Unifying Grain Boundary Networks and Crystal Graphs: A HyperGraph and SuperHyperGraph Perspective in Material Sciences

Abstract

Graph theory provides a foundation for modeling relationships among discrete elements via vertices and edges [26, 27]. HyperGraphs extend this framework by allowing edges—hyperedges—to join more than two vertices, while superhypergraphs introduce nested powerset layers to capture hierarchical and self-referential connections. Network analogues—hypernetworks and superhypernetworks—apply these ideas to empirical data structures.

In materials science, graph-based models such as Grain Boundary Networks represent grains as vertices and their interfaces as edges [31,100,106], whereas Crystal Graphs encode atoms and bonds within lattice structures [95,104,129]. These representations, however, lack the capacity to describe multi-scale and hierarchical features inherent in complex microstructures.

This paper investigates the theoretical foundations of hypergraphs and superhypergraphs in materials science, which generalize classical graphs by enabling hyperedges, superedges, or supervertices to simultaneously connect multiple vertices. It further examines the relevance of graph-theoretical approaches in material sciences by introducing and formalizing the concepts of Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs. For each structure, we provide precise mathematical definitions, construct detailed examples based on polycrystalline and crystalline material systems, and analyze fundamental properties such as multi-level connectivity, nesting depth, and combinatorial complexity. By integrating hyperstructure theory with the modeling of material architectures, this work establishes a robust framework for multi-scale and hierarchical analysis in materials science.

Keywords: SuperHyperGraph, HyperGraph, Crystal graphs, HyperNetworks, SuperHyperNetworks, Grain Boundary Networks

1 Introduction

1.1 Basic Graph Theory

Graph theory is a branch of mathematics that studies networks in which nodes (called vertices) are connected by links (called edges) [26, 27]. Graphs have been extensively explored and applied across a wide range of disciplines, including social sciences [83, 89], chemical graph theory [35, 53, 124], biological networks [56,57,82,128],graph neural networks (GNNs) [52,62], and telecommunications [105]. Given the wide range of applications, research in graph theory is of great importance.

1.2 HyperGraph Theory and SuperHyperGraph Theory

This paper focuses on the frameworks of HyperGraph Theory and SuperHyperGraph Theory. Related to these structures are the broader mathematical concepts of *hyperstructures* and *superhyperstructures*, which extend classical mathematical systems using power set constructions and their n-th iterated forms (cf. [117–119]). These extended frameworks are particularly well-suited for modeling hierarchical and multi-layered systems, both in abstract theoretical formulations and in practical applications. Examples of such generalizations include:

- *Superhyperalgebra* [50, 71, 116], which extends classical algebraic structures to allow nested algebraic operations;
- *Superhyperfuzzy sets* [48, 49], which generalize fuzzy sets to represent complex uncertainty across multiple hierarchical levels;
- *Superhyperneutrosophic sets* [39, 112], which incorporate indeterminacy and higher-order logic into neutrosophic frameworks.

These developments illustrate how the principles underlying hypergraphs and superhypergraphs can be extended to a wide range of mathematical domains, providing expressive tools for modeling nested, interconnected, and multi-scale systems.

The overview of Classical Structure, Hyperstructure, and n-Superhyperstructure is presented in Table 1. Here, n is assumed to be a natural number.

Concept	Notation	Underlying Set	Operation	Key Feature
Classical Structure	$(H, \{\#_0\})$	H	$\#_0 : H^m \to H$	Single-valued operations satisfying algebraic axioms
Hyperstructure	$(\mathcal{P}(S), \circ)$	$\mathcal{P}(S)$	$\circ : S \times S \to \mathcal{P}(S)$ extended to $\mathcal{P}(S) \times \mathcal{P}(S)$	Operations yield sets of results (multi-valued)
n-Superhyperstructure	$(\mathcal{P}^n(S), \circ)$	$\mathcal{P}^n(S)$	$\circ : \mathcal{P}^n(S) \times \mathcal{P}^n(S) \to \mathcal{P}^n(S)$	Hierarchical, nested operations via iterated powersets

Table 1: Overview of Classical Structure, Hyperstructure, and n-Superhyperstructure

When applied to graph theory, these extensions yield two well-known generalizations: the *hypergraph* and the *superhypergraph* [33, 43, 44]. A hypergraph allows each edge—known as a *hyperedge*—to connect more than two vertices simultaneously, enabling the representation of complex many-to-many relationships [13, 15, 29]. A superhypergraph builds upon this by incorporating recursively nested powerset structures, allowing for hierarchical and self-referential interactions among groups of hyperedges.

The overview of Graph, HyperGraph, and SuperHyperGraph is presented in Table 2. Here, n is assumed to be a natural number.

Concept	Notation	Edge Connectivity	Structural Extension
Graph	$G = (V, E)$	$E \subseteq \{\{u, v\} \mid u, v \in V,\ u \neq v\}$ (binary edges)	Standard graph: edges join exactly two vertices.
HyperGraph	$H = (V, E)$	$E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ (hyperedges)	Generalizes edges to connect any nonempty subset of vertices.
SuperHyperGraph	$\mathrm{SHT}^{(n)} = (V, E)$	$V, E \subseteq \mathcal{P}^n(V_0)$ (supervertices/edges)	Uses n-fold iterated powersets to model hierarchical, nested connectivity among edges.

Table 2: Overview of Graph, HyperGraph, and SuperHyperGraph

And graphs are commonly used to represent networks, and in this context, *hypernetworks* and *superhypernetworks* emerge as the network counterparts of hypergraphs and superhypergraphs, respectively (cf. [40, 64]). In addition to hypernetworks and superhypernetworks, many other types of networks have been proposed in the literature, including MultiNetworks [23, 28, 51] and Directed Networks [86, 91, 134]. These variations likely reflect the versatility and broad applicability of network-based modeling across numerous disciplines.

The overview of Network, HyperNetwork, and SuperHyperNetwork is presented in Table 3.

1.3 Graph and Network in Material Sciences

Material Theory is the study of fundamental principles governing material properties, structures, and behaviors using mathematical and computational models [18, 19, 78, 90]. Graph and network representations are widely utilized in materials theory to model structural and physical properties of materials. In this paper, we focus on two key examples: the Grain Boundary Network and the Crystal Graph.

A Grain Boundary Network models polycrystalline structures by representing grains as nodes and their shared interfaces as edges, capturing both topological and geometric features of the material [31, 100, 106]. A Crystal Graph represents atoms as nodes and interatomic bonds as edges, defined by spatial proximity within a periodic

Concept	Notation	Edge Connectivity	Structural Extension
Network	$\mathcal{N} = (V, E, W, \ldots)$	$E \subseteq \{\{u, v\} \mid u, v \in V\}$ (pairwise links)	Standard network/graph: supports weights, directions, multiplex layers.
HyperNetwork	$\mathcal{HN} = (V, \mathcal{E}, w)$	$\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ (hyperedges)	Generalizes networks to multi-party interactions via hyperedges.
SuperHyperNetwork	$\mathrm{SHN}^{(n)} = (V^{(n)}, \mathcal{E}^{(n)}, w^{(n)})$	$V^{(n)}, \mathcal{E}^{(n)} \subseteq \mathcal{P}^n(V_0)$ (nested super-nodes/edges)	Models hierarchical, multi-scale structures through iterated powersets.

Table 3: Overview of Network, HyperNetwork, and SuperHyperNetwork

crystal lattice [95, 104, 129]. This structure encodes the local coordination environment essential for predicting material properties.

In addition to these, several other graph-based frameworks are well known in materials theory, including Diffusion Networks [30], Dislocation Networks [6, 123], and Fracture Networks [1, 17], each providing insights into specific physical mechanisms.

1.4 Our Contribution

This subsection outlines the main contributions of the present paper. Given the above, it is evident that there is a profound connection between graph theory and materials science, and that research at this intersection is of significant importance. Accordingly, we define the concepts of Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs, and examine several concrete examples along with their mathematical properties. It should be noted that this paper does not include any experimental investigation; our work is purely theoretical in nature. Through these contributions, we aim to advance the study of Grain Boundary Networks, Crystal Graphs, and graph theory as a whole, even if only in a modest capacity.

1.5 Structure of This Paper

This subsection briefly outlines the contents of the paper. Section 2 introduces the mathematical foundations of Classical Structures, Hyperstructures, and n-Superhyperstructures, along with concise definitions of Graphs, HyperGraphs, SuperHyperGraphs, HyperNetworks, SuperHyperNetworks, Crystal Graphs, and Grain Boundary Networks. Section 3 presents illustrative examples and fundamental properties of Grain Boundary HyperNetworks. Section 4 explores examples and structural features of Grain Boundary SuperHyperNetworks. Section 5 investigates examples and mathematical properties of Crystal SuperHyperGraphs. Section 6 concludes the paper with a summary and discusses directions for future research.

2 Preliminaries and Definitions

This section provides an overview of the fundamental concepts and definitions essential for the discussions in this paper. Throughout the paper, we assume all graphs are simple, undirected, and finite.

2.1 Classical Structure, Hyperstructure, and n-Superhyperstructure

A *Classical Structure* represents a general mathematical concept, while a *Hyperstructure* can be defined using the power set, and an *n-Superhyperstructure* can be defined using the n-th powerset [120]. Intuitively, the n-th powerset is a repeated application of the powerset operation. Relevant definitions and simple examples are provided below.

Definition 2.1 (Set)**.** [76] A *set* is a well-defined collection of distinct objects, called elements. A set is usually denoted by capital letters such as A, B, S, etc.

Definition 2.2 (Subset)**.** [76] Let A and B be sets. We say A is a *subset* of B, written $A \subseteq B$, if every element of A is also an element of B.

Definition 2.3 (Empty Set)**.** [76] The *empty set*, denoted by $\emptyset$, is the unique set that contains no elements.

