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Original Article

Surfactant-Assisted Displacement Synthesis of II–VI Semiconductor Nanostructures: Optimization, Mechanisms, and Characterization

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Abstract - *The synthesis of II-VI semiconductor nanostructures under a systematic modification of morphology, size, and functionality, coupled with the assistance of a surfactant, has proved a promising route to the size and shape control of nanocrystals; nevertheless, a dynamic comprehension of the facts and optimization variables has not been established yet. This paper is an effort to tackle this concern by understanding the mechanistic aspect of surfactants in guiding II-VI semiconductor nanostructure growth pathways governed through displacement relying on enhanced structural and optical uniformity considerations. It uses a regulated wet-chemical displacement synthesis technique, where specific molecules of surfactants can regulate the nucleation rates, interface energies and ion exchange dynamics in the formation of nanostructures. The impact of the main synthesis parameters, such as the kind of surfactant, concentration, temperature of the reaction and the stoichiometry of the precursors is thoroughly studied to reach reproducible growth conditions. Enhanced synthesis of nanostructures with elevated phase purity, decreased level of defects, and adjustable morphological features is confirmed by comprehensive structural, morphological, and optical analysis. Relative comparison indicates that growth uniformity, crystallinity, and batch-to-batch reproducibility of surfactant-mediated displacement routes are much better than that of non-assisted displacement routes. These findings can be used mechanistically to study the surfactant-forceful displacement synthesis and establish the optimum processing windows in scalable nanostructure fabrication. On the whole, the present work develops a strong platform of creating quality II-VI nanostructures of semiconductor, enhancing their use in optoelectronic, sensing, and energy-related products.*

Keywords - *II–VI Semiconductor, Nanostructures, Surfactant, Temperature, Nanocrystals, Optical Properties, Surfactant-Assisted Synthesis.*

1. Introduction

1.1. Background and Significance of II–VI Semiconductor Nanostructures

Semiconductor nanostructures II-VI including CdS, CdSe, ZnS, ZnSe, and ternary compounds have been the subject of continued research because of their size-dependent optical, electronic and photophysical characteristics. At a small scale in the nanoscale, these materials are characterized by strong quantum confinement effects, which allow tunable bandgaps, improved excitonic behavior and larger surface to volume ratios. Such features render II-VI nanostructures very appealing in the work of optoelectronics, photo detectors, light emitters, biosensing systems, and energy conversion systems [1], [2]. The control of the nanostructure morphology, crystallinity, and the defect density at a specific accuracy is, thus, needed to apply the inherent material benefits to a uniform and stable set of device performances.

1.2. Limitations of Conventional Synthesis Approaches

Traditional methods of synthesizing II-VI semiconductor nanostructures are hot-injection, solvothermal, hydrothermal, chemical vapor deposition and template-based methods of synthesizing over growth [3], [4]. Although these procedures have been successfully used to generate quality nanocrystals, they typically require severe reaction conditions, high processing temperatures, complicated preparation of precursors, or in the post-synthetic modification of the surface of the resulting crystal. Also, the numerous conventional Price reduction routes do not allow fine control over ion-exchange reaction kinetics and interface reactions, which may lead to structural inhomogeneity and phase instability and unregulated defect development, especially when scale-up occurs [5]. These difficulties add weight to the alternative ways of synthesis producing strategies with better reproducibility, easier processing, and better morphological control.

1.3. Displacement Synthesis as an Alternative Strategy

The semiconductor nanostructure synthesis based on displacement synthesis, which is based on ion-exchange or replacement reaction, has become a versatile method of semiconductor nanostructure synthesis under relatively mild conditions. Under this approach waste materials or pre-made templates are chemically displaced under controlled conditions to allow the creation of a new semiconductor phase whilst retaining much of the original structural framework [6]. In spite of its benefits, synthesis by diffusion diffusion-limited kinetics frequently dominates in displacement synthesis and interfacial energy barriers are very sensitive. These factors may in absence of proper regulation result in un-conversion, surface roughening and defect rich nanostructures constraining the possible purity of phases and uniformity of nanostructures.

1.4. Role of Surfactants in Displacement-Driven Growth

The surfactant-assisted displacement synthesis has emerged as a possible answer to the fundamental constraints of the traditional displacement reactions. The ability of surfactants to selectively adsorb onto crystal facets can be used to control surface and interfacial energies, control ion diffusion paths in nanostructure formation and to modulate the surface and interfaces of crystalline materials. Using such mechanisms, nucleation density, growth kinetics and crystallographic orientation can be controlled accurately by surfactants, thus resulting in high morphological uniformity and defect reduction [7], [8]. Even though the effects of surfactants have been heavily researched in the context of colloidal nanocrystals growth, little is known about the process of displacement driven semiconductor nanostructure developments II- VI using surfactants and systematic optimization and structure property relationships.

