 1345 cm-1 also it is assigned to CN stretching modes. CH out-of-plane bending vibration takes place in the region of 919.08 cm-1. The FTIR absorption spectrum of 3,5DNB is shown in Fig. 4.

3.4 Dielectric Studies

The grown crystal is Polished and silver plated on the opposite faces were two probe connected to a 3532-50 Hioki LCR Meter (Japan). Dielectric Constant and dielectric loss were recorded at room temperature Fig. 5(a) and 5(b) shows the variation of dielectric constant and loss with log frequency. The dielectric constant is very high at lower frequency range and found to decrease with the increase in frequency due to the presence of space charge polarization [6]. The dielectric loss is very low at high frequency this shows that the crystal contains low level defects. The low value of dielectric loss at high frequency suggests the sample posses an enhanced optical quality which is of vital importance for optoelectronic applications.

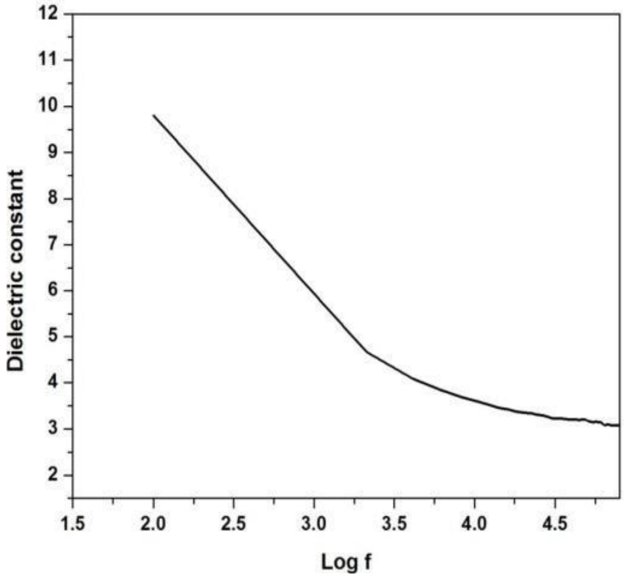

Figure 5. Dielectric constant Vs log f

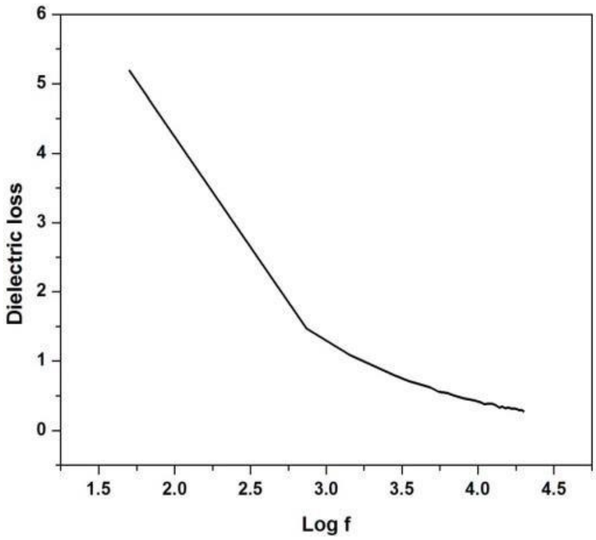

Figure 6. Dielectric loss Vs log f

3.5 Microhardness Studies

Vickers microhardness test was carried out for the grown crystals. The measurements were made at room temperature at constant indentation time of 5s. Indentation impressions were measured using leitz Wetzlar miniload hardness tester, fitted with a diamond pyramidal Vickers indenter. The microhardness was calculated using the formula Hv=1.854p/d2 (kg/mm2). Where p is the applied load in kilogram and d is the diagonal length of the indent in mm. for applied load above 100g micro cracks were observed around the impression [7-8]. It is observed from the Fig. 6 that when load increases hardness also increases this may be due to the release of internal stresses.

