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Review

The Role of Atomic-Scale Disorder in Tailoring the Functional Properties of Crystalline Materials: A Comprehensive Review

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Abstract: It has long been believed that crystalline solids will always have atomic-scale disorder, which includes vacancies, interstitials, andesite defects, local strain fields, short-range compositional changes, and amorphous pockets. The functional qualities of materials can be controlled by redefining disorder as a flexible and adjustable design parameter. Across classes of crystalline materials (oxides, chalcogenides, perovskites, semiconductors, and two-dimensional crystals), we synthesize experimental and theoretical advances demonstrate how particular types and distributions of atomic-scale disorder alter charge-carrier dynamics, optical absorption and emission, magnetic ordering, ionic conductivity, thermal transport, and mechanical response. Mechanistic relationships are highlighted, including how correlated defect complexes and local strain mediate polaron generation and carrier mobility, how interface disorder and grain-boundary structure control ion transport and catalytic activity, and how point defects alter electronic band edges and trap states. From total-scattering PDF analysis and advanced spectroscopies to aberration-corrected TEM, atom probe tomography, and scanning probe microscopies, we go over characterization tools and how data-driven models, large-scale molecular dynamics, and first-principles calculations are coming together to predict and direct disorder engineering. Successful methods for improving device performance such as defect-enabled light emission, dopant-activated ionic conductors, and disorder-stabilized phases are highlighted in case studies. We conclude with useful recommendations for intentional disorder design and point out unresolved issues, such as in-operando characterization, multiscale modelling, and controlled defect synthesis, providing a roadmap for utilizing atomic-scale disorder to develop next-generation functional materials.

Keywords: Atomic-Scale; Disorder; Properties; Crystalline materials; Defects.

1. Introduction

Crystalline materials are often idealized as perfectly periodic lattices; however, real solids inevitably contain atomic-scale disorder in the form of vacancies, interstitials, andesite defects, compositional fluctuations, and local strain fields [1]. Such disorder is not merely a structural irregularity it plays a critical role in governing phonon transport, ionic migration, carrier scattering, exciton dynamics, and magnetic interactions across semiconductors, oxides, perovskites, chalcogenides, and emerging two-dimensional crystals [2]. This shift in understanding has reframed disorder from an undesirable flaw to a functional design variable capable of tuning optical, electrical, magnetic, and catalytic properties [3].

Although numerous studies have examined isolated defect types or specific material systems, a unified understanding of how diverse forms of atomic-scale disorder influence structure property relationships remain incomplete [4]. Existing literature often focuses on material-specific phenomena, lacks cross-comparison, or relies on characterization methods that individually capture only partial aspects of disorder [5]. As a result, the broader principles linking local disorder configurations to macroscopic properties remain fragmented [6].

This challenge persists largely because atomic-scale disorder is inherently difficult to quantify. Bulk diffraction obscures short-range variations, local microscopy often lacks statistical representativeness, spectroscopic methods are chemically sensitive but spatially limited, and computational approaches face system-size and data constraints [7]. These limitations hinder predictive control of defect landscapes during synthesis and operation [8].

Recent advances provide a natural path to resolving this gap. State-of-the-art techniques such as aberration-corrected TEM, atom probe tomography, synchrotron-based scattering, and advanced spectroscopic probes combined with first-principles calculations, molecular dynamics, and machine-learning-assisted simulations now enable unprecedented access to the structural and energetic signatures of disorder [9]. Integrating these experimental and computational perspectives offers a unified framework for understanding and engineering atomic-scale disorder across crystalline materials.

The main contribution of this paper lies:

- Provides a unified review of how atomic-scale disorder influences the functional properties of crystalline materials.
- Integrates knowledge across multiple material classes (metals, ceramics, semiconductors, and functional oxides).
- Explains the mechanistic links between disorder types (vacancies, substitutions, distortions) and changes in electronic, optical, thermal, and mechanical behavior.
- Highlights how processing routes control the formation and evolution of atomic-scale disorders.
- Summarizes recent advances in characterization techniques (TEM, XRD, atom probe, spectroscopy) and computational modeling for quantifying disorder.
- Proposes a general process → disorder → microstructure → property framework for rational material design.
- Identifies emerging opportunities for tailoring high-performance materials through intentional introduction and control of disorder.

