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Role of Crystallinity in Determining the Electrical and Optical Properties of Nanomaterials

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Abstract

The idea of crystallinity is among the best factors that dictate electronic and optical properties of nano-materials since it directly dictates distribution of defects, density of grain boundaries and quantum confinement effects. The interaction of the sequence of the crystalline state and electronic terms is a significant aspect in the determination of charge elimination, carrier mobility, and light absorption and light emission. Here, we provide a review of how the specific crystalline characteristics impact the physical properties of various nanomaterials and groups, specifically metal oxide systems, semiconductors, 2D materials and perovskite compounds. The discussion is centred on the property correlations of the synthesis structure and how parameters of fabrication and incorporation of annealing and dopants influence the crystallinity and consequently properties of nanostructures. Recent developments of the enhanced characterizations of the X-ray diffraction, transmission electron microscope, Raman/photoluminescence spectrums are given to quantify and compare crystallinity with optoelectronics response. In addition, the contribution of the crystal disorder to the band structure and defect electronic states is interpreted by theoretical view of density functional theory (DFT) and molecular simulations. Lastly, the methods of managing large area crystallinity such as interfacial architecture, heteroepitaxy and laser annealing are discussed, and a prognostication presented regarding their future usage in electronic and optoelectronic products. The review therefore fills the vacuum between the crystallographic structure and functional properties and forms the basis of rational design of nanomaterials.

Keywords: *Nanomaterials; Electrical Conductivity; Optical Band Gap; Grain Boundaries; Quantum Confinement.*

I. Introduction

The concept of crystallinity is a basic determinant of the physical properties of nanomaterials, which dictate the manner in which atoms are organized and interact on the nanoscale [1]. In crystalline solid, the atoms are arranged in a long-range periodic arrangement, whereas in amorphous or poorly crystalline materials, the arrangement of atoms is disordered [2]. This order-disorder correlation has a direct influence on the behavior of electrons, phonon and photons in the material. Since nanomaterials have an extraordinarily high surface/volume ratio and size-dependent characteristics, even minor modifications in their crystallinity cause considerable alterations in electrical conductivity, carrier mobility, optical absorption and emission efficiency [3]. Hence, the crystallinity control has become a critical approach to nanomaterials tuning to electronic and optoelectronic applications.

The importance of investigating crystallinity effect lies in the fact that the influence of crystallinity is directly related to the formation of defects as well as the dynamics of charge carrier. The lower concentration of defects in high crystalline materials enables the carrier mobility and electronic performance to improve [4]. On the other hand, when in disordered or amorphous nanostructures, these defects concentrate charge carriers or cause band tail states, they cause a change in electrical and optical response. Therefore, the knowledge of the crystallinity degree gives important information on how to maximize the structure-property association of high-performance devices, including solar cells, sensors, transistors, and LEDs.

Optically, crystallinity has a great effect on the interaction of light and matter. In well-ordered crystal, electronic band structure is well-defined and thus optical transitions are sharp, photoluminescence is efficient and exciton behaviour controlled [5]. Also, in nanocrystalline systems, which are smaller in size, quantum confinement effects are more intense, with the size of the particles and the crystalline domain boundaries determining the energy bandgap.

The area of this review is a detailed discussion of the role of crystallinity in determining the electrical and optical properties of different types of nanomaterials, such as metal oxides, semiconductors, two-dimensional (2D) materials, and perovskite compounds. This review seeks to offer a holistic view of crystallinity as an important design parameter of the next generation nanoelectronic and optoelectronic materials by bringing together theoretical knowledge with experimental evidence. Figure 1 illustrates the multifaceted impact of crystallinity on nanomaterials. The main Contributions are given as follows;

- The paper describes the relationship between the degree of crystallinity and the electrical and optical characteristics of nanomaterials through the connection between crystal order, defects and charge dynamics.

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- It involves both experimental and theoretical methods of knowing the structure effect on performance of various materials.
- It identifies emerging methods such as heteroepitaxy, laser annealing, and interface engineering to assist in the attainment of improved and larger control of crystallinity in future electronic and optical gadgets.