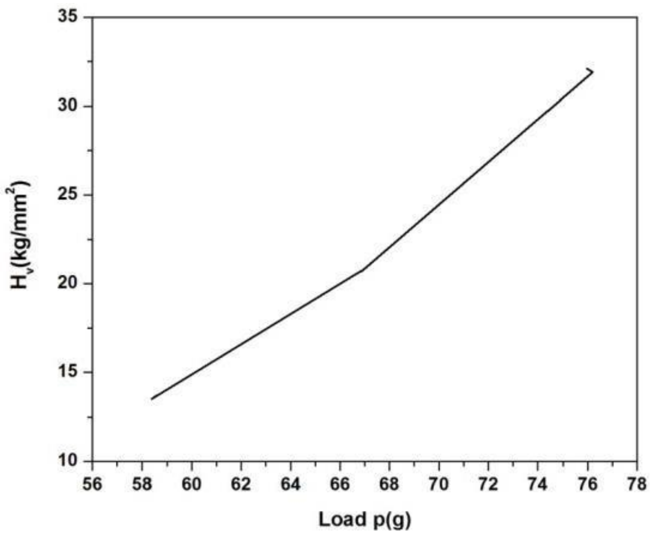

Figure 7. Vickers hardness Plot

3.6 Photoluminescence

Fluorescence may be expected generally in molecules that are aromatic which contains multiple conjugated double bonds with a high degree of resonance stability.

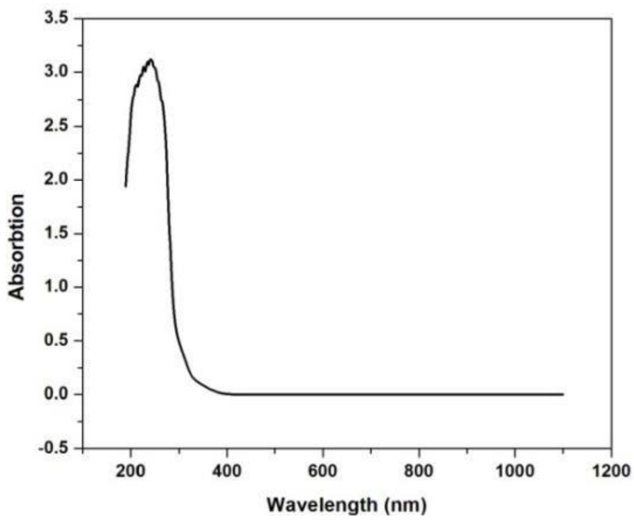

Figure 8. Excitation spectrum of 2AT, 3,5-DNB Crystals

The emission spectrum was recorded in the range of 200–1200 nm at room temperature. Spectra are displayed in Fig. 7(a) and 7(b). The sample was excited at 233 nm. The emission spectrum was measured in the range 250–500 nm. The maximum emission wavelength is observed to be at 435 nm. The results indicate that 2 AT 3,5 DNB crystals have a blue fluorescence emission. Also 2 AT 3,5 DNB crystals shows low UV absorption throughout the entire visible region which posses the crystal a suitable candidate for optical applications. The direct band gap of the material was calculated using the relations h, c, λ (Eg=2.852 ev).