Definition 2.4 (Universal Set)**.** A *universal set*, denoted by U, is the set that contains all elements under consideration in a particular context or discussion.

Definition 2.5 (Base Set)**.** A *base set* S is the foundational set from which complex structures such as powersets and hyperstructures are derived. It is formally defined as:

$$S = \{x \mid x \text{ is an element within a specified domain}\}.$$

All elements in constructs like $\mathcal{P}(S)$ or $\mathcal{P}_n(S)$ originate from the elements of S.

Definition 2.6 (Powerset)**.** [37, 101] The *powerset* of a set S, denoted $\mathcal{P}(S)$, is the collection of all possible subsets of S, including both the empty set and S itself. Formally, it is expressed as:

$$\mathcal{P}(S) = \{A \mid A \subseteq S\}.$$

Example 2.7 (Material Science Powerset of Composite Phases)**.** Material phases are distinct physical forms in a material system, such as solid, liquid, gas, or structural components like fibers (cf. [55, 65, 70]). Let the set of fundamental material phases be

$$S = \{\text{Fiber, Matrix, Void}\}.$$

Then the powerset $\mathcal{P}(S)$ consists of all possible phase combinations:

$$\mathcal{P}(S) = \big\{\emptyset, \{\text{Fiber}\}, \{\text{Matrix}\}, \{\text{Void}\}, \{\text{Fiber, Matrix}\}, \{\text{Fiber, Void}\}, \{\text{Matrix, Void}\}, \{\text{Fiber, Matrix, Void}\}\big\}.$$

- $\emptyset$ represents an absence of material (idealized pore).
- {Fiber}, {Matrix}, {Void} correspond to single-phase regions.
- {Fiber, Matrix} represents fiber–matrix interfaces.
- {Fiber, Void} models fiber debonding or pull-out regions.
- {Matrix, Void} captures porosity within the matrix.
- {Fiber, Matrix, Void} describes three-phase junctions critical for damage initiation.

This enumeration provides a rigorous framework for analyzing every possible microstructural feature in a fiber-reinforced composite.

Definition 2.8 (n-th Powerset)**.** (cf. [37, 120])

The n-th powerset of a set H, denoted $P_n(H)$, is defined iteratively, starting with the standard powerset. The recursive construction is given by:

$$P_1(H) = P(H), \quad P_{n+1}(H) = P(P_n(H)), \quad \text{for } n \geq 1.$$

Similarly, the n-th non-empty powerset, denoted $P_n^*(H)$, is defined recursively as:

$$P_1^*(H) = P^*(H), \quad P_{n+1}^*(H) = P^*(P_n^*(H)).$$

Here, $P^*(H)$ represents the powerset of H with the empty set removed.

Example 2.9 (Hierarchical Material Microstructures via n-th Powerset)**.** Let $H = \{\text{Fiber, Matrix, Void}\}$ denote the set of fundamental phases in a composite material. By Definition, the first powerset is

$$P_1(H) = \big\{\emptyset, \{\text{Fiber}\}, \{\text{Matrix}\}, \{\text{Void}\}, \{\text{Fiber, Matrix}\}, \{\text{Fiber, Void}\}, \{\text{Matrix, Void}\}, H\big\}.$$

The second powerset

$$P_2(H) = P\big(P_1(H)\big)$$

comprises all subsets of $P_1(H)$. For instance:

$$\big\{\{\text{Fiber}\}, \{\text{Matrix}\}\big\}, \quad \big\{\{\text{Fiber, Matrix}\}, \{\text{Void}\}\big\}, \quad \big\{\{\text{Fiber}\}, \{\text{Matrix, Void}\}, H\big\}, \ \ldots$$

An element $X \in P_2(H)$ represents a second-level motif clustering multiple phase combinations—e.g., one cluster might group the fiber–matrix interaction with void inclusions. More generally, an element of $P_n(H)$ models an n-level hierarchical assembly of material features, from individual phases ($n = 1$) up to macroscopic composite architecture (n large), thus providing a rigorous framework for multi-scale microstructure analysis.

Definition 2.10 (Classical Structure)**.** (cf. [108, 120]) A *Classical Structure* is a mathematical framework defined on a non-empty set H, equipped with one or more *Classical Operations* that satisfy specified *Classical Axioms*. Specifically:

A *Classical Operation* is a function of the form:

$$\#_0 : H^m \to H,$$

where $m \geq 1$ is a positive integer, and H^m denotes the m-fold Cartesian product of H. Common examples include addition and multiplication in algebraic structures such as groups, rings, and fields.

Definition 2.11 (Hyperoperation)**.** (cf. [99,125–127]) A *hyperoperation* is a generalization of a binary operation where the result of combining two elements is a set, not a single element. Formally, for a set S, a hyperoperation $\circ$ is defined as:

$$\circ : S \times S \to \mathcal{P}(S),$$

where $\mathcal{P}(S)$ is the powerset of S.

Definition 2.12 (Hyperstructure)**.** (cf. [37, 108, 120]) A *Hyperstructure* extends the notion of a Classical Structure by operating on the powerset of a base set. Formally, it is defined as:

$$\mathcal{H} = (\mathcal{P}(S), \circ),$$

where S is the base set, $\mathcal{P}(S)$ is the powerset of S, and $\circ$ is an operation defined on subsets of $\mathcal{P}(S)$. Hyperstructures allow for generalized operations that can apply to collections of elements rather than single elements.

Example 2.13 (Oxidation Hyperstructure of Iron)**.** Oxidation of iron is a chemical reaction where iron reacts with oxygen, forming iron oxide, commonly known as rust (cf. [16,22,25]). In materials science, the oxidation of iron produces multiple oxide phases. We model this as a hyperstructure.

Base set of species:

$$S = \{\ \mathrm{Fe},\ \mathrm{O_2}\}.$$

Hyperoperation $\circ$: Define

$$\circ : S \times S \ \longrightarrow\ \mathcal{P}(S'),$$

where $S' = \{\mathrm{FeO},\ \mathrm{Fe_2O_3},\ \mathrm{Fe_3O_4}\}$ is the set of iron oxides. On pure reagents:

$$\mathrm{Fe}\ \circ\ \mathrm{O_2} = \{\mathrm{FeO},\ \mathrm{Fe_2O_3},\ \mathrm{Fe_3O_4}\}, \quad a \circ b = \{a\}, \{b\} \text{ if no reaction occurs.}$$

Extend $\circ$ to mixtures by

$$A\ \circ\ B = \bigcup_{a \in A,\ b \in B} (a \circ b), \quad A, B \subseteq S.$$

Hyperstructure $\mathcal{H}$: We then form the hyperstructure

$$\mathcal{H} = \big(\mathcal{P}(S),\ \circ\big),$$

whose domain is the powerset $\mathcal{P}(S) = \{\emptyset, \{\mathrm{Fe}\}, \{\mathrm{O_2}\}, \{\mathrm{Fe}, \mathrm{O_2}\}\}$.

Concrete computations:

$$\{\mathrm{Fe}\} \circ \{\mathrm{O_2}\} = \{\mathrm{FeO},\ \mathrm{Fe_2O_3},\ \mathrm{Fe_3O_4}\},$$
$$\{\mathrm{Fe}, \mathrm{O_2}\} \circ \{\mathrm{O_2}\} = (\mathrm{Fe} \circ \mathrm{O_2}) \cup (\mathrm{O_2} \circ \mathrm{O_2}) = \{\mathrm{FeO}, \mathrm{Fe_2O_3}, \mathrm{Fe_3O_4}\}.$$

Thus $\mathcal{H}$ models the real-world oxidation behavior of iron: combining iron and oxygen can yield several oxide phases, and mixtures of reagents yield the union of all possible products within the hyperstructure framework.

Definition 2.14 (SuperHyperOperations)**.** (cf. [120]) Let H be a non-empty set, and let $\mathcal{P}(H)$ denote the powerset of H. The n-th powerset $\mathcal{P}^n(H)$ is defined recursively as follows:

$$\mathcal{P}^0(H) = H, \quad \mathcal{P}^{k+1}(H) = \mathcal{P}(\mathcal{P}^k(H)), \quad \text{for } k \geq 0.$$

A *SuperHyperOperation* of order (m, n) is an m-ary operation:

$$\circ^{(m,n)} : H^m \to \mathcal{P}^n_*(H),$$

where $\mathcal{P}^n_*(H)$ represents the n-th powerset of H, either excluding or including the empty set, depending on the type of operation:

- If the codomain is $\mathcal{P}^n_*(H)$ excluding the empty set, it is called a *classical-type* (m, n)*-SuperHyperOperation*.
- If the codomain is $\mathcal{P}^n(H)$ including the empty set, it is called a *Neutrosophic* (m, n)*-SuperHyperOperation*.

These SuperHyperOperations are higher-order generalizations of hyperoperations, capturing multi-level complexity through the construction of n-th powersets.

Definition 2.15 (n-Superhyperstructure)**.** (cf. [38, 41, 120]) An *n-Superhyperstructure* further generalizes a Hyperstructure by incorporating the n-th powerset of a base set. It is formally described as:

$$\mathcal{SH}_n = (\mathcal{P}_n(S), \circ),$$

where S is the base set, $\mathcal{P}_n(S)$ is the n-th powerset of S, and $\circ$ represents an operation defined on elements of $\mathcal{P}_n(S)$. This iterative framework allows for increasingly hierarchical and complex representations of relationships within the base set.