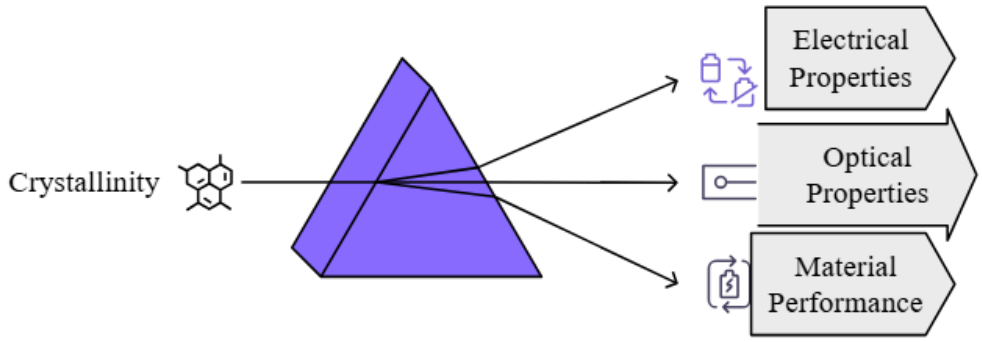

Figure 1: Unveiling the Multifaceted Impact of Crystallinity on Nanomaterials

II. Fundamentals of Crystallinity in Nanomaterials

Crystallinity is the extent of structural organization of a material, which is determined by the regularity and periodicity of atoms in a crystal structure. Conversely the amorphous materials do not exhibit any long-range atomic order and hence have different electronic and optical properties. [6] Discussed different definitions of nanomaterials that are provided by ISO and the European Commission. Discusses the role of the nanoscale grain size in improving mechanical strength in contrast to the coarse-grained materials. [7] Emphasized the increase in the use of nanomaterials in liquid crystals other than display technologies. [8] Research article on the development of heterogeneous photocatalysis in forty years of energy and environmental applications. Concentrates on such applications as solar water splitting and air/water purification. [9] Analysed nanomaterials-Electroceramics in batteries, sensors, capacitors and superconductors. Concentrates on ferroelectric and piezoelectric nanomaterials such as BaTiO3, SrTiO3 and ZnO that have special dielectric characteristics. [10] Prepared nanostructured MnOx materials with catalytic activity of pollutant degradation which resembled laccase. Finds that g-MnO2 has the best catalytic activity of the tested materials. Employs cyclic voltammetry to make a correlation between structure and catalytic behavior. [11] How internal stresses and crystallite sizes are measured utilizing the Bragg peak broadening. Gives a description of progress in X-ray detectors and sources to do high-resolution diffraction. [12] Explored reactions of Postsynthetic modification of semiconductor nanocrystals, using cation exchange. Information Thermodynamic and kinetic laws that govern ion exchange in lattices of nanocrystals. [13] had an article about the application of MnO2 nanomaterials in flexible supercapacitors to Next-generation electronics. Emphasize their benefits, which are flexibility, low weight, reliability, and high-power density. [14] Produced nanocrystalline soft magnetic materials in different forms such as nanoparticles, nanowires and thin films. Explains synthesis through mechanical alloying, high-rate solidification, and electrochemical. [15] studied the synergies of photocatalytic activity of anatase and rutile TiO2 phases. Prepares TiO2 samples in controlled phase, morphology and surface area by the soft-chemical techniques. Table I depicts the summary on fundamentals of crystallinity in nanomaterials.

Table I: Summary on Fundamentals of Crystallinity in Nanomaterials

Material/ System	Focus Area	Crystallinity Aspect Studied	Techniques Used	Key Outcomes / Insights	Ref
General nanomaterials	Structural & surface properties	Grain size, surface effects, quantum behavior	Theoretical / ISO & EC standards	Defines nanoscale effects on melting, strength, and catalytic activity	[6]
LC–nanomaterial composites	Self-organization & anisotropy	Ordering via LC templating	LC studies, optical analysis	Nanoparticles tune liquid crystal orientation and responsiveness	[7]
Photocatalysts (TiO_2, ZnO)	Energy & environmental catalysis	Charge transport, phase structure	Photocatalytic analysis, reactor design	Phase control enhances charge separation and reactivity	[8]
Electroceramics ($BaTiO_3$, ZnO)	Dielectric & ferroelectric behavior	Phase transition, domain ordering	XRD, SEM, impedance analysis	Size-dependent ferroelectricity for nanoscale energy devices	[9]