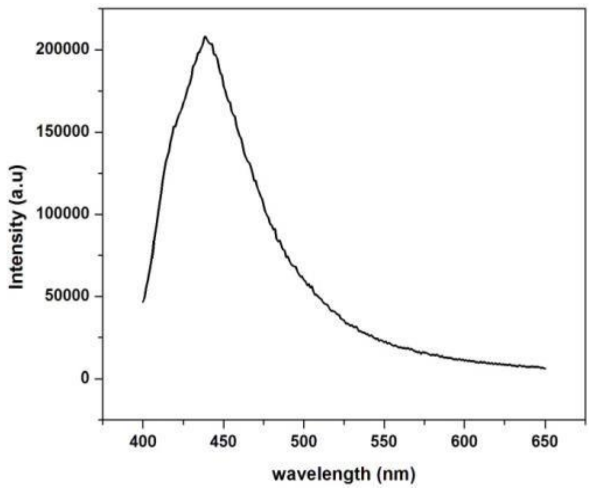

Figure 9. Emission spectrum of 2AT, 3,5-DNB Crystals

Conclusions

The 2-Aminothiazole and 3,5-Dinitrobenzoic acid complex has been prepared and grown by slow evaporation technique. The UV–Visible spectrum reveals that the grown crystals have a cut-off wavelength of 240 nm, which can be employed in the optical applications in the entire visible region and the near IR region. The presence of various functional groups was confirmed by FTIR spectrum. Powder X-ray diffraction studies confirm the crystallinity and show that 2-AT 3,5-DNB crystal has monoclinic structure. Dielectric constant increases in the lower frequency and the low value of dielectric loss indicates the purity of the crystal. The Microhardness value increases with the applied load. From photoluminescence study the direct band gap of the material has been calculated and crystals have a blue fluorescence emission.

In this work, we briefly introduce the fields of reinforcement and curriculum learning and highlight curriculum-based deep reinforcement learning methods and their robotics applications. While the conceptual curriculum generation is a wide topic[1], we focus on recent works where a curriculum is utilized in a strict sense and the method is demonstrated for a robotics environment with a neural network-based reinforcement learning agent.

4. Reinforcement Learning

In the last couple of decades, the field of Deep Reinforcement Learning (DRL) has established itself as a vital paradigm of Machine Learning (ML) and Artificial Intelligence (AI)[2]. Fueled by the recent advancements in processing hardware technology, the potential of the field has attracted research interest and scientific contributions from several domains like robotics, chemistry, neuroscience, gaming, business services and web management industries[3]. The field boasts an extremely powerful framework that allows for a software learner (dubbed agent) to observe and manipulate the world (dubbed environment). The outcome of the interaction between the agent and the environment, if successful, is a trained agent that maps simulated data into real-world actions. The nature of the framework and its ability to train an agent without an explicit supervisor poses a significant advantage, which however is surmounted by its need for colossal amounts of data. While reinforcement learning continues to dominate the simulation-based applications, there is a principal need to study and apply sample-efficient extensions to the field, viz. curriculum learning, to enable applicability in practical and real-world scenarios[4].

5. Curriculum Learning

Formally proposed in 2009[5], curriculum learning derives its inspiration from human learning style and the intuition that it is easier to learn by accumulating knowhow through simple tasks rather than trying to tackle a complex task directly. Figure 1 demonstrates the process as a flow diagram, where a given task (π) is broken down in multiple subtasks ($\pi 1$, $\pi 2$,… $\pi 5$) and presented to the learning RL agent in a particular order. Sometimes studied as a specific case of continuation methods and dynamic programming[5], curriculum learning strategies have been widely employed to improve supervised and reinforcement learning algorithms. Curriculum-based Reinforcement Learning (CRL) agents have shown significant improvement in convergence rates, training time and generalization capabilities when compared to standalone RL agents[6]. Moreover, CRL agents have also been able to solve tasks where standalone RL agents prove intractable[7]. While the nature of the curriculum itself has a myriad of possibilities, the curriculum design process can be either domain-expert specified [8] or automatic[9]. Domain-expert specified curricula rely heavily on human knowledge and thus lack new knowledge discovery, scalability, and robustness to unseen scenarios and may exhibit bias towards certain tasks. Automatic curricula, on the other hand, can offer what the latter lacks but are extremely difficult to generate and implement. The amalgamation of curriculum learning with reinforcement learning allows an agent to train in complex scenarios and learn a range of tasks, for which the domain of robotics stands to be the perfect recipient.

6. Adaptive Rpbotics

Evolved from traditional industrial robots and static automation, adaptive robots boast the ability to adapt to dynamic environmental changes, handle numerous tasks and safely collaborate with human agents. The interconnectivity and interoperability of adaptive robots further enable them to be an indispensable discipline for modern and future industrial, manufacturing, medical and assistive technological needs. Nonetheless, advancing robots beyond conventional automation pose unparalleled challenges like autonomous decision-making and semantic perception, specially for real-world implementations. Through the introduction of artificial intelligence and machine learning, the current state-of-the-art adaptive robots show tremendous potential and invites interest from numerous research domains.