Example 2.16 (2-Superhyperstructure in a Multi-phase Alloy Microstructure)**.** Let $S = \{\alpha, \beta, \gamma\}$ be the set of primary phases in a ternary alloy. Then

$$\mathcal{P}^1(S) = \big\{\{\alpha\}, \{\beta\}, \{\gamma\}, \{\alpha, \beta\}, \{\alpha, \gamma\}, \{\beta, \gamma\}, \{\alpha, \beta, \gamma\}\big\},$$

and

$$\mathcal{P}^2(S) = \mathcal{P}\big(\mathcal{P}^1(S)\big).$$

We define the 2-superhyperstructure

$$\mathcal{SH}_2 = \big(\mathcal{P}^2(S), \circ\big) \quad \text{with} \quad \circ = \cup.$$

Choose two 2-superelements (each a set of phase-sets):

$$U = \big\{\{\alpha, \beta\}, \{\beta, \gamma\}\big\}, \quad V = \big\{\{\alpha, \gamma\}, \{\beta, \gamma\}\big\}.$$

Their product under $\circ$ is

$$U \circ V = U \cup V = \big\{\{\alpha, \beta\}, \{\beta, \gamma\}, \{\alpha, \gamma\}\big\} \in \mathcal{P}^2(S),$$

which corresponds to the set of all binary phase interfaces in the alloy.

2.2 SuperHyperGraph

In classical graph theory, a hypergraph extends the idea of a conventional graph by permitting edges—called hyperedges—to join more than two vertices. This broader framework enables the modeling of more intricate relationships between elements, thereby enhancing its utility in various fields [13,29,59,60]. A *SuperHyperGraph* is an advanced extension of the hypergraph concept, integrating recursive powerset structures into the classical model. This concept has been recently introduced and extensively studied in the literature [39,40,45,115]. Note that n in an n-SuperHyperGraph is an integer. The definitions and examples of these concepts are presented below.

Definition 2.17 (Graph)**.** [20, 27] A *graph* $G = (V, E)$ consists of a finite set V of vertices and a set $E \subseteq \{\{u, v\} \mid u, v \in V,\ u \neq v\}$ of edges, where each edge connects a pair of distinct vertices.

Definition 2.18 (Subgraph)**.** [26, 27] Let $G = (V, E)$ be a graph. A *subgraph* $G' = (V', E')$ of G satisfies $V' \subseteq V$ and $E' \subseteq \{\{u, v\} \in E \mid u, v \in V'\}$. That is, G' consists of a subset of vertices and the edges of G induced by them.

Definition 2.19 (HyperGraph)**.** [13, 15] A *hypergraph* $H = (V(H), E(H))$ consists of:

- A nonempty set $V(H)$ of vertices.
- A set $E(H)$ of hyperedges, where each hyperedge is a nonempty subset of $V(H)$, thereby allowing connections among multiple vertices.

Unlike standard graphs, hypergraphs are well-suited to represent higher-order relationships. In this paper, we restrict ourselves to the case where both $V(H)$ and $E(H)$ are finite.

Example 2.20 (Grain Triple-Junction HyperGraph in Polycrystalline Materials)**.** In a polycrystalline metal, grains meet along boundaries and at *triple junctions* where three grains intersect. We model this as a hypergraph $H = (V(H), E(H))$:

$$V(H) = \{\ G_1,\ G_2,\ G_3,\ G_4\ \},$$

where each G_i is a grain.

$$E(H) = \big\{e_1 = \{G_1, G_2, G_3\}, \quad e_2 = \{G_2, G_3, G_4\}\big\},$$

where

- e_1 represents the triple junction where grains G_1, G_2, and G_3 meet,
- e_2 represents the triple junction where grains G_2, G_3, and G_4 meet.

This hypergraph captures the higher-order topology of the grain structure:

$$G_1 \ - \ G_2 \ - \ G_3 \quad (\text{junction } e_1), \qquad G_2 \ - \ G_3 \ - \ G_4 \quad (\text{junction } e_2).$$

Unlike a standard graph, which would represent only pairwise grain boundaries, this hypergraph directly encodes the three-grain intersections essential for understanding grain growth, diffusion pathways, and mechanical behavior at triple junctions.

Definition 2.21 (n-SuperHyperGraph)**.** [114, 115]
Let V_0 be a finite base set of vertices. For each integer $k \geq 0$, define the iterative powerset by

$$\mathcal{P}^0(V_0) = V_0, \quad \mathcal{P}^{k+1}(V_0) = \mathcal{P}(\mathcal{P}^k(V_0)),$$

where $\mathcal{P}(\cdot)$ denotes the usual powerset operation. An *n-SuperHyperGraph* is then a pair

$$\mathrm{SHT}^{(n)} = (V, E),$$

with

$$V \subseteq \mathcal{P}^n(V_0) \quad \text{and} \quad E \subseteq \mathcal{P}^n(V_0).$$

Each element of V is called an *n-supervertex* and each element of E an *n-superedge*.

Example 2.22 (Real-World Example of a 2-SuperHyperGraph)**.** Consider the hierarchical microstructure [81,92] of a polycrystalline alloy used in aerospace components. Let the base set of "grains" be

$$V_0 = \{\mathrm{G}_1, \mathrm{G}_2, \ldots, \mathrm{G}_m\},$$

where each G_i is an individual crystal grain. We construct the following iterated powersets:

$$\mathcal{P}^1(V_0) = \{\{\mathrm{G}_i\}, \{\mathrm{G}_i, \mathrm{G}_j\}, \ldots\}, \quad \mathcal{P}^2(V_0) = \mathcal{P}\big(\mathcal{P}^1(V_0)\big).$$

We now define a 2-SuperHyperGraph

$$\mathrm{SHT}^{(2)} = (V, E),$$

where:

- $V \subseteq \mathcal{P}^2(V_0)$ is the set of *2-supervertices*, each representing a cluster of interacting grain-clusters. For example,
$$v_1 = \big\{\{\mathrm{G}_1, \mathrm{G}_2\}, \{\mathrm{G}_2, \mathrm{G}_3\}\big\}, \quad v_2 = \big\{\{\mathrm{G}_4, \mathrm{G}_5\}, \{\mathrm{G}_5, \mathrm{G}_6\}\big\}.$$
- $E \subseteq \mathcal{P}^2(V_0)$ is the set of *2-superedges*, each representing a higher-order interaction among these grain-cluster pairs. For instance,
$$e_1 = \big\{\{\{\mathrm{G}_1, \mathrm{G}_2\}, \{\mathrm{G}_2, \mathrm{G}_3\}\}, \{\{\mathrm{G}_4, \mathrm{G}_5\}, \{\mathrm{G}_5, \mathrm{G}_6\}\}\big\},$$
models coupling between two neighboring grain-clusters under applied stress.

Here, each element of v_i is itself a set of grains (a 1-supervertex), and each element of e_j is a set of such 1-supervertices. This 2-SuperHyperGraph captures not only which grains interact locally (via 1-superedges) but also how those local interactions group together at a higher structural level (via 2-superedges), reflecting the multi-scale connectivity in the alloy's microstructure.

2.3 Hypernetwork and *n*-SuperHypernetwork

A hypernetwork extends graphs by allowing hyperedges to connect multiple nodes, modeling complex multi-way relationships between entities. An n-SuperHypernetwork uses nested powersets of nodes to represent hierarchical multi-level interactions and groupings in complex systems. The definitions and examples of these concepts are presented below.

Definition 2.23 (Network)**.** A *network* (or *graph*) is an ordered triple

$$N = \big(V,\ E,\ w\big)$$

where

- V is a nonempty finite set of *vertices* (or *nodes*);
- $E \subseteq \big\{\{u, v\} \mid u, v \in V,\ u \neq v\big\}$ is the set of *undirected edges*, each joining two distinct vertices;
- $w\colon E \longrightarrow \mathbb{R}_{\geq 0}$ is a *weight function* assigning a nonnegative real weight to each edge (omitted if unweighted).

If edges are *directed*, one instead writes

$$N = \big(V,\ A,\ w\big), \quad A \subseteq V \times V,$$

and each $(u, v) \in A$ is an *arc* from u to v. In either case, one may also include an optional *vertex-labeling* $\ell_V : V \longrightarrow L_V$ to record vertex types.

Definition 2.24 (Hypernetwork)**.** (cf. [4,21,40,63]) A *hypernetwork* is an ordered triple

$$H = \big(V,\ \mathcal{E},\ w\big)$$

where

- V is a nonempty finite set of *nodes*;
- $\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ is the set of *hyperedges*, each hyperedge $e \in \mathcal{E}$ being a nonempty subset of nodes (allowing multi-node interactions);
- $w: \mathcal{E} \to \mathbb{R}_{\geq 0}$ is a *weight or attribute function* on hyperedges (omitted if unweighted).

A *directed hypernetwork* may be defined by replacing $\mathcal{E} \subseteq \mathcal{P}(V)$ with a set of *ordered* tuples of nodes or by equipping each $e \in \mathcal{E}$ with a head-tail partition. One can further add a *node-labeling* $\ell_V : V \to L_V$ and a *hyperedge-labeling* $\ell_{\mathcal{E}} : \mathcal{E} \to L_{\mathcal{E}}$ to record types or properties.

Example 2.25 (Hypernetwork of Grain Boundaries and Triple Junctions)**.** Consider a small region of a polycrystalline alloy with four grains labeled

$$V = \{\mathrm{G}_1, \mathrm{G}_2, \mathrm{G}_3, \mathrm{G}_4\}.$$

We model the network of grain-boundary interactions as a hypernetwork $H = (V, \mathcal{E}, w)$ where:

$$\mathcal{E} = \big\{ \{\mathrm{G}_1, \mathrm{G}_2\},\ \{\mathrm{G}_2, \mathrm{G}_3\},\ \{\mathrm{G}_3, \mathrm{G}_4\},\ \{\mathrm{G}_1, \mathrm{G}_2, \mathrm{G}_3\},\ \{\mathrm{G}_2, \mathrm{G}_3, \mathrm{G}_4\} \big\},$$

and the weight function $w: \mathcal{E} \to \mathbb{R}_{\geq 0}$ assigns:

- For each pair $\{\mathrm{G}_i, \mathrm{G}_j\}$: the measured grain-boundary energy per unit area,
  $$w\big(\{\mathrm{G}_i, \mathrm{G}_j\}\big) = \gamma_{ij} \quad (\mathrm{J/m^2}),$$
  e.g. $\gamma_{12} = 0.60$, $\gamma_{23} = 0.55$, $\gamma_{34} = 0.62$.
- For each triple $\{\mathrm{G}_i, \mathrm{G}_j, \mathrm{G}_k\}$: the triple-junction line energy per unit length,
  $$w\big(\{\mathrm{G}_i, \mathrm{G}_j, \mathrm{G}_k\}\big) = \tau_{ijk} \quad (\mathrm{J/m}),$$
  e.g. $\tau_{123} = 1.20$, $\tau_{234} = 1.15$.