2. Types of Atomic-Scale Disorder in Crystalline Materials

One of the most basic forms of atomic-scale disorder in crystalline materials is point defects [10]. They contain vacancies, which occur when atoms are absent from their normal lattice locations. These vacancies can be mixed, cation, or anion vacancies, and they all have different

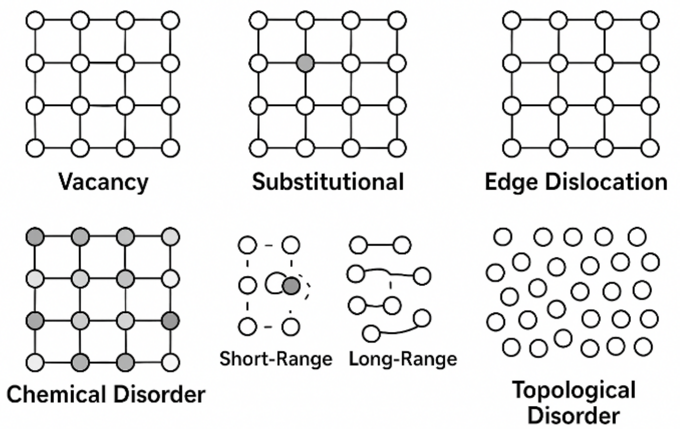

Figure 1. Schematic illustration of the types of atomic scale disorder

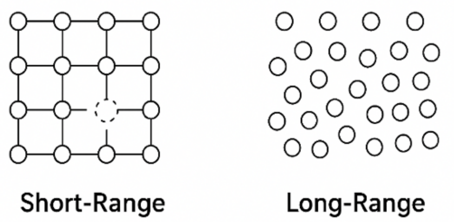

Figure 2. Visual comparison between short-range and long-range disorder.

effects on local bonding, charge balance, and carrier concentration. Atoms known as interstitials occupy ordinarily vacant regions in the crystal lattice, frequently causing local lattice distortions and altering mechanical, ionic, and electronic characteristics. Andesite defects, which can drastically change electronic structure, magnetic interactions, and optical properties, are frequently seen in ordered alloys, perovskites, and semiconductors when one atom occupies the lattice site of a different species.

When atoms in a crystal lattice are swapped out for other species, often purposefully done by dopants to modify material properties substitute disorder results [11]. Substitutions can be is valent, preserving charge neutrality, or aliovalent, adding extra charges that alter carrier concentration, defect formation, and local lattice strain, depending on the dopant's valence in relation to the host atom. Another way to categorize substitutional disorder is by spatial arrangement: ordered substitution, in which dopants occupy lattice locations in a periodic or quasi-periodic fashion, and random substitution, in which dopant atoms are dispersed randomly throughout the lattice. Substitutional disorder is a flexible tool for functional tuning because the electronic, optical, magnetic, and ionic characteristics of crystalline materials are significantly influenced by the kind and arrangement of substituted atoms.

When local lattice structure is disturbed by atomic-scale disorder, local strain fields that may span many unit cells are created, leading to disorder-induced distortions [12]. These distortions frequently show up as variations in bond lengths and angles, which modify the material's mechanical, optical, and electrical properties. These small structural changes frequently combine with other forms of disorder, including point defects or substitute atoms, and can affect charge-carrier mobility, phonon scattering, and defect interactions. Disorder-induced distortions are a crucial lever in materials design because they may be carefully controlled through doping, defect engineering, or thermal treatment to fine-tune the functional properties of crystalline solids.

The spatial extent of correlation between atomic-scale abnormalities in a crystal is referred to as short-range and long-range disorder. Ionic mobility, optical transitions, and local electronic states can all be impacted by short-range disorder, which usually involves local compositional changes such dopant or vacancy clustering within a few lattice spacings [13]. Long-range disorder, on the other hand, affects macroscopic characteristics like conductivity, mechanical strength, and magnetic ordering and is frequently linked to structural abnormalities at grain borders, interfaces, or extensive defect networks. It also spans greater distances. Since both forms of disorder interact and collectively affect a material's performance, it is crucial to comprehend and manage the balance between short-range and long-range disorder to customize the functional behavior of crystalline materials.

In Figure 1, the schematic illustration provides a concise and intuitive visualization of the various types of atomic-scale disorder discussed in the manuscript. Although these concepts are described in detail within the text, atomic-scale phenomena are often difficult to imagine without visual support. The figure helps readers from beginners to experts quickly understand how different defects differ structurally and how they can influence physical properties.

