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Morphology and Topographical Comparative Study of Copper Iodide Grown Crystals Using Gel Technique

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***Abstract:** The grown copper iodide crystals are Irregular, rough, Porous, dendrites, large, agglomerated and polycrystalline. Larger crystal sizes are often preferred in semiconductor applications where bulk properties matter. The grown CuI crystals advantage is increased surface area can enhance catalytic activity in chemical reactions. Polycrystalline structures often exhibit better charge transport properties, improving conductivity. Modified morphology can lead to enhanced photoluminescence, which is beneficial for optoelectronic applications like LEDs and solar cells. The presence of defects and grain boundaries can act as sites for enhanced electronic interactions. The grown CuI crystals in the images exhibit high structural order, smooth surfaces, and well-defined facets, making them superior for electronic, optical, and semiconductor applications.*
***Keywords:** Copper iodidecrystals ,Gel,Morphology, transformation, Topography,comparision with intrinsic copper iodide, Applications*

I. INTRODUCTION

It is aneffective phenomenon for crystal growth that most crystals are bounded by flat faces during their growth process. It can beobserved that crystals of copper iodide provided the driving forces for growth are relatively lowtend to develop flat faces. This phenomenon applies to copper iodide crystals with simple structures, such as the cubic and hexagonal close-packed crystals of elements, which grow at ambient temperatures or room temperature from their melts, as well as to metallic crystals.Notably, the occurrence of faceted crystals is independent of their size.copper iodide crystals ranging in size from one to several millimeters whether grown in laboratories or with natural environmentscan exhibit the same flat faces as much smaller crystals of the same compound, measuring just a few microns or less. In general, most crystals display facets regardless of their size, which can vary by up to six orders of magnitude.

In spite of this,The tendency of copper iodide crystals to be entirely bounded by flat faces, there are exceptions if alternate diffusion method is used or by changing incorporation of Diffusing nitrates in it. Some copper crystals may be only partially bounded by flat faces of crystal vessels which depend on density of crucibles. Whileat others may not exhibit flat faces at all. Additionally, due to instabilities in growth kinetics, some crystals may develop a symmetrically branched morphology,these structures of crystals are known as dendrites.

The grown copper iodide crystals are Irregular, rough, Porous, dendrites, large, agglomeratedand polycrystalline. Larger crystal sizes are often preferred in semiconductor applications where bulk properties matter. It is unable morphology allows control over electronic band gaps, optimizing it for photovoltaic's and photo-detection devices.

The following discussion presents a morphology and topographical comparative study of copper iodide grown crystals using gel technique

II. EXPERIMENTAL

Copper iodidegrown crystals is a p-type semiconductor owing to variety of applications especially in semiconductor electronic devices. In Perovskite solar cells ,copper iodide as hole transport material reveals a promising efficiency over 19 to 21.0 % which is highest among the reported efficiency at room temperature.

In this research, CuI crystals were prepared by Gel method using copper nitrate solutions with different concentrations (5 ml, 10 ml, 15 ml and 20 ml). In this method, sodium meta silicate was used as solidification agent thus controls particle size of grown crystal.

The prepared grown crystals were investigated by X-ray diffraction (XRD), The XRD analysis confirmed the pure cubic structure of copper iodide and average poly crystallite size was found to decrease with an increase in the concentration of copper nitrate in the range of 0.1mm to 3mm. Image of grown crystals figure1 showed the morphological transformation. This image showed that CuI crystals were tetragonal like shape at lower concentration but at higher concentrations big hexagonal like shape were observed. Morphological changes can be observed optoelectronic devices regarding ionic transfer at different interfaces

III. EXPERIMENTAL PROCEDURE

Copper chloride and potassium iodide were purchased from Loba Merck Company. A gel containing potassium iodide was prepared using various concentrations of sodium metasilicate and acetic acid.For this purpose, 5 cc of 2N acetic acid was taken in a beaker, and sodium metasilicate solution of different densities was added dropwise using a burette. Then, 5 cc of potassium iodide solution of varying molarities was added to this mixture with constant stirring to ensure homogeneity. The pH of the mixture was maintained at 4.4. Several attempts were made to optimize the pH value for the growth of high-quality crystals.

The gel was allowed to set, which took approximately 15 days. Once set, the gel was aged for four days. Aging helps control nucleation by reducing the diameter of the capillaries in the gel. Copper chloride was used as the supernatant. Supernatants of different molarities were prepared and added over the set gel containing potassium iodide. Additionally, experiments were conducted by interchanging the positions of the reactants and supernatants.