MnOx polymorphs	Catalytic activity & redox properties	Phase–reactivity correlation	XRD, CV, BET	γ-MnO_2 phase shows superior catalysis via defect chemistry	[10]
Metals & polymers	Structural defect analysis	Crystallite size, dislocations	XRD line profile analysis	Quantitative stress & microstrain evaluation in nanocrystals	[11]
Semiconductor nanocrystals	Postsynthetic ion exchange	Lattice substitution, phase control	TEM, EDX, XRD	Enables compositional tuning without shape loss	[12]
MnO_2–based electrodes	Supercapacitor performance	Crystallinity & oxygen vacancies	Electrochemical testing, XRD	Improved conductivity & flexibility via defect modulation	[13]
Magnetic nanocrystals	Magneto-structural correlation	Grain refinement, anisotropy	Sputtering, magnetometry	Nanostructuring enhances soft magnetic properties	[14]
TiO_2 heterostructures	Mixed-phase photocatalysis	Phase ratio (anatase: rutile)	XRD, UV–Vis, BET	7:3 phase ratio maximizes photocatalytic efficiency	[15]

III. Influence of Crystallinity on Electronic Properties

The electronic properties of nanomaterials are highly dependent on their crystallinity, as atomic order directly influences charge transport pathways. In highly crystalline structures, fewer defects and grain boundaries enable smooth carrier movement, resulting in enhanced conductivity and mobility. Conversely, in disordered or amorphous systems, defects act as traps or Crystallinity is the most important electronic property of nanomaterials because the atomic order has a direct effect on the pathways of charge transport. [16] Structural and electronic order-disorder effects in TiO2 nanoparticles synthesized by sol-gel and solvothermal methods with the aid of microwaves. Such characterization methods as XRD, TEM, Raman, and XPS provided the mixed phases of anatase-brookite with Ti4+ oxidation state. [17] Investigated the size-related crystallinity development in TiO2 nanoparticles by the ab initio calculation. Low-energy (TiO2) N structures of N = 1-38 were discovered in global optimization and data mining. [18] Examined the influence of the graphene orientation, CNF edge structure and surface groups on catalytic behavior. Prismatic and basal sites ratio is very strong and it determines the CNF-metal nanoparticle interactions. [19] Reported on nanomaterials that have at least one nanoscale dimension, and metal halide perovskites. The quantum dots are high quantum efficiency perovskite tunable emission sources of LEDs and single-photon sources. [20] Reported the variety and relevance of oxide nanomaterials in the development of nanotechnology. Indicates that they have a large variety of structures, morphologies, and physicochemical characteristics. [21] Researched the influence of the sputtering power on the Al-doped ZnO (AZO) transparent conducting oxide films. Has all films with >80% visible transmittance and c-axis orientation. Increased power causes larger grain size, conductivity and bandgap and reduces carrier mobility. [22] Synthesis of undoped and Sb-doped ZnO nanostructures by sol-gel. Maximizes reaction time to get high-aspect-ratio nanorods (aspect ratio =12 at 24 h). [23] Investigated mixed-halide-based lead perovskites CsFA1-Pb (BrI1)3 to be used as photovoltaic and LED. Optimal Cs concentration (0.10 < y 0.30) produces high crystallinity, long lifetimes and high mobility. [24] The research problem will be examining the influence of crystalline order on the Seebeck coefficient and the electrical conductivity of P3HT films doped with F4TCNQ. Findings indicate that the Seebeck coefficient increases and then decreases with the increase in crystallinity, but conductivity is always improved with increased charge mobility. This leads to the fact that the thermoelectric power factor increases by a factor of order of magnitude in case of the most crystalline films. [25] To regulate the crystallinity of conjugated polymers, a novel method of branched polyethylene additives was invented. The additive decreased the crystallinity and favored aggregation and phase separation resulting in stable charge mobility without thermal annealing. This blending technique can be used to do low-concentration processing and scalable fabrication of organic semiconductors. Figure 2 represents the influence of crystallinity on nanomaterial properties.