In this hypernetwork:

- 2-node hyperedges $\{\mathrm{G}_i, \mathrm{G}_j\}$ represent individual grain boundaries.
- 3-node hyperedges $\{\mathrm{G}_i, \mathrm{G}_j, \mathrm{G}_k\}$ represent triple junctions where three grains meet.
- The weights encode the respective interfacial energies measured experimentally.

Such a hypernetwork captures both pairwise and multi-grain interactions, facilitating analysis of energy distributions and topological constraints in the alloy's microstructure.

Definition 2.26 (n-SuperHypernetwork)**.** [40] Let V_0 be a finite base set of *nodes*. Define the n-th iterated powerset recursively by

$$\mathcal{P}^0(V_0) = V_0, \qquad \mathcal{P}^{k+1}(V_0) = \mathcal{P}\big(\mathcal{P}^k(V_0)\big) \quad (k \geq 0).$$

An *n-superhypernetwork* is a tuple

$$\mathcal{N}^{(n)} = \big(V,\ \mathcal{E},\ w\big)$$

where

- $V \subseteq \mathcal{P}^n(V_0)$ is a finite set of *n-supernodes*;
- $\mathcal{E} \subseteq \mathcal{P}^n(V_0)$ is a finite set of *n-superedges*, each superedge $e \in \mathcal{E}$ being a nonempty subset of V;
- $w: \mathcal{E} \to \mathbb{R}_{\geq 0}$ is an optional *weight function* assigning a nonnegative real weight (or confidence) to each superedge.

In other words, both vertices and hyperedges of the network are drawn from the n-th powerset of the base node set, capturing up to n levels of hierarchical grouping.

Example 2.27 (2-SuperHypernetwork in Polycrystalline Microstructure)**.** A polycrystalline microstructure consists of numerous small crystals or grains, each with different orientations, separated by grain boundaries (cf. [102, 107, 121]). Consider a polycrystalline alloy whose microstructure consists of five grains:

$$V_0 = \{\mathrm{G}_1, \mathrm{G}_2, \mathrm{G}_3, \mathrm{G}_4, \mathrm{G}_5\}.$$

First iterated powerset (grain-boundary pairs):

$$\mathcal{P}^1(V_0) \supseteq \{\{\mathrm{G}_1, \mathrm{G}_2\},\ \{\mathrm{G}_2, \mathrm{G}_3\},\ \{\mathrm{G}_3, \mathrm{G}_4\},\ \{\mathrm{G}_4, \mathrm{G}_5\}\}.$$

Second iterated powerset (clusters of boundary pairs):

$$\mathcal{P}^2(V_0) = \mathcal{P}\big(\mathcal{P}^1(V_0)\big).$$

Define the 2-superhypernetwork

$$\mathcal{N}^{(2)} = \big(V,\ \mathcal{E},\ w\big)$$

by:

$$\begin{aligned} V &= \big\{\, v_1,\ v_2 \big\} \ \subseteq\ \mathcal{P}^2(V_0), \\ v_1 &= \big\{\{\mathrm{G}_1, \mathrm{G}_2\},\ \{\mathrm{G}_2, \mathrm{G}_3\}\big\}, \\ v_2 &= \big\{\{\mathrm{G}_3, \mathrm{G}_4\},\ \{\mathrm{G}_4, \mathrm{G}_5\}\big\}, \end{aligned}$$

and

$$\mathcal{E} = \big\{\, e_1 \big\} \ \subseteq\ \mathcal{P}^2(V_0), \qquad e_1 = \{\, v_1,\ v_2\},$$

where the weight function

$$w(e_1) = \gamma$$

assigns to e_1 the measured coupling coefficient $\gamma \geq 0$ between the two triple-junction clusters.

In this construction:

- Each G_i is a single crystal grain (node at level 0).
- Each 1-supernode $\{\mathrm{G}_i, \mathrm{G}_j\}$ is a grain-boundary pair.
- Each 2-supernode v_k is a cluster of neighboring boundaries (a set of 1-supernodes) representing a triple-junction region.
- The single 2-superedge e_1 links the two triple-junction clusters, modeling their mechanical interaction under load.

This 2-superhypernetwork captures both local grain-boundary connectivity (level 1) and higher-order cluster interactions (level 2) in the alloy's microstructure.

2.4 Grain Boundary Network

A Grain Boundary Network represents grains as nodes and shared interfaces as edges, modeling the topological and geometric properties of polycrystalline materials [31, 100, 106]. If we were to define it mathematically, it could be expressed as follows.

Definition 2.28 (Grain Boundary Network)**.** Let $\Omega \subset \mathbb{R}^d$ be a polycrystalline domain partitioned into N disjoint grains

$$\Omega = \bigcup_{i=1}^{N} G_i, \qquad G_i \cap G_j = \emptyset \quad (i \neq j),$$

each G_i a connected open set with Lipschitz-boundary. Define the *grain boundary network* as the undirected graph

$$\mathcal{G} = (V, E, W, \Theta, \mathbf{n}),$$

where:

- $V = \{1, 2, \ldots, N\}$ indexes the grains G_i.
- $$E = \big\{\{i, j\} : \mathcal{H}^{d-1}\big(\partial G_i \cap \partial G_j\big) > 0\big\}$$
  is the set of *grain-boundary edges*, each connecting two grains that share a nonzero-measure interface.
- $W = [w_{ij}] \in \mathbb{R}^{N \times N}$ is the *boundary-area weight matrix*, with
  $$w_{ij} = \mathcal{H}^{d-1}\big(\partial G_i \cap \partial G_j\big) \quad (\{i, j\} \in E),$$
  and $w_{ij} = 0$ otherwise, where $\mathcal{H}^{d-1}$ is the $(d-1)$-dimensional Hausdorff measure.
- $\Theta = \{\theta_{ij}\}$ is the set of *misorientation angles*, with $\theta_{ij} \in [0, \pi]$ the minimum rotation angle taking the crystal orientation of G_i to that of G_j.
- $\mathbf{n} = \{\mathbf{n}_{ij}\}$ assigns to each edge $\{i, j\}$ a *unit normal* $\mathbf{n}_{ij}$ to the boundary $\partial G_i \cap \partial G_j$.

Example 2.29 (Grain Boundary Network of a Triple-Junction Microstructure)**.** A triple junction is the point or line where three distinct grains in a polycrystalline material meet, influencing microstructural evolution (cf. [61, 136]). Consider a 2D polycrystalline domain Ω partitioned into three wedge-shaped grains meeting at the origin:

$$G_1 = \{(r, \theta) : 0 < r \le 1,\ 0 \le \theta < 120^\circ\},$$
$$G_2 = \{(r, \theta) : 0 < r \le 1,\ 120^\circ \le \theta < 240^\circ\},$$
$$G_3 = \{(r, \theta) : 0 < r \le 1,\ 240^\circ \le \theta < 360^\circ\}.$$

Label the grains $V = \{1, 2, 3\}$. The nonzero-measure pairwise boundaries are three straight segments of length 1:

$$E = \big\{\{1, 2\}, \{2, 3\}, \{1, 3\}\big\},$$

where

$$\partial G_1 \cap \partial G_2 = \{(r, 120^\circ) : 0 < r \le 1\}, \quad \partial G_2 \cap \partial G_3 = \{(r, 240^\circ) : 0 < r \le 1\}, \quad \partial G_1 \cap \partial G_3 = \{(r, 0^\circ) : 0 < r \le 1\}.$$

The boundary-area weight matrix $W = [w_{ij}]$ has

$$w_{12} = w_{23} = w_{13} = 1,$$

and zeros elsewhere. Assume the crystal orientations of G_i differ by 60° at each interface, giving misorientation angles

$$\theta_{12} = \theta_{23} = \theta_{13} = 60^\circ.$$

The outward unit normals (pointing into the lower-indexed grain) are

$$\mathbf{n}_{12} = \big(\cos 120^\circ, \sin 120^\circ\big),$$
$$\mathbf{n}_{23} = \big(\cos 240^\circ, \sin 240^\circ\big),$$
$$\mathbf{n}_{13} = \big(\cos 0^\circ, \sin 0^\circ\big).$$

Thus the Grain Boundary Network is

$$\mathcal{G} = \big(V, E, W, \Theta, \mathbf{n}\big),$$

fully encoding the topology, boundary lengths, misorientations, and normal directions of the three-grain microstructure.

2.5 Crystal Graph and Crystal HyperGraph

A Crystal Graph represents atoms as nodes and interatomic bonds as edges based on spatial proximity within a periodic crystal lattice [95, 104, 129]. If we were to define it mathematically, it could be expressed as follows.

Definition 2.30 (Crystal Graph)**.** Let C be a periodic crystal structure with atom set $V = \{v_1, \ldots, v_N\}$ in a unit cell and lattice vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$. Fix a cutoff radius $r_c > 0$. The *crystal graph* is the directed graph

$$G = (V, E),$$

where

$$E = \big\{(v_i, v_j) \in V \times V : \exists \mathbf{R} \in \Lambda,\ 0 < \|\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i\| \leq r_c\big\},$$

with $\mathbf{r}_i$ the position of atom v_i and $\Lambda = \{n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 : n_k \in \mathbb{Z}\}$. Each edge (v_i, v_j) carries a feature vector $\mathbf{e}_{ij} = [\ \|\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i\|, \ldots]$ encoding the interatomic distance (and possibly angular or chemical attributes).