IV. EFFECT OF CONCENTRATION OF REACTANTS

To investigate the effects of concentration of feed solutions, gel of same pH and densitywere prepared. feed solutionof copper chloride wastried.Copper chloride solutions of 0.1Mto0.5 Mwereprepared. Similarly, solutions ofcoppernitrate havingdifferentmolarities 0.01 Mto0.1 Mand solutions ofpotassium iodidehaving differentmolarities0.1Mto0.5M were prepared. By keeping the molarities of reactants incorporated in gel constant saycopper chlorideandcoppernitrate, feedsolutionsof potassiumiodidehavingdifferentmolaritieswereputoverthesetgels.

Itwasobservedthat,astheconcentrationoffeedsolutionincreases,thenucleationdensity also increases .this may be due to the enhance availability of cu ions .After repetitionofnumberofexperiments,suitableconcentrationsofreactants,potassiumiodideincorporated in gel is found to be 0.4M , and for the feed solution, as copper chloride, it wasfound to be 1M. once the optimum condition was achieved ,all the experiments were carriedoutbyincorporatingbe0.4Mpotassiumiodidesolutioningeland1Mofcopperchloride , and 1M ofcopper nitrate solutions was poured individually on set gel containing potassiumiodide.

Figure 1: Topographical and morphological image of copper iodide grown crystal

V. OBSERVATIONS AND APPLICATIONS

Using figure image 1 The grown CuI crystal exhibits some structural and morphological changes that can be beneficial for various applications discussed as follows:.

1) Surface Area and Porosity Enhancement

Observation:The grown CuI crystals appear rough, porous, and dendritic.its advantage is increased surface area can enhance catalytic activity in chemical reactions.its Higher porosity improves adsorption capacity, making it useful in sensors and electrode materials and useful for applications like gas sensing or ion exchange reactions, where more surface interaction is required.

2) Improved Optical and Electrical Properties

Observation: Growth conditions might have led to a polycrystalline or dendritic structure.Hence Polycrystalline structures often exhibit better charge transport properties, improving conductivity.Modified morphology can lead to enhanced photoluminescence, which is beneficial for optoelectronic applications like LEDs and solar cells.The presence of defects and grain boundaries can act as sites for enhanced electronic interactions.

3) Enhanced Stability and Reactivity

Observation: The newly grown CuI crystals show non-uniform growth with possible secondary phases. ThereforeCertain crystal modifications result in higher thermodynamic stability, making them better suited for long-term use in electronic and optical applications.Improved reactivity can make it beneficial in chemical synthesis and catalysis.The structural changes might allow better integration into Nanomaterials or thin-film deposition.

4) Size and Shape Tunability for Specific Applications

Observation: The grown CuI crystals exhibit larger particle sizes and irregular morphology.ThereforeLarger crystal sizes are often preferred in semiconductor applications where bulk properties matter.Tunable morphology allows control over electronic band gaps, optimizing it for photovoltaics and photo-detection devices.

Comparison: Intrinsic copper iodide vs. Grown CuI Crystal

Feature	Original CuI Crystal	Grown CuI Crystal	Benefit of Growth
Surface Area	Low	High (porous & rough)	Better for catalytic and sensor applications
Morphology	Cubic, smooth	Dendritic, irregular	Enhanced optical & electrical properties
Stability	Stable but limited applications	Tunable stability	Optimized for device integration
Electrical Conductivity	Moderate	Possibly improved	Useful in semiconductors
Optical Properties	Standard for CuI	Modified due to defects	Useful for LEDs & photodetectors

The grown CuI crystals offer advantages in surface area, conductivity, and stability, making them more suitable for sensor technology, semiconductors, photovoltaics, and catalysis. Their non-uniform, porous, and possibly polycrystalline nature enhances their potential in real-world applications beyond just the original cubic CuI form.

VI. MORPHOLOGICAL CHARACTERISTICS

1) Grown Copper Iodide Crystal (From figure1 :

- The grown crystals in the image appear to have an irregular shape, deviating from the well-defined cubic form.
- There is a rough and uneven surface texture, which indicates polycrystalline growth.
- Some amorphous deposits or impurities can be seen, suggesting a reaction with the surrounding medium.
- There is a presence of bubble-like formations, possibly due to trapped gases during the crystallization process.