The robotics research community investigating the notion of behavioral adaptivity is actively seeking solutions to alleviate challenges including efficient and automatic curriculum generation, multitask learning and sim-to-real curriculum generation to improve applicability and implementation across a wide range of domains. Curriculum-based reinforcement learning methods allow the field of adaptive robotics to surpass its era of explicitly programmed robots with limited functionalities and thrust the progress in automation towards a true behaviorally adaptive machine intelligence to train and implement sophisticated and hard-to-engineer behaviors.

Work in [10] extends the work of [11] to design a curriculum based on Hindsight Experience Replay (HER) transitions. The design of curriculum is based on the measure of similarity between the intended and achieved goals while tuning the measure for diversity among goals to aid exploration. On the other hand, [12]argues that a natural curriculum can be learnt in competitive multi-agent environments and that such a setting can produce complex behaviours that surpass the complexity of the environment itself. Similarly, cooperative multi-agents[13], diverse environments [14] and self-plays [15] have demonstrated better generalization and faster training using intrinsic and natural curriculums. Work in proposes a curriculum of start states for a constant goal state while the work in [16] estimates the next or intermediary goal of the appropriate complexity using a Generative Adversarial Network (GAN). [17]uses the backward reachability decomposition between different goal and start states to estimate reachability and obtain a measure of complexity of the task [18] quantifies the complexity of different training environments (teacher network) and generates a curriculum for the student networks to learn. [19]masks certain features of the goal vector to reduce its complexity and trains the agent on the reduced complexity goal states. It has also been shown that the development of a simple curriculum based on the accuracy requirements of a given task, on basis of a measure of a degree of competence like[20], leads to faster and more efficient training[21]. An extension to the work with Universal Value Function Approximators (UVFA) [22] is studied in[23]. While the current state of research mostly focusses on simulated objectives, notable efforts are being put into introducing simulation-trained intelligent and highly adaptive agents to the real-world[24-26].

In learning-based robotics, end-to-end autonomy often involves three principle components-perception, cognition, and control. The components are complementary in nature which allows for intelligent perception and cognition algorithms to enable autonomous control. Compared to traditional robotics where planning is an independent phase, the cognition phase is often embedded within the control framework of the learning-based robotics. In this way, the combination of cognition and control constitute the decision making process[27]. The curriculum-based reinforcement learning methods strictly focus on the decision-making framework of autonomous agents. Depending on the nature of the training data available, the decision-making agent framework can range from an end-to-end solution that also includes perception to one that only captures a low-dimensional control strategy. An example of the former can be the implementation of deep drive that replaces all the steps of a traditional Autonomous Vehicle (AV) process. A comparison of different implementations of learning-based AV can be found in[28]. In the same way, RL-based training is a quintessential choice for implementation that can collapse different required processes of industrial robots into the decision-making process of an adaptive robot. Task-specific trajectory planning from traditional control methods have proven to be more efficient for designated tasks [29,30] though may lack the flexibility to repurpose a robot to cope with the changes of dynamic environments. On the other hand, optimization techniques from various trajectory planning methods[31], have effectively been adopted for reinforcement learning agents [32,33] that allow for better convergence and learning of the autonomous decision-making process. The introduction of curriculum to RL training process (CRL) helps learning by improving sample efficiency and generalization capabilities of the agent. The ability of CRL to train incrementally complex agents based on scheduled experiences allow for maximal learning required for the promotion of adaptive robots in practical applications.

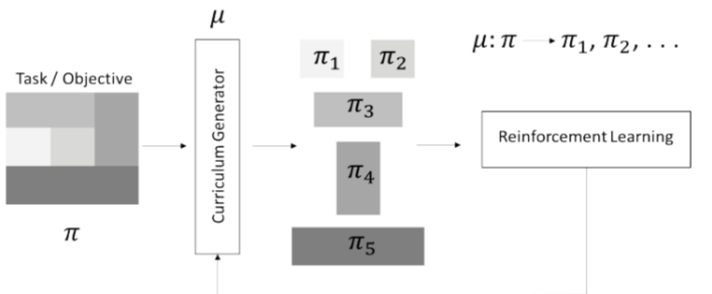

Figure 1. Curriculum interaction with the reinforcement learning process.

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