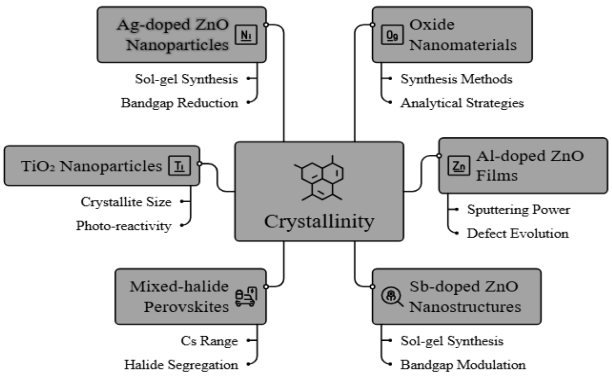

Figure 2: Influence of Crystallinity on Nanomaterial Properties

IV. Influence of Crystallinity on Optical Properties

Crystallinity is a highly influential factor that influences the optical properties of nanomaterials by controlling the interaction of light with the electronic structure. When the material is highly crystalline, the atomic structure is well-ordered resulting in sharp edges of the absorption, intense photoluminescence, and efficient exciton recombination. Contrarily, disordered or amorphous phases bring in defect states which bring about non-radiative losses and spectral broadening. [26] Thin films of Al-doped ZnO (AZO) (520-1420 nm) were sputtered on substrates of quartz using RF magnetron. Annealing of films (250-550 degC) was done with 30 min in vacuum to observe structural, optical and electrical changes. [27] AZO transparent films were deposited on glass by RF magnetron sputtering at 25-350 deg C. XRD, FESEM, HRTEM, and Hall tests revealed the structure of wurtzite with the c-axis orientation. [28] In-doped ZnO films (3 wt.% In) were sprayed onto glass with the ultrasonic spray at 300-400 degC. Using XRD, films were found to have wurtzite (002)-oriented films and a polycrystalline nature.

[29] Sol-gel method used to form ZnO thin films and annealed at different temperatures. XRD identified (002) preferred orientation with an increasing crystallinity and grain size with annealing. AFM disclosed that annealed roughened surfaces of the films improve gradually. [30] Sol-gel dip CdO Thin Films Al-doped CdO Thin Films CdO was deposited by sol-gel dip coating on glass (0-5 at. %). Al). XRD revealed a lower crystallinity and a decrease in the size of crystallites with increase in Al doping (37-11 nm).

[31] Thin films (pure, Ni-doped and La/Ni co-doped) of CuO were prepared using sol-gel spin coating. The XRD and FTIR confirmed the monoclinic CuO with the size of crystallites influenced by doping and thickness. [32] The films of al-doped ZnO were prepared using the spray pyrolysis method and subjected to electron beam of 8 MeV. The reverse saturable absorption and negative nonlinear refractive index was observed using Z-scan technique. [33] Examined the influence of crystallinity and surface -OH density on TiO2 photocatalysis. The commercial and home-made powders were compared through the XRD, TG and EPR analysis. [34] Eu3+ doped Mg2SiO4 nanophosphors were made through the combustion method and annealed at different temperatures. FESEM and HRTEM were used to verify these phase-pure Mg2SiO4 nanosized spherical particles by XRD. [35] The hydrothermal method of the synthesis of CeO2 nanoparticles was based on the use of SDS, PEG, and CTAB surfactants. XRD had cubic fluorite structure with crystallites of 12-16 nm. Table II determines the crystallinity and optical properties in nanomaterials.

Table II: Crystallinity and Optical Properties in Nanomaterials

Synthesis / Treatment	Crystallite Size (nm)	Band Gap (Eg, eV)	Optical Transmittance (%)	Resistivity (Ω·cm)	Mobility ($cm^2/V·s$)	Ref
RF magnetron sputtering; annealed 250–550 °C (30 min, vacuum)	25–38	3.25–3.30	82–88	$1.2\times10^{-2} \rightarrow 2.7\times10^{-3}$	4.88 → 7.86	[26]
RF sputtering at 25–350 °C	28–40	3.26–3.28	85–90	3.6×10^{-4}	10.2	[27]
Ultrasonic spray pyrolysis, 300–400 °C; annealed 500 °C	32–45	3.31 → 3.36	75–88	4.8×10^{-3}	6.5	[28]
Sol–gel spin coating; annealed 300–600 °C	20–35	3.24–3.27	90 (300 °C) → 82 (600 °C)	—	—	[29]
Sol–gel dip coating	11–37	2.45–2.70	80–92	$5.0\times10^{-3} \rightarrow 1.2\times10^{-3}$	3.1 → 5.4	[30]
Sol–gel spin coating	18–30	~2.0	70–85	8.0×10^{-2}	1.8	[31]
Spray pyrolysis + 8 MeV electron irradiation	25–33	3.23–3.27	78–84	—	—	[32]
UV photocatalysis, varied crystallinity & surface OH	15–25	3.10–3.20	—	—	—	[33]
Combustion synthesis + annealing	30–50	—	—	—	—	[34]
Hydrothermal synthesis	12–16	3.40–3.60	—	—	—	[35]

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V. Crystallinity–Structure–Property Correlations in Different Nanomaterial Systems

Crystallinity, structure, and properties do not have a consistent correlation in different nanomaterial systems. When the metal oxide is ZnO and TiO2, increased crystallinity results in an increase in carrier transport and optical transparency due to a decrease in defect scattering.