3. Characterization Techniques For Atomic-Scale Disorder

To fully comprehend atomic-scale disorder, complementing experimental and computational methods that can probe both local and long-range structural properties must be combined. Deviations from perfect periodicity are revealed by diffraction-based techniques including X-ray diffraction (XRD) and neutron scattering. Peak broadening sheds light on crystallite size and macrostrain, while diffuse scattering captures correlated disorder. When it comes to identifying structural and magnetic disorders in systems that contain light elements, neutron scattering is especially helpful. Extended X-ray absorption fine structure (EXAFS) resolves small atomic environments by providing quantitative data on bond lengths, coordination numbers, and local disorder. Atom probe tomography (APT) provides three-dimensional compositional maps to show dopant clustering and chemical inhomogeneity, while real-space imaging methods such as aberration-corrected TEM and HAADF-STEM allow direct visualization of defects, dislocations, and dopant distributions at sub-angstrom resolution. Short-range correlations that are invisible in traditional diffraction are captured by total scattering and pair distribution function (PDF) analysis. Spectroscopic techniques like Raman, IR, photoluminescence, Mössbauer, and NMR are used to further investigate bonding conditions, defect-related electrical or optical effects, and dynamic disorder. By forecasting defect energetics, evolution, and their impact on material characteristics, computational methods such as density functional theory (DFT), molecular dynamics (MD), and Monte Carlo simulations supplement observations. Thus, a multiscale framework connecting atomic-level disorder to macroscopic functional behavior is provided by the integration of diffraction, spectroscopy, microscopy, and modelling. By combining these methods, researchers can improve the trustworthiness of defect models by using direct experimental evidence to validate theoretical predictions. Cross-verification of structural characteristics that would not be identified by a single technique is also made possible by the combination of several probes.

Short-range disorder refers to small, localized disruptions in an otherwise ordered crystal lattice. Only a few neighboring atoms are displaced or missing, but the overall long-range periodicity of the material remains intact Long-range disorder occurs when disorder extends throughout the entire structure. The atomic arrangement loses periodicity over large distances, leading to a globally distorted or non-crystalline (amorphous-like) structure. A visual comparison between short-range and long-range disorder has been shown in Figure 2.

4. Role of Disorder in Tailoring Functional Properties

Atomic-scale disorder has a significant impact on the electronic characteristics of crystalline materials, affecting carrier concentration, mobility, and energy levels [14]. By introducing localized states within the bandgap and serving as charge traps or recombination centers, point defects including vacancies, interstitials, and andesite defects can alter conductivity and carrier lifetime. By using is valent or aliovalent dopants, substitutional disorder can introduce regulated impurity bands, regulate carrier density, and tailor the Fermi level. Disorder-induced lattice distortions and local strain fields can alter the electronic band structure, modifying effective masses, band edges, and mobility pathways. Additionally, short-range compositional fluctuations and grain boundary disorder affect carrier scattering and percolation pathways, which are critical in polycrystalline semiconductors. A conceptual diagram illustrating how disorder influences the functional properties of materials are shown in Figure 3.

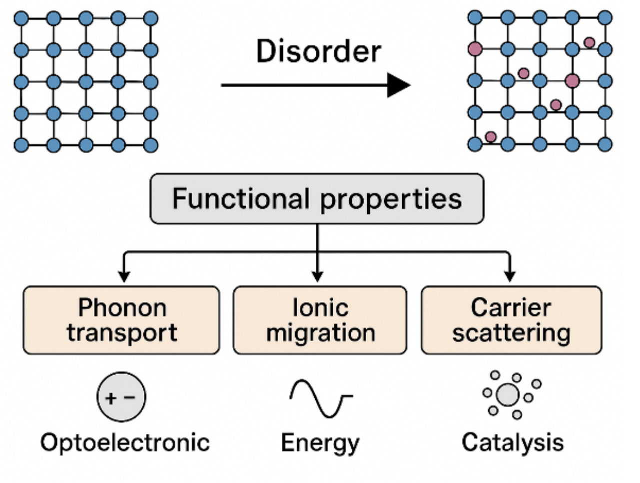

Figure 3. Conceptual diagram illustrating how disorder influences the functional properties of materials.

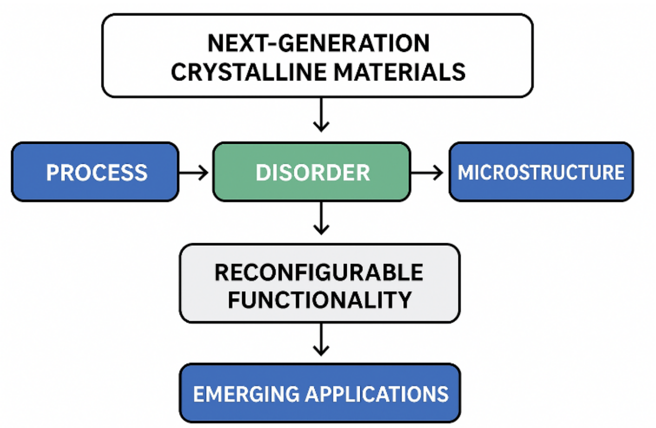

Figure 4. Visual Roadmap for Next-Generation Crystal-line Materials.