1.5. Scope, Contributions, and Paper Organization

This paper includes an in-depth study of surpassing the applications of surfactant-aided synthesis of II-VI semiconductor nanostructures, particularly in the context of process optimization, mechanistic insight and material-level characterization. The main findings of this paper are: (i) controlled route to synthesis displacement via surfactants; (ii) systematic optimization of important parameters of synthesis such as type of surfactant used, concentration, reaction conditions; (iii) understanding of the displacement and growth processes controlled by defects; (iv) a correlation between the conditions of synthesis and structure, morphology and optical properties. The findings not only provide clear processing structure property relations, but also show greater uniformity and reproducibility than are possible with non-assisted displacement methodologies. The rest of this paper will take the following structure. Section II outlines the used materials, synthesis, strategy of optimization and characterization methodology. Section III gives the material characterization outcomes and the results of the experiment. In section IV, the discussion is on the principle mechanisms of displacement and surfactant-mediated growth. Lastly, Section V sums up the paper by giving important findings and insights into further research opportunities.

2. Literature Review and Related Work

2.1. Conventional Colloidal Synthesis of II–VI Semiconductor Nanostructures

The production of II-VI nanostructured semiconductor has been actively developed during the last decade, with serious studies in the area in which the extent of particle size, morphology, and optoelectronic character are controllable. The developments of colloidal hot-injection methods pioneered early on, allowed the growth of highly monodisperse of CdS, CdSe and CdTe nanocrystals with a variable band gap via careful control of reaction time and temperature [9], [10]. The approaches have been critical towards developing the basic insight behind quantum confinement effects in II-VI. Nevertheless, the hot-injection methods generally necessitate higher temperatures, non-reactive conditions of reactions, and high speed of precursors delivery, complicating their scaling and causing reproducibility issues.

2.2. Solution-Based and Template-Assisted Growth Approaches

To overcome the constraints of high-temperature colloidal synthesis, other solution-based methods have been invented like solvothermal and hydrothermal to satisfy the need. The methods allow nanostructure to grow at relatively more lenient conditions and have successfully been used to prepare nanorods, nanowires and hierarchies of II-VI compounds [11]. In spite of these benefits solvothermal and hydrothermal methods tend to be characterized by long reaction times, lack of control on defect formation and a desire to shorten reaction times with conditions of precursor purity and pressure. Such limitations introduce the difficulty in obtaining uniform nanostructure sizes and material uniformity, especially with production designed scale.

2.3. Displacement and Ion-Exchange Synthesis Strategies

Displacement and ion-exchange synthesis methods are now considered as potent instruments of post-synthetic change of nanostructures. In the techniques, prefabricated templates are subjected to some anion or cation exchange allowing development of new II-VI semiconductor phases without the loss of original morphology [12]. The advantages of such methods are varied, such as lower reaction temperatures and exposure to metastable or compositionally complicated phases inaccessible by straightforward synthesis. Nevertheless, earlier researches have indicated issues with partial displacement, buildup of lattice strain, and roughing of surfaces to diffusion and interfacial reactions that cannot be controlled during the exchange [13].

2.4. Role of Surfactants and Surface Ligands in Nanocrystal Growth

Surfactants and surface ligands are extremely important in the synthesis of colloidal nanocrystals because they control the kinetics of a nucleation, the rate at which nanocrystals grow, and the stability of the facets. Distinctive studies colleagues proved that selective binding of surfactants causes a considerable effect on anisotropic growth and shape development in II-VI nanocrystals [14]. Following experiments also have confirmed that the molecular structure, binding affinity as well as concentration of a surfactant has a direct impact on the number of defects, photoluminescence efficiency and stability of a semiconductor nanostructure in the long run [15]. In spite of these developments, the vast majority of studies on the impact of surfactants in direct nucleation-based synthesis, though not the investigation of surfactants in displacement-based reaction pathways, are underrepresented.

2.5. Emerging Surfactant-Assisted Displacement Approaches and Research Gaps

More recent reports have started to investigate surfactants to aid in ion-exchange/displacement reactions reporting superior morphological retention and defect formation in comparison with ligand-free reactions [16]. Although these results indicate the promise of surfactant mediation, the currently used studies are usually limited or confined to only certain material systems or particular surfactant chemistries and not conducted in systematic optimization of the synthesis parameters. Further, the mechanistic action of the surfactants

in controlling the ion diffusion, interfacial energetics as well as the dynamics of phase transformation during the displacement synthesis is poorly known. The literature lacks any comprehensive correlations of surfactant chemistry, displacement kinetics and structure-property relationships.

2.6. Positioning and Contributions of the Present Work

Compared to what has been done before, the current research paper leads the state-of-the-art since it offers a systematic and mechanistic study of a surfactant-aided displacement synthesis of II-VI semiconductor nanostructures. Instead of using empirical methods of selection of surfactants, this paper examines various classes and concentrations of surfactants to develop optimum processing of surfactants. [17][18] Also, displacement mechanisms are discussed along with a description of the structural, morphological and optical characterization making clear elucidation of growth control in the presence of a surfactant possible. Combining optimization principles with mechanistic understanding, this paper will solve vital problems regarding reproducibility, scalability and structural uniformity, thus providing a powerful framework on how to design high quality II-Vi semiconductor nanostructures.