Nanothermodynamics [36] is the extension of the classical thermodynamics to nanoscale systems connecting macroscopic and nanoscopic behavior. It describes physicochemical property which depends on size, such as stability, magnetism, and conductivity. Quantitative models are associated with bond dangling and cohesive energy changes. [37] Photocatalysts Bismuth oxyhalide nanomaterials with layered structures hold promise because of their special layered structures. The exposure to the facet, phase transitions and photoactivity tailored using layer configuration controls. [38] The extensive application of nanotechnology has caused an issue concerning the effects of nanotechnology on the environment and biology. The toxicity of nanomaterials is based on the physicochemical characteristics such as size, shape, surface energy and stability.

[39] It is important to comprehend the interactions between nanomaterials and the biological and environmental systems to be able to regulate them in a safe manner. The paper determines the important physicochemical descriptors that affect toxicity. It suggests the application of quantitative nanostructure-activity relationships (QNARs) to predictive modeling. [40] Layered double hydroxides (LDHs) have adjustable composition, morphology and structure to catalyze and adsorb. Their interlayer and self-assembly properties are unique giving them high-performance in nanomaterial design. Active sites, defects, and morphologies of tailors are controlled. [41] TiO2 nanomaterials in the form of Cu-doped nanomaterials were produced using flame aerosol reactors with regulated parameters.

[42] Hydrothermal synthesis of manganese oxides was performed at different ratios of the reactants, temperature and additives. Phase formation (OMS-7, OMS-2) relied on effect of complexation and potassium ions. [43] Photocatalytic phenol degradation of different TiO2 nanostructures under UV light was tested. Adsorption was followed by quasi-second-order and Langmuir-Hinshelwood models. Facet exposure had an effect on reactivity; P25 TiO2 was better compared to others when it came to breaking phenol. [44] This study demonstrates advances in crystal-phase engineering noble and non-noble metal nanomaterials, and its effects on their physical and electronic characteristics. It talks about synthesis techniques, phase changes and phase-related phenomena. The work also defines issues and future trends of the realization of the accurate control of crystal phases. [45] The article looks into the effect of length scale, crystallinity as well as surface reactivity of nanocellulose on the biological interactions and immune responses. CNCs of higher crystallinity and intermediate length were more cellularly uptaken and inflamed. These results highlight the necessity to take into account structural parameters of safe biomedical application of nanocellulose. Figure 3 depicts the nanomaterials properties and applications.

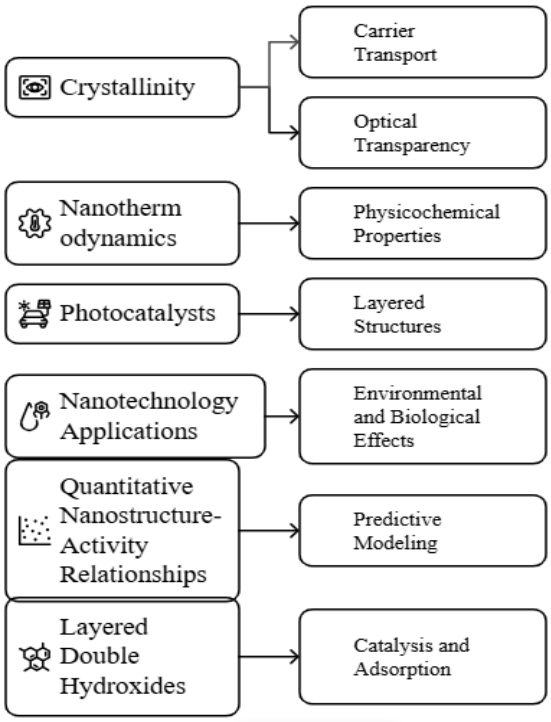

Figure 3: Nanomaterial Properties and Applications

VI. Synthesis and Processing Routes Affecting Crystallinity

Synthesis and processing pathways that define the atomic arrangement and defect formation play a major role in determining the crystallinity of nanomaterials. Precursor chemistry, reaction temperature and substrate type are among other factors that are critical in regulating crystal growth and orientation. Methods such as sol-gel, hydrothermal and chemical vapor deposition (CVD) tune nucleation and grain size with precision and has an impact on the quality of overall crystal.