Example 2.31 (Crystal Graph of a 2D Square Unit Cell)**.** Consider a 2D square lattice with one atom per corner of the unit cell:

$$V = \{v_1, v_2, v_3, v_4\},$$

with positions

$$\mathbf{r}_1 = (0, 0), \quad \mathbf{r}_2 = (1, 0),$$
$$\mathbf{r}_3 = (1, 1), \quad \mathbf{r}_4 = (0, 1),$$

and lattice vectors $\mathbf{a}_1 = (1, 0)$, $\mathbf{a}_2 = (0, 1)$. Fix cutoff radius $r_c = 1.1$. Then the crystal graph $G = (V, E)$ has directed edges

$$E = \{(v_1, v_2),\ (v_2, v_1),\ (v_2, v_3),\ (v_3, v_2),$$
$$(v_3, v_4),\ (v_4, v_3),\ (v_4, v_1),\ (v_1, v_4)\},$$

since only nearest-neighbor distances $\|\mathbf{r}_j - \mathbf{r}_i\| = 1 \leq r_c$ are included (with $\mathbf{R} = \mathbf{0}$ in Λ). Each edge (v_i, v_j) carries the feature

$$\mathbf{e}_{ij} = \big[\|\mathbf{r}_j - \mathbf{r}_i\|\big] = [1].$$

Thus G is a directed 4-cycle capturing the nearest-neighbor connectivity of the square lattice.

A Crystal HyperGraph models each atom and its nearest neighbors as hyperedges, capturing higher-order local structures in periodic crystal lattices (cf. [68]). If we were to define it mathematically, it could be expressed as follows.

Definition 2.32 (Crystal HyperGraph)**.** Let C and Λ be as above, and let V be the atom set. For a chosen coordination number k, define for each atom v_i the ordered neighbor set $\mathcal{N}_i = \{v_{i_1}, \ldots, v_{i_k}\}$ of the k closest neighbors (including periodic images). The *crystal hypergraph* is the hypergraph

$$H = (V, \mathcal{E}),$$

where the hyperedge set

$$\mathcal{E} = \big\{\, e_i : i = 1, \ldots, N\big\}, \quad e_i = \{v_i\} \cup \mathcal{N}_i$$

connects each central atom v_i with its k-nearest neighbors. Each hyperedge e_i is equipped with a feature vector $\mathbf{h}_{e_i} = [\ d_{i,i_1}, \ldots, d_{i,i_k}, \alpha_{i,i_1,i_2}, \ldots]$ that encodes all pairwise distances $d_{i,i_j} = \|\mathbf{r}_{i_j} + \mathbf{R}_j - \mathbf{r}_i\|$ and selected bond angles α_{i,i_j,i_ℓ} among neighbors.

Example 2.33 (Crystal HyperGraph of the 2D Square Lattice (Coordination $k = 2$))**.** Let the base atom set and positions in one unit cell be

$$V = \{v_1, v_2, v_3, v_4\}, \quad \mathbf{r}_1 = (0, 0),\ \mathbf{r}_2 = (1, 0),$$

$$\mathbf{r}_3 = (1, 1),\ \mathbf{r}_4 = (0, 1),$$

with periodic lattice vectors $\mathbf{a}_1 = (1, 0)$, $\mathbf{a}_2 = (0, 1)$. Choose coordination number $k = 2$, i.e. each atom connects to its two nearest neighbors (using periodic images). The neighbor sets are:

$$\mathcal{N}_1 = \{v_2, v_4\}, \quad \mathcal{N}_2 = \{v_1, v_3\},$$
$$\mathcal{N}_3 = \{v_2, v_4\}, \quad \mathcal{N}_4 = \{v_1, v_3\}.$$

Form the hyperedges

$$e_i = \{ v_i \} \cup \mathcal{N}_i, \quad i = 1, 2, 3, 4,$$

so explicitly

$$e_1 = \{v_1, v_2, v_4\}, \quad e_2 = \{v_2, v_1, v_3\},$$
$$e_3 = \{v_3, v_2, v_4\}, \quad e_4 = \{v_4, v_1, v_3\}.$$

Then the *crystal hypergraph* is

$$H = (V, \mathcal{E}), \quad \mathcal{E} = \{e_1, e_2, e_3, e_4\}.$$

Each hyperedge e_i carries a feature vector

$$\mathbf{h}_{e_i} = \left[d_{i,i_1},\ d_{i,i_2},\ \alpha_{i,i_1,i_2}\right],$$

where $\{i_1, i_2\} = \mathcal{N}_i$,

$$d_{i,i_j} = \left\|\mathbf{r}_{i_j} - \mathbf{r}_i\right\| = 1, \qquad \alpha_{i,i_1,i_2} = \measuredangle(v_i, v_{i_1}, v_{i_2}) = 90^\circ.$$

Thus each hyperedge encodes the two equal bond lengths and the right angle between them, capturing the local square-lattice motif in the hypergraph representation.

3 Result: Grain Boundary HyperNetwork

The Grain Boundary HyperNetwork is a hypernetwork model that represents interfaces between grains in a polycrystalline material. In this model, hyperedges correspond to shared boundaries among multiple grains, and each hyperedge is weighted according to the geometric intersection measure of the associated grain boundaries. The definition, examples, and mathematical properties of this concept are presented below.

Definition 3.1 (Grain Boundary HyperNetwork)**.** Let $\Omega \subset \mathbb{R}^d$ be a polycrystalline domain partitioned into N disjoint grains

$$\Omega = \bigcup_{i=1}^{N} G_i, \qquad G_i \cap G_j = \emptyset \quad (i \neq j),$$

each G_i a connected open set with Lipschitz boundary. Define the set of grains

$$V = \{1, 2, \ldots, N\}.$$

For any nonempty subset $e \subseteq V$ with $|e| = k \geq 2$, let

$$J_e = \bigcap_{i \in e} \partial G_i$$

be the geometric intersection of their boundaries. If the $(d-k+1)$-dimensional Hausdorff measure $\mathcal{H}^{d-k+1}(J_e)$ is positive, declare e a *grain-boundary hyperedge*. The *Grain Boundary HyperNetwork* is the weighted hypernetwork

$$\mathcal{H} = \big(V,\ \mathcal{E},\ w\big),$$

where

$$\mathcal{E} = \left\{ e \subseteq V : |e| \geq 2,\ \mathcal{H}^{d-k+1}(J_e) > 0 \right\},$$

and the weight function $w : \mathcal{E} \to \mathbb{R}_{>0}$ is given by

$$w(e) = \mathcal{H}^{d-k+1}(J_e).$$

Example 3.2 (Grain Boundary HyperNetwork of a Triple-Junction in 2D)**.** Let $\Omega \subset \mathbb{R}^2$ be the unit disk, partitioned into three wedge-shaped grains meeting at the origin:

$$G_1 = \{(r, \theta) : 0 < r \leq 1,\ 0 \leq \theta < \tfrac{2\pi}{3}\},$$
$$G_2 = \{(r, \theta) : 0 < r \leq 1,\ \tfrac{2\pi}{3} \leq \theta < \tfrac{4\pi}{3}\},$$
$$G_3 = \{(r, \theta) : 0 < r \leq 1,\ \tfrac{4\pi}{3} \leq \theta < 2\pi\}.$$

Label the grains $V = \{1, 2, 3\}$. The pairwise grain-boundary intersections are radial segments:

$$J_{\{1,2\}} = \{(r, \theta) : 0 < r \leq 1,\ \theta = \tfrac{2\pi}{3}\},$$

$$J_{\{2,3\}} : \theta = \tfrac{4\pi}{3}, \quad J_{\{1,3\}} : \theta = 0 \text{ or } 2\pi,$$

each of length 1. The triple-junction is

$$J_{\{1,2,3\}} = \bigcap_{i=1}^{3} \partial G_i = \{(0, \theta) : \theta \in [0, 2\pi)\},$$

a single point (the origin). Thus the hyperedges are

$$\mathcal{E} = \big\{\{1, 2\},\ \{2, 3\},\ \{1, 3\},\ \{1, 2, 3\}\big\},$$

with weights

$$w(\{i, j\}) = \mathcal{H}^1(J_{\{i,j\}}) = 1, \quad w(\{1, 2, 3\}) = \mathcal{H}^0(J_{\{1,2,3\}}) = 1.$$

Therefore the Grain Boundary HyperNetwork is

$$\mathcal{H} = \big(V,\ \mathcal{E},\ w\big),$$

where each two-grain boundary and the single triple-junction are represented as hyperedges with the corresponding Hausdorff measure as weight.

Example 3.3 (Grain Boundary HyperNetwork of a 2×2 Grid of Square Grains)**.** Let $\Omega = [0, 2] \times [0, 2] \subset \mathbb{R}^2$ be partitioned into four unit-square grains:

$$G_1 = [0, 1] \times [0, 1], \quad G_2 = [1, 2] \times [0, 1],$$
$$G_3 = [0, 1] \times [1, 2], \quad G_4 = [1, 2] \times [1, 2].$$

Define the vertex set $V = \{1, 2, 3, 4\}$. We compute boundary intersections:

- $\partial G_1 \cap \partial G_2 = \{(1, y) : 0 < y < 1\}$, a segment of length 1. Hence $\{1, 2\} \in \mathcal{E}$ with $w(\{1, 2\}) = 1$.
- $\partial G_1 \cap \partial G_3 = \{(x, 1) : 0 < x < 1\}$, length 1. Hence $\{1, 3\} \in \mathcal{E}$ with $w(\{1, 3\}) = 1$.
- $\partial G_2 \cap \partial G_4 = \{(x, 1) : 1 < x < 2\}$, length 1. Hence $\{2, 4\} \in \mathcal{E}$ with $w(\{2, 4\}) = 1$.
- $\partial G_3 \cap \partial G_4 = \{(1, y) : 1 < y < 2\}$, length 1. Hence $\{3, 4\} \in \mathcal{E}$ with $w(\{3, 4\}) = 1$.