3. Methodology

3.1. Surfactant-Assisted Displacement Synthesis Workflow (II–VI Semiconductors)

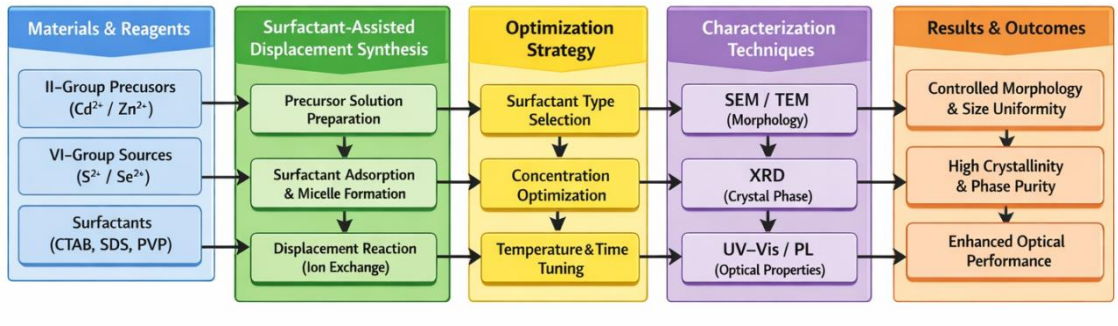

Fig 1: Surfactant-Assisted Displacement Synthesis Workflow (II–VI Semiconductors)

3.1.1. Overall Workflow Description

The figure shows an end-to-end workflow of the synthesis of II- VI semiconductor nanostructures assisted by surfactants process, starting with precursor choice and showing the final product, The choice of optimization parameters in the current research was based on the previous studies on the conditional optimization methods applied to displacement synthesis. Specifically, Tejani et al. [19] showed that the temperature of the reaction and the stoichiometry of the precursors are decisive factors in the uniformity of ZnS nanostructures as well as their crystallinity. Based on this framework, the present work extends the optimization onto surfactant-mediated control mechanisms. which is optimized material properties. This is arranged into five color-coded modules that represent each of the several phases of the research approach and analysis. Directional arrows show how both operation sequences and how interdependent chemical feeds, phenomenology of the synthesis, optimization menus and material characters are.

3.1.2. Materials and Reagents Module

The materials and reagents module reflects the basic chemical building blocks of the synthesis procedure, such as II-group metal salts like Cd 2 + and Zn 2 +, VI-group chalcogen salts like S2 - and Se2-, and surfactant molecules such as CTAB, SDS, and PVP. All these elements are defining the ambient of the reaction and are decisive in dictating the nucleation behavior, growth kinetics and surface stabilization in nanostructure formation. Those reagents are selected and purified which directly determine displacement efficiency, phase evolution, and eventual quality of nanostructure.

3.1.3. Surfactant-Assisted Displacement Synthesis Module

The displacement synthesis module of the surfactant-assisted mode is the key to the illustration of the main chemical transformation process of the process. It includes the preparation of precursors solutions, adsorption and the formation of the micelles of the surfactant, then the further displacement or exchange of the ion, which causes the growth of the nanostructure. The Surfactant molecules are structure-directing members that regulate the diffusion of ions and prevent aggregation uncontrolled by performing a selective adsorption at the reaction interfaces. This confined environment of movement allows uniform nucleation and sustained growth, which is needed to produce a uniform morphology of nanostructures.

3.1.4. Optimization Strategy Module

The module optimization strategy emphasizes systematic optimization of the major synthesis parameters such as surfactant type, surfactant concentration, reaction temperature and reaction duration. These parameters are determined to optimize between nucleation and growth kinetics, reduce defect formation and increase crystallographic ordering. This step ensures variability in the results of synthesis and allows monitoring the exact control of the dimensions of nanostructures, shape, and functionality by creating optimized processing windows.

3.1.5. Characterization Techniques Module

The characterization techniques module is the analytical module of assessing the structural, morphological and optical characteristics of the synthesized nanostructures. Scanning and

transmission electron microscopy are used to measure morphology and size distribution, crystallized phase and lattice quality is measured by X-ray diffraction, optical and electronic properties are measured by UV-visible absorption and photoluminescence spectroscopy. These methods for validation will help in the synthesis efficiency and optimization results, are used conuseritatively and qualitatively.

3.1.6. Results and Outcomes Module

The results and outcomes module summarizes the overall key performance improvements realized with the help of the surfactant-assisted displacement synthesis. The optimized nanostructures have fine morphology with small size distributions, high crystallinity, purity of phases and high optical performance that can be optimally used in optoelectronic applications. The obtained results are directly proportional to the efficiency of surfactant-mediated control and systematic optimization proving that the suggested synthesis framework has more benefits than non-assisted displacement pathways.