[46] Sn-Beta crystallization in fluoride medium is highly dependent on the content of tin and the type of source. Addition of Sn to the medium increases the crystallization time and morphology of crystalline products. Low Sn forms bipyramidal-shaped crystals after 4 days, and high Sn forms plate-like crystal after 60 days. Tin is not uniformly distributed as it is more concentrated towards the surface. [47] Self-templating pore formation was used to develop a bottom-up synthesis of mesoporous crystalline silicon. The

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by-products of salt are removable templates, which do not require etchants. The resultant silicon has high surface area and adjustable pore/particle size. [48] ZIF-8 was grown at the room temperature in the presence of triethylamine (TEA) that affected the quality of crystals. Crystallinity and particle size were regulated by adjusting the TEA/ total molar ratio between 0.004-0.007.

[49] The g-C3N4 photocatalysts were crystalline, and their synthesis was rapid with the help of a microwave in minutes. This method substitutes the long and high temperature reactions (400-600 degC hours or days). [50]

[50] The study of the hybrid silicas in the synthesis of solvent-free zeolites found that the crystallinity depends heavily on silica structure and chemical nature. The various synthesis paths resulted in crystallinities of 0-100 percent with all of them constituting sodalite-type zeolites. Longer alkyl chains in hybrid silica retarded crystallization indicating their important role in zeolite formation dynamics. Figure 4 illustrates the nanomaterial manufacturing: challenges and innovations.

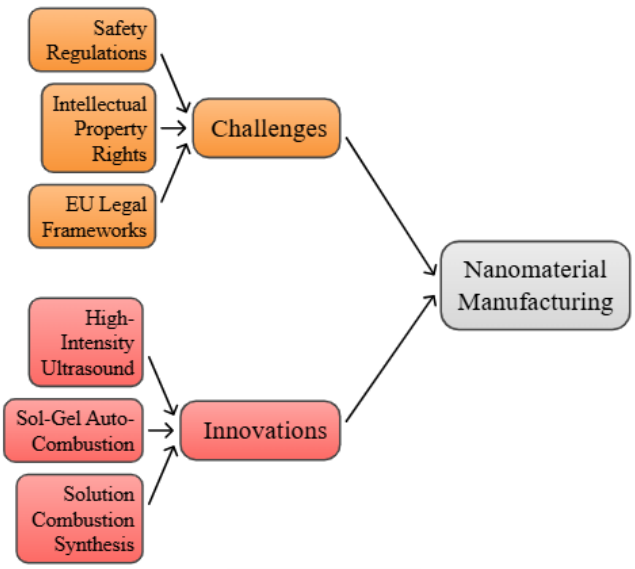

Figure 4: Nanomaterial Manufacturing: Challenges and Innovations

VII. Challenges, Emerging Strategies, and Future Perspectives

This is a significant problem in nanomaterial fabrication because it is not easy to have accurate and scaled control of the crystallinity. Other methods, including heteroepitaxy, interfacial engineering and laser-assisted growth are promising as ways to control the crystal orientation and reduce defects on large scales. Nevertheless, consistency and stability in the production of large scale remains challenging.

a. The core challenge: variability and defect control

Not only does controlling crystallinity at the nanoscale imply the creation of the desired crystal phase, but also the choice of orientation, grain size, boundary character, and the concentration of point defects and dislocations all of which have significant impact on electronic, optical, thermal and mechanical properties. At small scales growth kinetics, surface energies and local chemistry prevail and, therefore, small changes in precursor concentration, temperature, or condition of substrate generates significant changes in result. Furthermore, synthesis often produces populations of defects size- and shape-dependent; size- and shape-dependent defects in a synthesis pathway readily form what would otherwise form near-perfect crystals when carried out on an individual small scale; a synthesis method that works well on a single small sample not work when repeated or scaled.

b. Promising routes: heteroepitaxy and interfacial engineering

Two of the most potent levers of the control of crystallinity are heteroepitaxy and foresight in interfacial design. Heteroepitaxy involves the orientation and registry of the growing film or nanostructure to be grown by the use of a lattice-matched or commensurate substrate, and with the control of lattice mismatch and thermal expansion epitaxial growth yield single-crystal films or aligned arrays of nanowires with much reduced grain boundaries. The concept of interfacial engineering gets this point further: deliberately engineered buffer layers, self-assembled monolayers or chemically functionalized surfaces adjust nucleation energy barriers, regulate wetting as well as absorb misfit strain.