All four grains meet at the single corner point $(1, 1) = \bigcap_{i=1}^{4} \partial G_i$, so every triple and the quadruple intersection include this point:

$$J_{\{i,j,k\}} = \{(1, 1)\}, \quad J_{\{1,2,3,4\}} = \{(1, 1)\}.$$

Thus the hyperedge family also contains

$$\{1, 2, 3\},\ \{1, 2, 4\},\ \{1, 3, 4\},\ \{2, 3, 4\},\ \{1, 2, 3, 4\},$$

each with weight

$$w(e) = \mathcal{H}^0(J_e) = 1.$$

In total, the Grain Boundary HyperNetwork is

$$\mathcal{H} = \big(V,\ \mathcal{E},\ w\big),$$

where

$$\mathcal{E} = \big\{\{1, 2\}, \{1, 3\}, \{2, 4\}, \{3, 4\},\ \{1, 2, 3\}, \{1, 2, 4\}, \{1, 3, 4\}, \{2, 3, 4\},\ \{1, 2, 3, 4\}\big\},$$

and each hyperedge carries the corresponding Hausdorff measure as its weight. This example illustrates both pairwise grain boundaries and higher-order junctions in a simple polycrystalline microstructure.

Theorem 3.4 (Hypernetwork Structure)**.** *The Grain Boundary HyperNetwork $\mathcal{H} = (V, \mathcal{E}, w)$ is a hypernetwork: V is finite, $\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$, and $w : \mathcal{E} \to \mathbb{R}_{>0}$.*

Proof. By construction, V is the finite set of grain indices. Each hyperedge $e \in \mathcal{E}$ is a nonempty subset of V (with $|e| \geq 2$) such that the intersection of the corresponding boundaries has positive $(d - |e| + 1)$-measure. The weight $w(e)$ is defined for every such e and is strictly positive. Hence $(V, \mathcal{E}, w)$ satisfies the definition of a (finite, undirected, weighted) hypernetwork. □

Theorem 3.5 (Generalization of Grain Boundary Network)**.** *If one restricts to hyperedges of size two, the Grain Boundary HyperNetwork $\mathcal{H}$ reduces to the classical Grain Boundary Network $\mathcal{G} = (V, E_2, W)$ with*

$$E_2 = \big\{\{i, j\} \in \mathcal{E} : |\{i, j\}| = 2\big\}, \qquad W_{ij} = w(\{i, j\}).$$

Conversely, any Grain Boundary Network arises in this way as the 2-section of some Grain Boundary HyperNetwork.

Proof. By definition, every size-2 hyperedge $\{i, j\} \in \mathcal{E}$ corresponds to two grains sharing a boundary of positive $(d-1)$-measure. Collecting exactly these pairs yields

$$E_2 = \big\{\{i, j\} : \mathcal{H}^{d-1}(\partial G_i \cap \partial G_j) > 0\big\},$$

and setting $W_{ij} = w(\{i, j\})$ recovers the boundary-area weights. This is precisely the Grain Boundary Network. Conversely, given any Grain Boundary Network (V, E_2, W), one may define $\mathcal{E} = E_2$ (and possibly add higher-order hyperedges for triple or higher junctions) and $w(e) = W_{ij}$ on pairs to embed it as the 2-hyperedge subnetwork of a Grain Boundary HyperNetwork. Therefore the hypernetwork construction both generalizes and specializes to the classical network. □

Theorem 3.6 (Downward Closure)**.** *Let $\mathcal{H} = (V, \mathcal{E}, w)$ be a Grain Boundary HyperNetwork. If $e \in \mathcal{E}$ and $f \subseteq e$ with $|f| \geq 2$, then $f \in \mathcal{E}$.*

Proof. By definition $e \in \mathcal{E}$ implies $\mathcal{H}^{d-|e|+1}(J_e) > 0$, where

$$J_e = \bigcap_{i \in e} \partial G_i.$$

If $f \subseteq e$ and $|f| = k \geq 2$, then

$$J_e \subseteq J_f = \bigcap_{i \in f} \partial G_i,$$

so J_f is a superset of J_e. The $(d-k+1)$-dimensional Hausdorff measure of any superset of a positive-measure set is itself positive. Hence $\mathcal{H}^{d-k+1}(J_f) > 0$, and so $f \in \mathcal{E}$. □

Theorem 3.7 (Weight Monotonicity)**.** *In the same setting, if $f \subseteq e$ then*

$$w(e) \ = \ \mathcal{H}^{d-|e|+1}(J_e) \ \leq \ \mathcal{H}^{d-|f|+1}(J_f) \ = \ w(f).$$

Proof. Since $J_e = \bigcap_{i \in e} \partial G_i \subseteq J_f = \bigcap_{i \in f} \partial G_i$ and $d - |e| + 1 < d - |f| + 1$, the $(d - |e| + 1)$-measure of the smaller-dimensional set J_e cannot exceed the $(d - |f| + 1)$-measure of the larger-dimensional set J_f. Therefore $w(e) \leq w(f)$. □

Theorem 3.8 (Abstract Simplicial Complex)**.** *The hyperedge family $\mathcal{E}$ of a Grain Boundary HyperNetwork is an abstract simplicial complex on V.*

Proof. Downward closure shows that if $e \in \mathcal{E}$, then every nonempty subset $f \subset e$ with $|f| \geq 2$ also lies in $\mathcal{E}$. Since simplicial complexes require closure under all nonempty subsets, and singletons $\{i\}$ are excluded by $|e| \geq 2$, $\mathcal{E}$ satisfies the definition of a simplicial complex on the vertex set V. □

Theorem 3.9 (Induced Subhypernetwork)**.** *Let $U \subseteq V$. Then*

$$\mathcal{H}[U] := \big(U, \ \{\, e \in \mathcal{E} : e \subseteq U\}, \ w|_{\mathcal{E}[U]}\big)$$

is a Grain Boundary HyperNetwork corresponding to the subdomain $\bigcup_{i \in U} G_i$.

Proof. Restricting to grains with labels in U yields a valid partition of the subdomain $\bigcup_{i \in U} G_i$. Every hyperedge $e \subseteq U$ shares a positive-measure intersection J_e by assumption, so $\mathcal{E}[U]$ and w satisfy the hypernetwork definition. Hence $\mathcal{H}[U]$ is again a Grain Boundary HyperNetwork. □

Theorem 3.10 (Connectivity of the Incidence Graph)**.** *If the 2-section graph of $\mathcal{H}$ is connected, then the bipartite incidence graph between V and $\mathcal{E}$ is also connected.*

Proof. The 2-section graph connects any two vertices $i, j \in V$ by a path of length-2 edges through hyperedges in $\mathcal{E}$. In the bipartite incidence graph, each such 2-section edge $\{i, k\} \in \mathcal{E}$ becomes a path i–$\{i, k\}$–k. Concatenating these paths shows that any two vertices in V remain connected in the bipartite graph by alternating vertex–hyperedge–vertex sequences. Thus the incidence graph is connected. □

4 Result: Grain Boundary n-SuperHyperNetwork

The Grain Boundary n-SuperHyperNetwork, on the other hand, is a hierarchical generalization that organizes grain boundary structures using nested powersets. This framework captures not only direct grain interactions but also higher-order junctions and complex interrelations among grain clusters at multiple scales. The definition, examples, and mathematical properties of this concept are presented below.

Definition 4.1 (Grain Boundary n-SuperHyperNetwork)**.** Let $\Omega \subset \mathbb{R}^d$ be a polycrystalline domain partitioned into N disjoint grains $\{G_i\}_{i=1}^N$ with Lipschitz boundaries, and set

$$V_0 = \{1, 2, \ldots, N\}.$$

For each integer $k \geq 0$, define the iterated powerset

$$\mathcal{P}^0(V_0) = V_0, \qquad \mathcal{P}^{k+1}(V_0) = \mathcal{P}\big(\mathcal{P}^k(V_0)\big).$$

A *Grain Boundary n-SuperHyperNetwork* is a triple

$$\mathcal{N}^{(n)} \;=\; \big(V^{(n)},\, \mathcal{E}^{(n)},\, w\big)$$

where:

- $V^{(n)} \subseteq \mathcal{P}^n(V_0)$ is a finite set of *n-supernodes*.
- $\mathcal{E}^{(n)} \subseteq \mathcal{P}^n(V_0)$ is a finite set of *n-superedges*, each $e \in \mathcal{E}^{(n)}$ a nonempty subset of $V^{(n)}$.
- $w : \mathcal{E}^{(n)} \to \mathbb{R}_{>0}$ assigns to each superedge e the $(d - k + 1)$-dimensional measure of the common intersection of all base-level grain boundaries indexed by the elements of e:

  $$w(e) = \mathcal{H}^{\,d-|\operatorname{flat}(e)|+1}\Big(\bigcap_{i\in \operatorname{flat}(e)} \partial G_i\Big),$$

  where $\operatorname{flat}(e) \subseteq V_0$ is the union of all base-nodes appearing (possibly nested) in e.

The incidence relation is the natural membership of supernodes in superedges.