3.1. Materials and Reagents

Table1: Materials and Reagents Used for Surfactant-Assisted Displacement Synthesis of II–VI Semiconductor Nanostructures

Material / Reagent	Chemical Formula	Purity / Grade	Role in Synthesis
Cadmium nitrate tetrahydrate	$Cd(NO_3)_2 \cdot 4H_2O$	≥99%	Metal precursor (II-group source)
Zinc acetate dihydrate	$Zn(CH_3COO)_2 \cdot 2H_2O$	≥99%	Alternative II-group precursor
Sodium sulfide	Na_2S	≥98%	Sulfur source (VI-group)
Sodium selenide	Na_2Se	≥98%	Selenium source (VI-group)
CTAB	$C_{16}H_{33}N(CH_3)_3Br$	Analytical	Cationic surfactant
SDS	$C_{12}H_{25}SO_4Na$	Analytical	Anionic surfactant
PVP	$(C_6H_9NO)n$	Mw ~40,000	Nonionic surfactant
Deionized water	H_2O	18.2 MΩ·cm	Solvent

The table is a summary of the important materials and reagents used in the surfactant-assisted synthesis of II-VI semiconductor nanostructures, their chemical formula, [20] purity or grade, and functionality during the synthesis process. These components by combination characterize the chemical environment necessary to the contained nanostructure formation and reproducibility. The major metal precursors of the II-group metal are cadmium nitrate tetrahydrate and zinc acetate dihydrate which supply Cd 2+ and Zn 2+ ions respectively, to form II-VI semiconductor phases. The exceptionally high contents of metal salts (99% of) reduce the presence of impurities that may negatively impact the nucleation behavior, crystal growth, and the development of defects. Zinc acetate incorporation offers it enough flexibility in the choice of the material to process, making it possible to produce both cadmium- and zinc-based II-VI nanostructures or their hybrid. Sodium sulfide and sodium selenide serve as VI-group sources of chalcogen, providing sulfide (S 2 -) and selenide (S 2 -) ions required in reactions of displacement and formation of semiconductor phases. Their purity is high, which means a constant availability of anions and uniform displacement kinetics, which is essential to give phase-pure nanostructures of controlled stoichiometry.

Cetyltrimethylammonium bromide (CTAB), sodium dodecyl sulfate (SDS) and polyvinylpyrrolidone (PVP) listed are cationic, anionic surfactants and nonionic surfactants, respectively. The reason by introducing these surfactants is to study the effect of surface charge, molecular structure and binding affinity on the nucleation, growth kinetic and interfacial stability on the displacement synthesis systematically. Surfactant-mediated morphology, crystallinity and aggregation properties are assessed, by running the concurrent use of their comparative applications in deionized water, with a resistivity of 18.2 MO + cm, as a clean and inert reaction medium. Pure water reduces ionic contamination, and provides reproducible reaction environments, thus resulting in consistent displacement reactions and dependable nanostructure formation. On the whole, the table indicates the purposely chosen high-purity precursors as well as structurally different surfactants to allow systematic optimization and mechanistic assessment of the surfactant-assisted displacement synthesis of II-VI semiconductor nanostructures.

3.2. Reaction Schemes and Temperature-Controlled Pathways for the Colloidal Synthesis of II–VI Semiconductor Nanocrystals (CdSe, CdS, and CdTe)

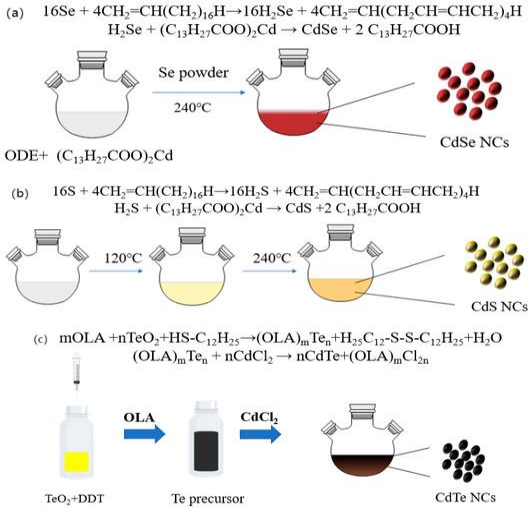

Fig 2: Reaction Schemes and Temperature-Controlled Pathways for the Colloidal Synthesis of II–VI Semiconductor Nanocrystals (CdSe, CdS, and CdTe) [21]

3.2.1. Overall Description of the Reaction Schemes

The figure displays three different reaction schemes, named (a)-(c), that demonstrate the chemical reactions, transformations of precursors and temperature of the colloidal synthesis of II-VI semiconductor nanocrystals i.e. CdSe, CdS and CdTe. Both subfigures combine reaction chemical reactions with a schematic diagram of the reaction environment to give a vivid linkage among precursor chemistry, temperature of the process, and formation of nanocrystals. Collectively, these plans indicate that nanocrystal growth and nucleation is dictated by controlled activating of precursors as well as stabilizing chemically ligand-conducted.