By carefully controlling the type and distribution of atomic-scale disorder, researchers can engineer materials with enhanced electronic performance, such as increased conductivity, optimized band alignment, and defect-enabled semiconducting behavior, making disorder a versatile tool in electronic materials design.

Optical properties of crystalline materials are strongly influenced by atomic-scale disorder, which can modify absorption, emission, and light–matter interaction processes [15]. Point defects, such as vacancies and interstitials, can introduce localized energy levels within the bandgap, acting as luminescent centers or nonradiative recombination sites, thereby controlling photoluminescence intensity and spectral position. Substitutional dopants can shift absorption edges, create defect-assisted emission, or induce color centers, while lattice distortions and local strain modify electronic band structures, exciton binding energies, and optical transition probabilities. Additionally, short-range disorder and compositional fluctuations can broaden absorption or emission spectra and influence light scattering, particularly in nanostructured or polycrystalline systems. By carefully engineering the type, concentration, and spatial distribution of disorder, materials can be designed for enhanced or tunable optical functionalities, including defect-mediated luminescence, bandgap modulation, and improved light-harvesting efficiency in optoelectronic and photonic applications.

Catalytic and surface properties of crystalline materials are strongly influenced by atomic-scale disorder, which can create active sites, modify adsorption energies, and alter reaction pathways. Point defects, such as vacancies and interstitials, often serve as high-energy sites that enhance catalytic activity by facilitating reactant binding and charge transfer. Substitutional dopants can tune the electronic structure of surface atoms, modulating catalytic selectivity and reaction kinetics. Lattice distortions, local strain, and compositional fluctuations can modify surface energies, defect formation energies, and electronic density at active sites, influencing both heterogeneous and electrocatalytic processes. In addition, grain boundaries and interface disorder provide unique structural motifs that are often more reactive than the bulk lattice. By deliberately engineering the type, concentration, and distribution of atomic-scale disorder, researchers can enhance surface reactivity, improve catalyst stability, and design materials with tailored selectivity, making disorder a key parameter in optimizing catalytic performance and surface-related functionalities.

5. Case Studies and Recent Advances

Material-specific examples illustrate how atomic-scale disorder can be purposefully exploited to tailor functional properties [16]. In oxide semiconductors such as ZnO, In_2O_3, and TiO_2, defect engineering including control over oxygen vacancies, cation interstitials, and dopant distribution enables simultaneous tuning of electrical conductivity and optical transparency, critical for transparent conducting oxides and optoelectronic devices. In perovskites, both halide and oxide types, control disorder at the atomic scale, including halide or cation vacancies and local lattice distortions, plays a crucial role in stability, charge-carrier dynamics, and optoelectronic performance, affecting photovoltaic efficiency and light-emitting properties. Transition metal dichalcogenides (TMDs) exhibit strong sensitivity to vacancy-induced disorder, where sulfur or metal vacancies can modulate electronic structure, enhance catalytic activity, and influence carrier mobility. These examples demonstrate that disorder is not merely an imperfection but a versatile design tool, enabling precise control over electronic, optical, and catalytic functionalities across diverse classes of crystalline materials. Advanced material classes further illustrate the functional role of atomic-scale disorder. In high-entropy alloys (HEAs), inherent atomic disorder arising from the random distribution of multiple principal elements on lattice sites acts as a fundamental design principle, enhancing mechanical strength, thermal stability, and corrosion resistance [17]. Disorders in HEAs also modifies electronic and magnetic properties, offering a pathway to multifunctional materials. In thermoelectric materials such as SnSe and skutterudites, atomic-scale disorder enhances phonon scattering, effectively reducing lattice thermal conductivity while preserving or improving electronic transport. This selective scattering improves the thermoelectric figure of merit (ZT), demonstrating how controlled disorder can optimize energy conversion efficiency [18]. These examples underscore that both intrinsic and engineered disorder can be deliberately leveraged to achieve superior functional performance across diverse material systems.

One visual roadmap has been providing for Next-Generation Crystalline Materials in Figure 4. The graphic roadmap offers a clear, step-by-step summary of how atomic-scale disorder can be intentionally controlled to build next-generation crystalline materials. It helps readers comprehend how each step contributes to property tuning and technical growth by highlighting the logical progression from processing settings to final material uses.