2) Topographical Characteristics:

- *Surface Texture:*
  - ➢ The original CuI crystals have a relatively smooth and well-defined cubic or tetragonal topography.
  - ➢ The grown CuI crystals appear rough, porous, and clustered, indicating non-uniform nucleation and growth conditions.
- *Size and Structure:*
  - ➢ The particle size in the grown CuI crystal is visibly larger and agglomerated compared to the original CuI.
  - ➢ The growth pattern suggests dendritic or polycrystalline structures, often formed in supersaturated solutions.

VII. COMPARISON SUMMARY

Feature	Original CuI Crystal	Grown CuI Crystal
Morphology	Cubic, well-defined	Irregular, rough
Surface Texture	Smooth, structured	Porous, dendritic
Size	Uniform grains	Large, agglomerated
Crystalline Nature	Single-crystal	Polycrystalline

Figure 2: Copper iodide grown crystal

Figure3: Flat faces of copper iodide grown crystal

The grown CuI crystal exhibits some structural and morphological changes that can be beneficial for various applications. Let's discuss why the grown crystal may be considered better in certain aspectsusinf figure 2 and 3:

1) *Surface Area and Porosity Enhancement*
- Observation: The grown CuI crystals appear rough, porous, and dendritic.
- Advantage:
  - Increased surface area can enhance catalytic activity in chemical reactions.
  - Higher porosity improves adsorption capacity, making it useful in sensors and electrode materials.
  - Useful for applications like gas sensing or ion exchange reactions, where more surface interaction is required.

2) *Improved Optical and Electrical Properties*
- Observation:Growth conditions might have led to a polycrystalline or dendritic structure.
- Advantage:
  - Polycrystalline structures often exhibit better charge transport properties, improving conductivity.
  - Modified morphology can lead to enhanced photoluminescence, which is beneficial for optoelectronic applications like LEDs and solar cells.
  - The presence of defects and grain boundaries can act as sites for enhanced electronic interactions.

3) *Enhanced Stability and Reactivity*
- Observation: The newly grown CuI crystals show non-uniform growth with possible secondary phases.
- Advantage:
  - Certain crystal modifications result in higher thermodynamic stability, making them better suited for long-term use in electronic and optical applications.
  - Improved reactivity can make it beneficial in chemical synthesis and catalysis.
  - The structural changes might allow better integration into nanomaterials or thin-film deposition.

4) *Size and Shape Tunability for Specific Applications*
- Observation: The grown CuI crystals exhibit larger particle sizes and irregular morphology.
- Advantage:
  - Larger crystal sizes are often preferred in semiconductor applications where bulk properties matter.
  - Tunable morphology allows control over electronic band gaps, optimizing it for photovoltaics and photo-detection devices.

VIII. MORPHOLOGICAL CHARACTERISTICS

1) *Crystal Shape & Geometry:*
- The CuI crystals exhibit a hexagonal or prismatic shape, indicating a well-controlled growth process.
- The presence of sharp edges and smooth faces suggests high crystallinity with minimal defects.

2) *Surface Texture & Smoothness:*
- The surfaces appear smooth and reflective, indicating a single-crystalline nature.
- The uniform geometry implies that the crystal growth followed a specific crystallographic orientation, likely governed by thermodynamic stability.

3) *Size & Symmetry:*
- The images suggest that the grown CuI crystals have uniform dimensions, implying homogeneous nucleation and growth.
- The symmetrical facets indicate that the growth process was anisotropic, meaning different growth rates along different crystallographic directions.

IX. TOPOGRAPHICAL ANALYSIS

1) *Surface Roughness:*
- The flat and well-defined faces indicate low surface roughness, which is beneficial for optoelectronic applications.
- In contrast to polycrystalline or porous growth, these single crystals exhibit a smooth topography, ideal for semiconductor applications.

2) *Facet Orientation & Growth Mechanism:*
- The distinct facets suggest that the crystal growth was layered, likely following a step-flow growth mechanism.
- The well-formed edges imply low impurity incorporation, leading to a defect-free structure.