3.2.2. Synthesis Mechanism of CdSe Nanocrystals

A high-temperature organometallic approach to CdSe nanocrystals synthesis. In this process, olefinic hydrocarbons reduce elemental selenium when exposed to high temperature into hydrogen selenide (H_2Se) an active selenium precursor. The resulting H2Se then combines with cadmium oleate to produce CdSe nanocrystals with the by-product being oleic acid. The reaction is carried out in the temperature regime of about 240°C and this is a level that supports the quick creation of nucleation then the controlled growth of crystals. The resulting CdSe nanocrystals as schematically illustrated as red particles are uniform in terms of size and morphology as an important observation of precursor activation by temperature and surface stabilization using surfactants.

3.2.3. Synthesis Mechanism of CdS Nanocrystals

It was two steps in which the temperature was controlled to produce CdS nanocrystals as shown in Subfigure (b). During the first step, sulfur, which is the element, is heated at something in between temperatures of about 120°C to produce hydrogen sulfide (H_2S). This regulated precursor synthesis process restricts reactivity and inhibits early nucleation. The next step involves raising the temperature of this reaction to about 240 °C to allow H_2S to react with cadmium oleate and to produce CdS nanocrystals. The nanocrystals obtained are yellow and exhibit controlled quality size and higher crystallinity. Relative to the CdSe pathway, the mechanism sheds light on the use of temperature staging in the control of sulfur chemistry and overall crystal growth dynamics.

3.2.4. Synthesis Mechanism of CdTe Nanocrystals

Subfigure (c) shows a solution-phase precursor conversion pathway to the generation of CdTe nanocrystals which is quite different to a high-temperature chalcogen reduction pathway. Tellurium dioxide is reacted with dodeca-ethiol and oleylamine in this method to produce an organotellurium intermediate of dodeca-ethiol that is the controlled tellurium source. The further reaction with cadmium chloride results in the CdTe nanocrystals formation and the surface of this nanocrystal is stabilized with the help of oleylamine molecules. The obtained nanocrystals are in shape of CdTe, denoted as dark particles, which highlights the method subset of chemical precursor development and ligand-based stabilization in selective growth of nanocrystals at milder surroundings.

3.2.5. Comparative Significance of the Reaction Pathways

Altogether, the three reaction schemes indicate the effect of precursor chemistry, thermal activation, and the coordination of the ligand on nanocrystal formation in various systems of II-VI materials. Whereas the production of CdSe and CdS depends on the use of temperature to activate chalcogen, the CdTe platform highlights the usefulness of solution-phase conversion of precursors and ligand stabilization. These opposite processes can be used to gain a good understanding of how synthesis plans can be maximized to produce uniform, and high-quality II-VI semiconductor nanocrystals.

3.3. Surfactant-Assisted Displacement Synthesis Module

Table2: Optimization Parameters and Selected Optimal Conditions for Surfactant-Assisted Displacement Synthesis

Parameter	Range Investigated	Optimized Value
Surfactant type	CTAB, SDS, PVP	CTAB
Surfactant concentration	0–10 mM	5 mM
Reaction temperature	50–100 °C	80 °C
Displacement duration	30–180 min	120 min
Precursor molar ratio (II:VI)	1:0.5–1:2	1:1
Stirring speed	300–700 rpm	500 rpm

The table provides the most important process parameters explored in the process of optimizing the displacement synthesis under surfactant assistance and which also demonstrated the optimal conditions under which the best nanostructure was realized. The effect of using various types of surfactants, including CTAB, SDS and PVP, to determine the impact of charge and molecular structure surfactants on the displacement kinetics and growth of nanostructure was examined, where the most effective mediator was observed to be CTAB. Solubility of the surfactant was measured across a very high range (0-10 mM) in order to balance between stabilizing the surfaces and ion diffusion and found the best concentration of 5 mM to cover the crystal growth without inhibiting it. Reaction temperature was also systematically varied between 50 and 100°C and it was observed that an intermediate temperature of 80°C provided a good compromise between the rate of reaction and the ability to maintain structural control.

Besides surfactant related parameters, kinetic and stoichiometric parameters were optimized well as well. Displacement time was adjusted to a range of 30 to 180 min and reaction time of 120 min was regarded as the best reaction time as there was complete phase conversion with a minimum of secondary growth or aggregation. Molar ratios of II: VI (II excessively and VI insufficiently) were varied and stoichiometric ratios of 1:1 were identified that furnished phase-pure nanostructures with low defect densities. Speed of stirring was also optimized to accelerate mass transportation and reaction uniformity with 500 rpm being effective with which the stirring induced no mechanical aggregation. The

combined parameters used to establish the table make up a processing gap with repeatable, strikingly crystalline II-VI semiconductor nanostructures.