Example 4.2 (Grain Boundary 2-SuperHyperNetwork of a Triple-Junction Polycrystal)**.** Let $\Omega \subset \mathbb{R}^2$ be the unit disk partitioned into three wedge-shaped grains meeting at the origin, as in the previous example. Label the grains

$$V_0 = \{1, 2, 3\}.$$

Level-1 hypernodes and hyperedges. The grain-boundary hypernetwork has hyperedges

$$\mathcal{E}^{(1)} = \big\{\{1, 2\}, \{2, 3\}, \{1, 3\}, \{1, 2, 3\}\big\},$$

with weights

$$w^{(1)}(\{i, j\}) = \mathcal{H}^1(J_{\{i,j\}}) = 1, \quad w^{(1)}(\{1, 2, 3\}) = \mathcal{H}^0(J_{\{1,2,3\}}) = 1.$$

Here $J_{\{i,j\}}$ are unit-length line segments and $J_{\{1,2,3\}}$ is the single triple point.

Level-2 supernodes. Form 2-supernodes by grouping each pair of overlapping hyperedges that include the triple-junction:

$$D_1 = \{\{1,2\},\{1,2,3\}\},$$
$$D_2 = \{\{2,3\},\{1,2,3\}\},$$
$$D_3 = \{\{1,3\},\{1,2,3\}\}.$$

Thus

$$V^{(2)} = \{D_1, D_2, D_3\}.$$

Level-2 superedges and weights. There is a single 2-superedge connecting all three 2-supernodes:

$$\mathcal{E}^{(2)} = \{\{D_1, D_2, D_3\}\}.$$

Its weight is the measure of the intersection of all base-level grain boundaries indexed by the flat set $\mathrm{flat}(\{D_1, D_2, D_3\}) = \{1,2,3\}$, namely the triple-junction:

$$w^{(2)}(\{D_1, D_2, D_3\}) = \mathcal{H}^0\Big(\bigcap_{i=1}^{3} \partial G_i\Big) = 1.$$

Resulting 2-SuperHyperNetwork. The Grain Boundary 2-SuperHyperNetwork is

$$\mathcal{N}^{(2)} = (V^{(2)},\ \mathcal{E}^{(2)},\ w^{(2)}) = \Big(\{D_1, D_2, D_3\},\ \{\{D_1, D_2, D_3\}\},\ w^{(2)}\Big),$$

which encodes the second-order meta-connection among the overlapping grain-boundary hyperedges via the common triple-junction.

Example 4.3 (Grain Boundary 3-SuperHyperNetwork of a Triple-Junction Polycrystal)**.** Let $\Omega \subset \mathbb{R}^2$ be the unit disk partitioned into three wedge-shaped grains meeting at the origin, as before, with

$$V_0 = \{1,2,3\}.$$

The level-1 hyperedges are

$$\mathcal{E}^{(1)} = \{\{1,2\},\{2,3\},\{1,3\},\{1,2,3\}\},$$

and $w^{(1)}(\{i,j\}) = \mathcal{H}^1(J_{\{i,j\}}) = 1$, $w^{(1)}(\{1,2,3\}) = \mathcal{H}^0(J_{\{1,2,3\}}) = 1$.

Form the level-2 supernodes by grouping each boundary hyperedge with the triple-junction:

$$D_1 = \{\{1,2\},\{1,2,3\}\}, \quad D_2 = \{\{2,3\},\{1,2,3\}\}, \quad D_3 = \{\{1,3\},\{1,2,3\}\}.$$

Then

$$V^{(2)} = \{D_1, D_2, D_3\}, \quad \mathcal{E}^{(2)} = \{\{D_1, D_2, D_3\}\}, \quad w^{(2)}(\{D_1, D_2, D_3\}) = \mathcal{H}^0(J_{\{1,2,3\}}) = 1.$$

Next form the level-3 supernodes by pairing overlapping level-2 supernodes:

$$A_1 = \{D_1, D_2\}, \quad A_2 = \{D_2, D_3\}, \quad A_3 = \{D_3, D_1\}.$$

Thus

$$V^{(3)} = \{A_1, A_2, A_3\}.$$

Finally, the single 3-superedge connects all three:

$$\mathcal{E}^{(3)} = \{\{A_1, A_2, A_3\}\}, \qquad w^{(3)}(\{A_1, A_2, A_3\}) = \mathcal{H}^0(J_{\{1,2,3\}}) = 1.$$

Therefore, the Grain Boundary 3-SuperHyperNetwork is

$$\mathcal{N}^{(3)} = (V^{(3)},\ \mathcal{E}^{(3)},\ w^{(3)}),$$

which encodes a third-order meta-connection among the three level-2 boundary clusters via their common triple-junction.

Theorem 4.4 (n-SuperHypernetwork Structure)**.** *Every Grain Boundary n-SuperHyperNetwork*

$$\mathcal{N}^{(n)} = (V^{(n)}, \mathcal{E}^{(n)}, w)$$

is an n-superhypernetwork on base set V_0:

$$V^{(n)} \subseteq \mathcal{P}^n(V_0), \quad \mathcal{E}^{(n)} \subseteq \mathcal{P}^n(V_0),$$

with the weight function w as above and incidence given by set membership.

Proof. By definition, $V^{(n)}$ and $\mathcal{E}^{(n)}$ are subsets of the nth iterated powerset of V_0. Each superedge $e \in \mathcal{E}^{(n)}$ is a nonempty subset of $V^{(n)}$, and the weight $w(e)$ is well-defined and positive whenever the corresponding geometric intersection has positive measure. The natural membership relation between supernodes and superedges provides the required incidence structure. Thus $\mathcal{N}^{(n)}$ satisfies all axioms of an n-superhypernetwork. □

Theorem 4.5 (Reduction to Grain Boundary HyperNetwork)**.** *If $n = 1$, then $\mathcal{N}^{(1)} = (V^{(1)}, \mathcal{E}^{(1)}, w)$ coincides with the Grain Boundary HyperNetwork $\big(V_0, \mathcal{E}, w\big)$, where*

$$V^{(1)} = V_0, \qquad \mathcal{E}^{(1)} = \Big\{ e \subseteq V_0 : \mathcal{H}^{d-|e|+1}\big(\bigcap_{i \in e} \partial G_i\big) > 0 \Big\},$$

and $w(e) = \mathcal{H}^{d-|e|+1}(\bigcap_{i \in e} \partial G_i)$. Conversely, any Grain Boundary HyperNetwork arises as the 1–superhypernetwork $\mathcal{N}^{(1)}$ for appropriate choice of $\mathcal{E}^{(1)}$ and w.

Proof. For $n = 1$, $\mathcal{P}^1(V_0) = \mathcal{P}(V_0)$. Setting $V^{(1)} = V_0$ and defining $\mathcal{E}^{(1)} \subseteq \mathcal{P}(V_0)$ exactly as those subsets whose grain-boundary intersections have positive measure yields the Grain Boundary HyperNetwork. The weight assignment agrees by construction. Conversely, any such hypernetwork on V_0 with weights given by boundary-intersection measures can be viewed as $\mathcal{N}^{(1)}$. Hence $\mathcal{N}^{(1)}$ and the Grain Boundary HyperNetwork are equivalent. □

Theorem 4.6 (Functoriality of SuperHypernetwork Levels)**.** *Let $\mathcal{N}^{(n)} = (V^{(n)}, \mathcal{E}^{(n)}, w^{(n)})$ be the Grain Boundary n-SuperHyperNetwork. Then for any $m, k \geq 0$,*

$$\big(\mathcal{N}^{(n)}\big)^{(m)} = \mathcal{N}^{(n+m)},$$

i.e. iterating the "super" construction m additional times on $\mathcal{N}^{(n)}$ yields the $(n+m)$-SuperHyperNetwork.

Proof. By Definition, each level increases the base-node set from $\mathcal{P}^k(V_0)$ to $\mathcal{P}^{k+1}(V_0)$. Applying m further iterations starting at level n gives

$$V^{(n+m)} \subseteq \mathcal{P}^{n+m}(V_0), \qquad \mathcal{E}^{(n+m)} \subseteq \mathcal{P}^{n+m}(V_0),$$

with weights defined by the same Hausdorff-measure rule on the flattened base-nodes. This matches precisely the result of applying the super-construction m times to $\mathcal{N}^{(n)}$, so the two procedures coincide. □

Theorem 4.7 (Cardinality Growth)**.** *If $|V_0| = N$, then for each $n \geq 1$,*

$$|V^{(n)}| \leq 2^{2^{\cdot^{\cdot^{2^N}}}} \quad \textit{(tower of n exponentials)},$$

and similarly $|\mathcal{E}^{(n)}|$ satisfies the same bound.

Proof. By construction $V^{(n)} \subseteq \mathcal{P}^n(V_0)$ and $|\mathcal{P}^n(V_0)| = 2^{|\mathcal{P}^{n-1}(V_0)|}$. Since $\mathcal{P}^{n-1}(V_0)$ has cardinality given by a tower of $n-1$ exponentials in N, adding one more powerset doubles the height. The same argument applies to $\mathcal{E}^{(n)} \subseteq \mathcal{P}^n(V_0)$. □

Theorem 4.8 (Injection and Projection)**.** *Define the singleton-embedding*

$$\iota_n : V^{(n-1)} \longrightarrow V^{(n)}, \quad \iota_n(x) = \{x\},$$

and the flattening projection

$$p_n : V^{(n)} \longrightarrow V^{(n-1)}, \quad p_n(X) = \bigcup_{x \in X} x.$$

Then ι_n is injective, p_n is surjective, and $p_n \circ \iota_n = \mathrm{id}_{V^{(n-1)}}$.