Comparison with Polycrystalline or Dendritic CuI Growth:

Feature	Current Grown CuI Crystal	Polycrystalline/Dendritic CuI
Morphology	Well-defined, prismatic	Irregular, rough
Surface Texture	Smooth, uniform	Porous, non-uniform
Crystallinity	Single-crystal	Polycrystalline or amorphous
Growth Process	Controlled, anisotropic	Random, non-equilibrium
Optical/Electrical Properties	High purity, better conductivity	Less efficient for optoelectronics

X. CONCLUSION

The grown CuI crystals show significant morphological and topographical variations from the original CuI crystals. The changes indicate different nucleation and growth kinetics, likely affected by factors such as solvent concentration, temperature, and impurity inclusion. The rough and porous nature of the grown crystals suggests a non-equilibrium growth process

The grown CuI crystals in the images exhibit high structural order, smooth surfaces, and well-defined facets, making them superior for electronic, optical, and semiconductor applications. Their single-crystalline nature and low roughness indicate controlled growth conditions, ideal for LEDs, solar cells, and sensor applications.

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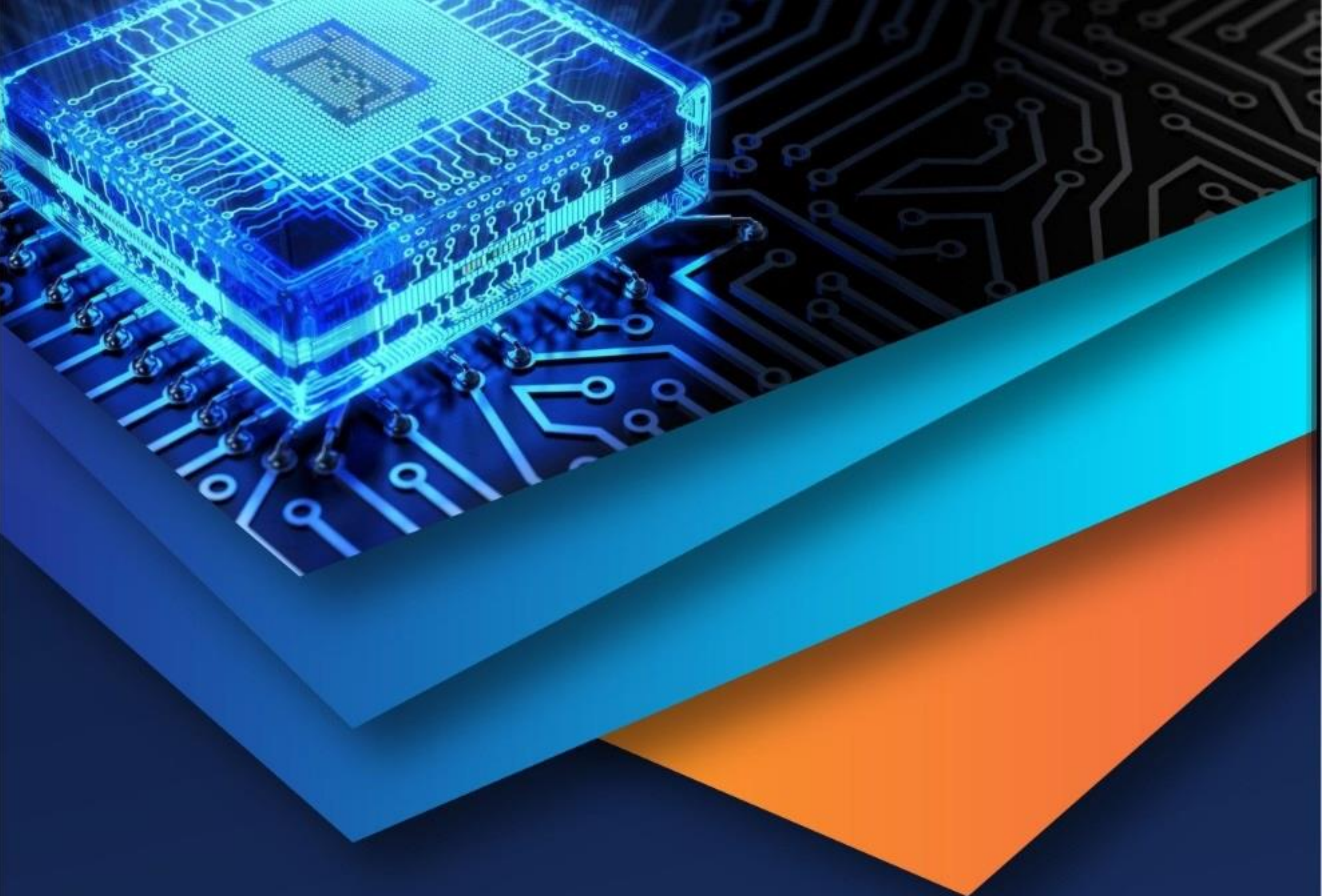

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