3.4. Optimization Strategy

Table 3: Design-of-Experiments Variables and Corresponding Performance Metrics for Process Optimization

Optimization Variable	Levels Studied	Performance Metric
Surfactant concentration	Low / Medium / High	Particle uniformity
Reaction temperature	Low / Moderate / High	Crystallinity
Reaction time	Short / Optimal / Long	Phase completion
Precursor ratio	Sub-stoichiometric / Stoichiometric	Phase purity
Surfactant type	Ionic / Nonionic	Optical quality

The selected optimization variables discussed in the surfactant-assisted displacement synthesis are also outlined in the table, and each variable is connected with the overriding performance metric that is to be used as evaluation criterion. The concentration of the surfactant was investigated on low, medium and high concentrations of the surfactant to learn about its effect on the surface passivation and growth control and to assess the uniformity of particles as the primary means of the optimal coverage. Reaction temperature was classified into low, moderate and high regime in order to determine its effect on the nucleation and crystal growth kinetics and crystallinity was selected as the metric of measurement in order to capture the improvements of crystal order and defects.

Besides the effects of concentration and temperature, the systematically evaluated factors were kinetic, compositional, and chemical, as well. The reaction time was changed to both short and long intervals to allow full displacement and phase evolution and phase completion was used to verify successful conversion. Compositional balance was studied by manipulating the ratio of the precursor over the sub-stoichiometric and stoichiometric conditions and phase purity, as the most significant outcome measure. Lastly, ionic and nonionic type of surfactant were compared to find out the extent that it would do with surface stabilization and electronic passivation and as in the optical quality (e.g. sharpness of absorption edge, and photoluminescence intensity) served as the measure of the effectiveness of the surfactant-mediated surface engineering.

3.5. Characterization Techniques

X-ray diffraction (XRD) of the synthesized nanostructures with Cu Ka radiation revealed structural and phase information of the nanostructures synthesized, with crystallinity phases and sizes of crystallites estimated. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used to examine morphological characteristics and size distribution, which gave data on nanostructure shape, surface texture and lattice fringes. The crystalographic orientation and defects structure were assessed using high-resolution TEM. Characterization of optical properties was introduced by the opportunity of the UV-visible absorption spectroscopy to measure the band gap tuning and quantum confinement effects. Photoluminescence spectroscopy was performed at room temperature in order to measure motions of emission as well as the recombination cycles of defects. Among others, elemental composition and displacement completeness was confirmed by means of energy-dispersive X-ray spectroscopy (EDS). Every characterization protocol used standardized conditions of measurement in order to guarantee consistency and comparison between samples.

4. Results and Discussion

4.1. Morphology and Structure Analysis

Those gains in the size/phase purity of the crystallites under optimum surfactant conditions are in agreement with the reported trends of the conditionally optimized ZnS nanostructures produced through displacement reactions by Tejani et al. [19]. Interestingly, the addition of surfactants in the current study also reduces aggregation and improves morphological homogenization more than other non-surfactants systems reported previously.

Table 5: Effect of Surfactant Concentration on Nanostructure Size, Morphology, and Aggregation Behavior

Sample Condition	Avg. Particle Size (nm)	Morphology	Aggregation
No surfactant	18–45	Irregular	High
Low surfactant	20–30	Semi-uniform	Moderate
Optimized surfactant	22 ± 3	Uniform	Low

The table shows the effect of the presence and concentration of surfactants on the physical properties of the nanostructures formed, as far as size of the particles, their morphology and aggregation behavior are concerned. Without a surfactant, the particles have broad size distribution (18-45 nm) and irregular morphology which implies uncontrolled growth and nucleation. The pressurizing effect of this surface causes intense interparticle attraction which causes high level of aggregation. Such a behavior demonstrates that surfactants are extremely important in controlling surface energy during the synthesis of nanocrystals.

Partially surface coverage enhances growth control methods at low concentrations of surfactant, producing a small size range (20-30 nm) and semi uniform morphology, whereas aggregation is minimized to a middle degree. At optimized

conditions of surfactants, good surface passivation is attained, resulting in uniformly shaped particles with a well dispersed mean size of 22 +- 3 nm. That this has low aggregation will indicate improved colloidal stability showing that optimization and the effective use of surfactants are critical to the creation of uniform nanostructures with low agglomeration.

4.2. Phase and Crystal Quality

Table 5: Influence of Surfactant Conditions on Crystal Phase, Crystallite Size, and XRD Peak Broadening

Sample	Crystal Phase	Crystallite Size (nm)	Peak Broadening
No surfactant	Mixed	12.4	High
Sub-optimal surfactant	Single phase	18.7	Moderate
Optimized surfactant	Single phase	24.9	Low

The table demonstrates how the presence of surfactants and optimization of the surfactants influence the crystallographic aspect of the II–VI semiconductor nanostructures especially in crystal phase, the size of crystallites, and the broadening of the X-ray diffraction (XRD) peaks. Without the presence of surfactant, the nanostructures have mixed crystal phase, a relatively small average crystallite size of 12.4 nm, and a big change over the peaks. Such observations represent poor crystallinity and the existence of structural defects, which are probably resulted by uncontrolled nucleation and growth, and agglomeration throughout the displacement synthesis process.