6. Theoretical Insights and Computational Approaches

Computational approaches play a crucial role in understanding and predicting the effects of atomic-scale disorder on material properties. Modelling disorder at the atomic scale can be achieved using supercell approaches, which explicitly include defects or dopants in a periodically repeated lattice, or special Quirino structures (SQS), which statistically mimic the random distribution of multiple species. First-principles simulations, such as density functional theory (DFT), enable detailed analysis of disorder property correlations, revealing how specific defects or local distortions influence electronic, optical, magnetic, and thermal behavior [19]. Recently, machine learning (ML) methods have emerged as powerful tools for predicting defect formation energies, mapping local structure property relationships, and guiding materials design with large datasets. By integrating traditional simulations with data-driven approaches, researchers can accelerate the identification and engineering of atomic-scale disorder to achieve targeted functional properties in complex crystalline materials [20].

Computational modelling and machine learning approaches provide powerful tools for understanding, predicting, and designing atomic-scale disorders in crystalline materials. One common strategy is the supercell approach, where a finite-size periodic cell explicitly includes defects, dopants, or vacancies [21]. This allows direct simulation of local lattice relaxations, electronic structure changes, and defect–defect interactions. For systems with high compositional complexity or random disorder, special Querandí structures (SQS) are used to statistically mimic the distribution of multiple atomic species while preserving average structural properties, enabling efficient simulations without requiring prohibitively large cells.

First-principles simulations, primarily based on density functional theory (DFT), allow quantitative evaluation of defect formation energies, electronic band structure modifications, charge localization, and magnetic interactions arising from disorder [22]. Combined with molecular dynamics (MD), these methods can capture temperature-dependent defective behavior, lattice vibrations, and dynamic disorder. Monte Carlo simulations provide additional insights into thermodynamic stability, defect clustering, and phase evolution in complex systems. ML models trained on high-fidelity simulation data can predict defect energetics, identify likely configurations of disordered atoms, and establish disorder–property correlations across large compositional and structural spaces [23]. These approaches allow researchers to screen materials and optimize functional properties without exhaustive first-principles calculations.

7. Challenges and Future Directions

Challenges and future perspectives in the study and engineering of atomic-scale disorder revolve around several key aspects. First, characterization challenges remain significant, particularly in distinguishing between similar defect types, identifying their precise location, and quantifying their concentration. Second, controlled synthesis is critical for translating insights into functional materials, requiring precise manipulation of defect density, type, and spatial distribution. A third challenge is correlating local disorder to macroscopic performance, which demands multiscale approaches linking atomic-level defects to electronic, optical, thermal, or catalytic behavior. Recent advances in artificial intelligence (AI) and high-throughput computational or experimental methods offer promising pathways to accelerate defect discovery, prediction, and optimization, enabling systematic defect engineering [24]. Finally, disorder in quantum materials presents unique opportunities: engineered atomic-scale defects and local disorder can stabilize superconductivity, enable topological phases, and manipulate spintronic properties, highlighting the potential of disorder as a design principle in next-generation quantum technologies. Addressing these challenges will require the integration of advanced synthesis, multiscale characterization, computational modelling, and data-driven design to fully harness the functional potential of atomic-scale disorder.

8. Conclusion

Atomic-scale disorder should no longer be viewed as a drawback in crystalline materials; rather, it represents a powerful lever for tailoring material functionality. By understanding how vacancies, interstitials, substitutional dopants, lattice distortions, and local strain influence electronic, optical, magnetic, catalytic, and mechanical properties, researchers can deliberately engineer disorder to achieve desired performance. Harnessing disorder opens new pathways for the design of next-generation semiconductors, energy materials, and quantum devices, including superconductors, topological phases, and spintronic systems. Realizing this potential requires integrated efforts combining advanced synthesis techniques, in-situ and multimodal characterization, and predictive computational modeling, supported by data-driven approaches and high-throughput screening. With these strategies, atomic-scale disorder can be transformed from a perceived limitation into a guiding principle for the rational design of functional crystalline materials.

9. Declarations

9.1. Author Contributions

Md Sultanur Rahman reviewed relevant journal papers and collected information. **Md Jasim Uddin** reviewed relevant journal papers and combined all information. **Md Sultanur Rahman** and **Md Jasim Uddin** wrote this manuscript together and made final draft. **Rakib Hasan** and **Md Mehedi Hasan Mia** revised it and make final version of manuscript.

9.2. Institutional Review Board Statement

Not applicable.

9.3. Informed Consent Statement

Not applicable.

9.4. Data Availability Statement

We wrote this manuscript by reviewing others manuscript which are added in reference section.

9.5. Acknowledgment

Not applicable.

9.6. Conflicts of Interest

The authors declare no conflicts of interest.

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