c. Laser-assisted and other advanced growth techniques for localized control

In laser-assisted, crystallization kinetics controlled locally and rapidly (impossible thermally over an entire wafer), particularly in the kinetics of nanoparticles. Lasers used to selectively melt or rearrange amorphous regions, rearrange phases, and repair defects by providing energy on ultrasonic or narrow focus timescales, and such capabilities are not possible with a high temperature substrate. This allows crystalline domain patterning, control of orientation on demand and repair of defects after deposition. Other more sophisticated methods also optimize the local thermodynamics and kinetics to achieve desired crystalline results.

d. Integration, scale-up, and the roadmap forward

It was necessary to match the precision of nanoscale with high throughput and robust process engineering in order to meet commercial needs. It necessary to monitor the processes in real time (in situ optical, electron or diffraction probe, and closed-loop control) in order to identify drift and actively correct deviations during growth. Lastly, materials-

agnostic schemes such as modular buffer schemes, scalable laser scanning schemes and defect-tolerant device structures reduce the adoption barrier in various material systems.

e. Comparative Analysis

A summary of important crystallinity-related parameters in the literature about nanomaterials is given in Table 5, including correlations between structure, optics, mechanics, and modeling observations. It incorporates the results of the effect synthesis conditions, doping, and annealing have on the grain size, band gap and defect density. This integrated summary is a combination of experimental and theoretical methods, where they are used together to optimize the performance of nanomaterials in the advanced functional application. Table V represents the summary of crystallinity parameters across nanomaterial studies. Figure 5 illustrates the distribution across crystallinity study categories.

Table V: Summary of crystallinity parameters across nanomaterial studies

Category	Parameter / Descriptor	Typical Range / Key Findings	Technique / Model Used	Representative References
Structural	Crystallite size	2–120 nm depending on synthesis and annealing	XRD (Scherrer), TEM, HRTEM	[15], [25], [27], [34]
	Grain size evolution	Increases with annealing (e.g., 12→38 nm)	SEM, AFM	[26], [29]
	Lattice strain / microstrain	0.05–0.3% (reduced after post-treatment)	Williamson–Hall, Rietveld refinement	[24]
	Phase composition	Wurtzite ZnO, Anatase TiO_2, Cubic CeO_2, etc.	XRD, Raman	[27], [33], [35]
	Morphology	Nanorods, nanosheets, spheres, porous scaffolds	SEM, FESEM, TEM	[22], [35], [47]
	Surface roughness (RMS)	2–10 nm (depends on doping/annealing)	AFM	[30], [31]
Optical / Electronic	Band gap (Eg)	2.0–3.6 eV depending on crystallinity and dopant	UV–Vi's absorption, Tauc plot, DFT	[4], [25], [28], [33]
	Optical transmittance	80–90% (visible range)	UV–Vi's spectroscopy	[26], [27], [29]
	Photoluminescence (PL) intensity	Strong in highly crystalline, weak in amorphous	PL spectroscopy	[33], [34], [35]
	Nonlinear optical coefficient (χ^3)	10^{-5}–10^{-3} esu (in Al: ZnO)	Z-scan	[32]
	Carrier mobility	4–8 $cm^2/V{\cdot}s$; enhanced with crystallinity	Hall effect	[26], [27]
	Resistivity	10^{-2}→10^{-4} Ω·cm (lower in crystalline films)	Hall / four-point probe	[25], [27], [30]
Thermal / Mechanical	Crystallization temperature (Tc)	250–550 °C typical; increases with order	DSC, in-situ XRD	[27], [34]
	Annealing effect	Improves grain growth, reduces defects	Vacuum/air annealing	[26], [29]
Chemical / Surface	Doping concentration	0–5 at. % (Al, In, Ni, La)	XPS, EDX, ICP-OES	[25], [30], [31], [35]
	Oxygen vacancies	Increase with defect formation or irradiation	XPS, PL emission	[15], [16], [33]
	Surface area (BET)	25–180 m^2/g depending on porosity	N_2 adsorption–desorption	[40], [42]
	Catalytic rate constant (k)	Enhanced with higher crystallinity (2–3×)	Photodegradation kinetics	[8], [33]