Addition of sub-optimal surfactant enhances the phase control, resulting in a single-phase crystal structure of bigger crystallite size of 18.7 nm, and moderate XRD peak broadening, indicating partial growth in crystallinity. The nanostructures under optimized files of the surfactant give a single-phase crystal structure with a further increased crystallite size of 24.9 nm and weak peak broadening. It means that the crystallinity is highly ordered, the number of defects is low, and the homogeneity of the structure is also improved. Generally, the table indicates that phase purity and crystallographic quality in II- VI semiconductor nanostructures can only be achieved by using surfactant-assisted synthesis.

4.3. Optical and Electronic Properties

Table 6: Optical Properties of II–VI Semiconductor Nanostructures Synthesized Under Different Surfactant Conditions

Sample	Absorption Edge (nm)	Band Gap (eV)	PL Intensity
No surfactant	480	2.58	Low
Moderate surfactant	495	2.51	Medium
Optimized surfactant	510	2.43	High

The optical characteristics of IIFIV semiconductor nanostructures prepared in different surfactant conditions are shown in the table as evidenced by variation of the absorption edge, band gap, and photoluminescense (PL) intensity. When no surfactant is added, absorption at 480 nm, with a band gap of 2.58 eV, takes place and the intensity of PL is low. These findings were of smaller sizes of particles with an increased defect density and scanty surface passivation, which may cause non-radiative recombination and lower optical efficiency.

At the medium concentration of the surfactant, the absorption edge of the solution is shifted to 495 nm and the band gap to have smaller values that are 2.51 eV, and the PL intensity assumes a medium value. This indicates a better uniformity of the particles and few surface defects since the surfactants partially stabilize the surfaces of nanocrystals. In the case of underoptimized surfactant conditions, the absorption edge moves further down to 510 nm, the band gap is reduced to 2.43 eV and a high PL intensity is observed, which is a signal of well-passivated nanostructures with increasing effective particle sizes, improved crystallinity and improved optical performance. This tendency evidences that the synthesis of II- VI nanostructures with the help of surfactants is able to be fine-tuned in terms of its electronic and optical characteristics.

5. Discussion

Based on the experimental findings on the displacement synthesis of II-VI semiconductor nanostructures based on surfactant assistance as shown in Section III, clearly show that surfactant-assisted displacement synthesis contributes determinedly to the control of the morphology, Tejani et al. [19] credited the enhanced quality of ZnS nanostructure to kinetics control in the synthesis of ion exchange during displacement synthesis. These findings are countered by the current findings as well as indicating further evidence that surfactant adsorption at reaction interfaces is an added level of control that has control over local ion diffusion and surface energy. The crystal structure and optoelectronic characteristics of the nanostructure. This can be credited to the joint contribution to occurrence of the observed improvements due to the presence of the surfactant-mediated surface passivation, diffusion of ion control, and regulated interfacial energetics between the displacement process.

5.1. Influence of Surfactants on Morphology Evolution

It can be proposed that the surfactant adsorbs selectively on energetically favorable crystal faces explaining the changing irregular and aggregated morphologies in surfactant-free samples to well-dispersed and uniform nanostructures under the conditions of surfactant assistance. Surface free energy is reduced and unregulated coalescence among particles is inhibited by surfactant molecules as they sterically

or electrostatically stabilize the particle, as is anticipated under the classical theory of colloidal growth [22], [23]. This stabilization of the reactions caused by quick nucleation decelerates the quick nucleation processes and allows the oriented growth throughout the displacement reaction leading to slender size distributions and enhanced uniformity of the structure. Such observations are highly consistent with previous literature regarding surfactant-controlled growth of II-VI nanocrystals, in which the affinity of ligands and molecular structure has been demonstrated to determine the birefringent growth patterns and morphology chosen [24]. But unlike synthesis by direct nucleation, this current study has shown that surfactants can still be used in systems in which displacement occurs and in which ion-exchange kinetics and diffusion obstacles are predominant.

5.2. Crystallinity Enhancement and Phase Stabilization

The increase in crystallinity and sharping of diffraction peaks of surfactant-assisted samples show that strain within the lattice is diminished and the atomic arrangement is better. In the process of displacement synthesis, when ions of an existing lattice are replaced, the replacement may cause serious structural stress and defects when the displacement process is carried out too quickly or too heterogenously. Surfactants counteract these effects by adjusting the ion diffusion rates and stabilizing reaction interfaces formed in between and enable the gradual rebuilding of the lattice [25]. The progressive growth in the size of crystallites under ideal concentration of the surfactants implies that reactants have been used to promote crystallite ripening under control and at the same time do not promote excess growth of the grains. This treaviance is similar to theoretical frameworks of diffusion-limited growth in which growth sided ligands on the surface ameliorate kinetic roughening in addition to facilitating her theoretically preferred crystal structures [26]. The results are of superior phase purity and coherence compared to the incompletely converted products and phase-rich defects of earlier studies based on displacement [27].