Characterization	XRD	Determines phase purity, crystallite size	Cu Kα radiation (λ = 1.5406 Å)	[15], [33],
	TEM / HRTEM	Reveals atomic lattice fringes	200–300 kV microscope	[35]
	Raman spectroscopy	Detects vibrational order/disorder	100–1500 cm^{-1} range	[33], [35]
Modeling / Computational	DFT simulations	Predicts band structure, charge density	PBE / HSE functionals	[16]

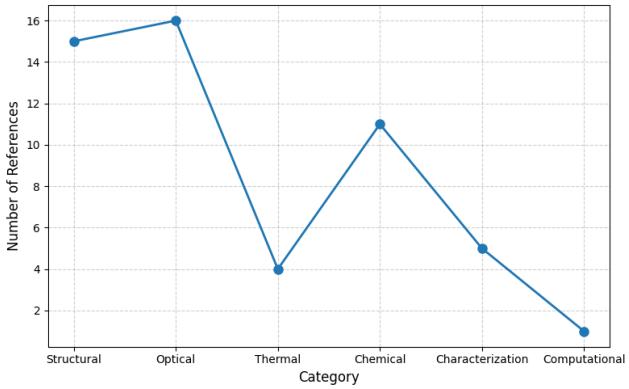

Figure 5: Distribution across crystallinity study categories

VIII. Research gaps

Although much has been achieved in the realization of the role of crystallinity in nanomaterials, there are a number of research gaps that are critical. To begin with, it is a little known how atomic-level processes control the amorphous crystal phase transition particularly when synthesizing under non-equilibrium conditions, like rapid laser annealing or chemical vapor deposition. The majority of modern research deals with the idea of the static characterization, and real-time, in situ observation of the crystallization kinetics and defects formation at the nanoscale remains insufficiently developed. Moreover, the interactions in the grain boundary dynamics, local strain and defect passivation in the determination of the charge transport and recombination losses have not been adequately modeled and experimentally verified.

Second, although a large number of studies have been conducted on individual material systems (ZnO, TiO2, or perovskites), comparative, cross-material studies on the relationship between crystallinity and common electronic and optical properties have not been done yet. The role of multi-element doping, compositional gradients and dimensional confinement on crystalline ordering and functional response is not known in detail. In addition, there are few scalable methods of synthesis with high crystallinity, low cost, and complexity, and it is harder to implement nanomaterials in electronic and optoelectronic products at scale than to incorporate materials at the smaller scale.

Lastly, in theoretical terms, the available models like DFT and molecular dynamics contain useful information but are usually limited by the size of computation and idealized assumptions. Multi-scale modeling frameworks based on machine learning that are capable of bridging between atomistic simulations and experimental observables are needed. Realistic disorder, interface effects and temperature dependent structural dynamics should be considered in such models to enhance prediction of material performance. Filling this modeling-experiment divide, as well as determining uniform crystallinity metrics, is one of the primary directions of the next-generation nanomaterials design with predictable and scalable functional qualities.

IX. Conclusion and Future Scope

In conclusion, crystallinity is a crucial factor to determine electrical and optical properties of nanomaterials, as it regulates charge transport, defect distribution, and energy band alignment. The review points out the fact that an increase in crystalline order increase carrier mobility, decrease recombination losses, and increase light-matter interactions and structural disorder create localized defect states that impede or program functionality. The knowledge of the crystallinity-property relationship, therefore, allows the rational design of nanomaterials to be used in high-performance devices. Although remarkable progress has been made in synthesis, characterization and modeling, it is still a daunting task to obtain uniform crystalline architectures in other classes and scales of materials.

Moving on, the future of crystallinity engineering would be the incorporation of modern synthesis methods and predictive modeling software. Heteroepitaxial growth, interfacial engineering, laser-assisted annealing and AI-guided simulations are some of the strategies that are likely to transform the control and scalability of crystals. The evolution of in situ and operando characterization technique also enhance the knowledge about the dynamic changes of crystal transformations in the real operating conditions. Further, integration of the experimental knowledge with data-driven solutions speeds up the identification of materials with adjustable crystallinity towards the next

generation of flexible electronics, photonics, and energy devices. Therefore, it necessary to have a multidisciplinary strategy of materials chemistry, computational modeling, and device engineering to maximize the potential of crystallinity in nanomaterial innovation.

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