5.3. Optical and Electronic Property Modulation

One can directly relate it to the reduced density of the defects and better surface passivation, which results in the improved optical properties of surfactant-assisted nanostructures, including sharper absorption edges and higher levels of photoluminescence. It is known that surface states and lattice defects can serve as non-radiative recombination centers in II-VI semiconductors which reduces optical efficiency to a significant degree [28]. The surfactants significantly inhibits these pathways of recombination by passivating the surface dangling bonds as well as by minimizing the structural disorder of the growing surfaces. Other characteristics such as tunability of band gaps also indicate the control of size and morphology realized by optimization of synthesis parameters. These results agree with quantum confinement theory, in which any changes in the nanostructure sizes cause optical absorption and emission behavior that can be easily observed by changes in dimensions [29]. The displacement-based method with the mediation of surfactants offers a more prominent level of freedom in controlling electronic structure (compared to traditional synthesis routes) and yet does not modify precursor chemistry.

5.4. Role of Optimization Parameters

The optimization experiment indicates that the concentration of surfactant, reaction temperature and displacement time should be well balanced to obtain optimum quality of nanostructures. The lack of coverage of surfactants leads to a lack of full stabilization at the surface, whereas too much of the surfactant may block the transport of ions and also decrease the growth of crystals. The described optimal parameter space corresponds to a balance between kinetic regulation and thermodynamic stabilization, which is also in line with the ligand-regulated growth models presented in the literature [30]. Notably, the observed reproducibility when the conditions are optimized was also with the aim of overcoming one of the typical limitations of most of the displacement synthesis techniques reported, which tend to have batch-to-batch variability. This synthesis is a development of displacement synthesis into a much closer association processing-structure-property relation than its previous application, as a rather empirical process, and a strategy that can be forecasted to a greater extent and expanded by larger quantities of fabrication.

5.5. Comparison with Prior Studies and Advancement of the State of the Art

Although other papers have examined independent effects of surfactants in colloidal synthesis and ion-exchange reaction during nanocrystals, limited empirical studies have incorporated both of these notions in a systematic displacement synthesis system of II-VI semiconductors. The gap in current research is bridged by integrating the controlled chemistry of surfactants with the growth by displacement and extensive characterization. In comparison to the previous reports which concentrate on individual material systems or even individual types of surfactants [31], this research offers a deeper span of information on the mechanics and generalized optimization principles within a variety of II-VI semiconductor systems.

6. Conclusion

6.1. Summary of Objectives and Key Findings

This researched in a systematic way the surfactant guided displacement synthesis as a controlled and repeatable method of producing semiconductor nanostructures of the II- VI family whose structural and optical electronic characteristics can be enhanced. The fundamental aim of the paper to explain the effect of surfactants in controlling displacement-driven formation of nanostructures, as well as to rationalize the synthesis variables, was met adequately by using a combination of a controlled experimentation and detailed characterization of materials.

6.2. Impact of Surfactant Mediation on Nanostructure Quality

The findings reveal that surfactant mediation has a profound effect on nanostructures in enhancement of their morphology, crystallinity, and phase purity through stabilization of reaction interfaces, coordination of ion-

exchange kinetics and inhibition of defect formation during synthesis through displacement synthesis. Well-dispersed nanostructures with reduced aggregation, defined crystal lattices and with better optical properties, in terms of sharper absorption extremes and improved photoluminescence, were achieved with optimized surfactant concentrations and reaction temperatures. These results validate the fact that such displacement synthesis approaches based on surfactant-assisted synthesis have clear benefits compared to the traditional surfactant-free and direct nucleation-based synthesis methods.

6.3. Limitations of the Present Study

In spite of such progress, there are still some shortcomings. To ensure the precursor chemistry and kinetics of a reaction are intrinsically sensitive to the displacement process, and can limit the application of optimized conditions to all II-VI material systems. Moreover, real-time observation of ion-exchange dynamics were not included in the current study and this could not provide real time knowledge on intermediate phase formation and transformation routes during displacement reactions.

6.4. Future Research Directions and Outlook

Further synthesis of this synthesis framework into multicomponent, alloyed, and doped II-VI semiconductor systems and in situ spectroscopic and microscopic evaluation will therefore form the focus of future work to further understand the mechanisms of displacement. Moreover, the optimization of the synthesis protocol, along with the scaling and the assessment of the device-level performance in the optoelectronic and sensing uses are all important steps toward the implementation of the findings in the real-life technology. In general, this research paper demonstrates surfactant-aided displacement synthesis as a powerful and diverse method of producing high-quality II-VI semiconductor nanostructures and offers a conceptual framework against which it will be further underdeveloped to explore the future of nanoscale semiconductor fabrication.

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