Proof. $\iota_n(\{x\}) = \{y\}$ implies $x = y$, so ι_n is injective. For any $y \in V^{(n-1)}$, $p_n(\{y\}) = y$, so p_n is surjective. Finally, for each $x \in V^{(n-1)}$,

$$(p_n \circ \iota_n)(x) = p_n(\{x\}) = \bigcup\{x\} = x,$$

establishing the retraction property. □

Theorem 4.9 (Strict Monotonicity of Levels)**.** *Assume $N \geq 1$. Then for every $n \geq 0$,*

$$V^{(n)} \subsetneq V^{(n+1)}, \qquad \mathcal{E}^{(n)} \subsetneq \mathcal{E}^{(n+1)}.$$

Proof. Since $V^{(n+1)} = \mathcal{P}(V^{(n)})$, each element of $V^{(n)}$ embeds as a singleton, giving $V^{(n)} \subseteq V^{(n+1)}$. Properness follows because $\emptyset \in V^{(n+1)}$ but $\emptyset \notin V^{(n)}$. The same argument applies to $\mathcal{E}^{(n)}$. □

Theorem 4.10 (Connectivity Preservation)**.** *If the base Grain Boundary HyperNetwork $\mathcal{H} = (V^{(1)}, \mathcal{E}^{(1)})$ is connected in the sense that its 2-section graph is connected, then for each $n \geq 1$, the 2-section of $\mathcal{N}^{(n)}$ is also connected.*

Proof. The 2-section of a hyper(super-)network has vertices $V^{(n)}$ and an edge between any two supernodes sharing a superedge. Since ι_2 embeds $V^{(n-1)}$ as a connected subgraph into the 2-section of level n, and every new supernode shares a superedge with some singleton image $\{x\}$ of a connected lower level, the graph remains connected by induction on n. □

Theorem 4.11 (Weight Consistency)**.** *For any superedge $e \in \mathcal{E}^{(n)}$, let $\mathrm{flat}(e) \subseteq V_0$ be the union of all base-nodes appearing in e. Then*

$$w^{(n)}(e) = \mathcal{H}^{d-|\mathrm{flat}(e)|+1}\Big(\bigcap_{i \in \mathrm{flat}(e)} \partial G_i\Big) = w^{(1)}\big(\mathrm{flat}(e)\big),$$

so the weight of e depends only on its flattened base intersection.

Proof. By definition $w^{(n)}(e)$ is the $(d-k+1)$-measure of the common boundary intersection of the base grains in $\mathrm{flat}(e)$, exactly the same quantity used to define $w^{(1)}$ on the hyperedge $\mathrm{flat}(e)$. Hence the equality holds. □

5 Result: Crystal n-SuperHyperGraph

A Crystal n-SuperHyperGraph models atomic structures using nested powersets, capturing hierarchical groupings of atoms and their multi-level interactions. The definition, examples, and mathematical properties of this concept are presented below.

Definition 5.1 (Crystal n-SuperHyperGraph)**.** Let C be a periodic crystal structure with atom set

$$V_0 = \{v_1, \ldots, v_N\}$$

in the unit cell and lattice Λ. For each integer $k \geq 0$, define the iterated powerset

$$\mathcal{P}^0(V_0) = V_0, \qquad \mathcal{P}^{k+1}(V_0) = \mathcal{P}\big(\mathcal{P}^k(V_0)\big).$$

A *Crystal n-SuperHyperGraph* is a pair

$$\mathrm{CSHT}^{(n)} = \big(V^{(n)}, E^{(n)}\big)$$

where

$$V^{(n)} \subseteq \mathcal{P}^n(V_0) \quad \text{(the } n\text{-supervertices)}, \qquad E^{(n)} \subseteq \mathcal{P}^n(V_0) \quad \text{(the } n\text{-superedges)},$$

together with the natural incidence relation $\{(v, e) \in V^{(n)} \times E^{(n)} : v \in e\}$.

Example 5.2 (Crystal 2-SuperHyperGraph of Square-Lattice Triangle Motifs)**.** Let the base atom set be

$$V_0 = \{v_1, v_2, v_3, v_4\},$$

with positions in the unit cell $\mathbf{r}_1 = (0, 0)$, $\mathbf{r}_2 = (1, 0)$, $\mathbf{r}_3 = (1, 1)$, $\mathbf{r}_4 = (0, 1)$. Form the level-1 hyperedges (3-atom motifs) by selecting all triangles sharing the central atom v_3:

$$e_1 = \{v_1, v_2, v_3\}, \quad e_2 = \{v_2, v_3, v_4\}, \quad e_3 = \{v_1, v_3, v_4\}.$$

Thus the Crystal HyperGraph is

$$\mathrm{CSHT}^{(1)} = (V_0, \{e_1, e_2, e_3\}).$$

Next form the level-2 supervertices by grouping each pair of overlapping triangles:

$$D_1 = \{e_1, e_2\}, \quad D_2 = \{e_1, e_3\}, \quad D_3 = \{e_2, e_3\}.$$

Since each pair of these supervertices shares exactly one hyperedge, the level-2 superedge set is

$$E^{(2)} = \big\{\{D_1, D_2\},\ \{D_1, D_3\},\ \{D_2, D_3\}\big\}.$$

Hence the Crystal 2-SuperHyperGraph is

$$\mathrm{CSHT}^{(2)} = \big(V^{(2)}, E^{(2)}\big) = \Big(\ \{D_1, D_2, D_3\},\ \{\{D_1, D_2\}, \{D_1, D_3\}, \{D_2, D_3\}\}\Big).$$

This 2-superhypergraph encodes the second-order grouping of triangular coordination motifs in the square lattice, yielding a complete 3-vertex meta-network among the three triangular clusters.

Example 5.3 (Crystal 2-SuperHyperGraph of Perovskite ABO_3 Octahedral Clusters)**.** Consider a perovskite crystal ABO_3 with three adjacent B-site octahedra in the unit cell. Let the base atom set be

$$V_0 = \{\ B_1, B_2, B_3,\ O_{11}, O_{12}, \dots, O_{16},\ O_{21}, \dots, O_{26},\ O_{31}, \dots, O_{36}\},$$

where B_i is the i-th metal cation and O_{ij} are the six oxygens coordinating B_i.

Level-1 hyperedges (octahedral motifs):

$$\begin{aligned} e_1 &= \{\ B_1, O_{11}, O_{12}, O_{13}, O_{14}, O_{15}, O_{16}\}, \\ e_2 &= \{\ B_2, O_{21}, O_{22}, O_{23}, O_{24}, O_{25}, O_{26}\}, \\ e_3 &= \{\ B_3, O_{31}, O_{32}, O_{33}, O_{34}, O_{35}, O_{36}\}. \end{aligned}$$

Each e_i is the set of bonds (here, cation–oxygen pairs) forming the i-th BO_6 octahedron.

Level-2 supervertices (pairs of neighboring octahedra): Adjacent octahedra share oxygen bridges. We define:

$$D_1 = \{e_1, e_2\}, \quad D_2 = \{e_2, e_3\}, \quad D_3 = \{e_1, e_3\}.$$

Each D_k collects two octahedral motifs that share some oxygens.

Level-2 superedges (inter-octahedral meta-connections): We connect any two supervertices that overlap in one hyperedge:

$$E^{(2)} = \big\{\ \{D_1, D_2\},\ \{D_2, D_3\},\ \{D_1, D_3\}\big\}.$$

Crystal 2-SuperHyperGraph:

$$\mathrm{CSHT}^{(2)} = \big(V^{(2)}, E^{(2)}\big) = \Big(\ \{D_1, D_2, D_3\},\ \{\{D_1, D_2\}, \{D_2, D_3\}, \{D_1, D_3\}\}\Big).$$

Here, $V^{(2)}$ comprises three 2-supervertices (pairs of octahedra), and $E^{(2)}$ encodes the overlapping relationships among them. This structure captures the second-order connectivity of BO_6 clusters in a perovskite, revealing meta-networks of corner-sharing octahedra essential for understanding electronic, ionic, and mechanical properties.

Example 5.4 (Crystal 3-SuperHyperGraph of Square-Lattice Third-Order Motif Clusters)**.** Let the base atom set and level-1 hyperedges be as in the 2-superhypergraph example:

$$V_0 = \{v_1, v_2, v_3, v_4\}, \quad e_1 = \{v_1, v_2, v_3\},\ e_2 = \{v_2, v_3, v_4\},\ e_3 = \{v_1, v_3, v_4\}.$$

Form the level-2 supervertices by pairing overlapping triangles:

$$D_1 = \{e_1, e_2\}, \quad D_2 = \{e_1, e_3\}, \quad D_3 = \{e_2, e_3\}.$$

Then form the level-3 supervertices by grouping overlapping level-2 supervertices:

$$A_1 = \{D_1, D_2\}, \quad A_2 = \{D_1, D_3\}, \quad A_3 = \{D_2, D_3\},$$

so that

$$V^{(3)} = \{A_1, A_2, A_3\}.$$

Finally, because each pair of these 3-supervertices overlaps, there is a single 3-superedge

$$S = \{A_1, A_2, A_3\},$$

giving

$$E^{(3)} = \{S\}.$$

Hence the Crystal 3-SuperHyperGraph is

$$\mathrm{CSHT}^{(3)} = (V^{(3)}, E^{(3)}) = \Big(\{A_1, A_2, A_3\}, \{\{A_1, A_2, A_3\}\}\Big).$$

This 3-superhypergraph captures a third-order meta-cluster linking all triangular coordination motifs in the square lattice into a single unified structure.

Example 5.5 (Crystal 4-SuperHyperGraph of Square-Lattice Fourth-Order Meta-Cluster)**.** Continuing the hierarchy from the 3-superhypergraph example, we construct the 4-superhypergraph for the same square-lattice atom set

$$V_0 = \{v_1, v_2, v_3, v_4\}, \quad e_1 = \{v_1, v_2, v_3\},\ e_2 = \{v_2, v_3, v_4\},\ e_3 = \{v_1, v_3, v_4\}.$$

Recall the level-2 supervertices:

$$D_1 = \{e_1, e_2\}, \quad D_2 = \{e_1, e_3\}, \quad D_3 = \{e_2, e_3\},$$

and the level-3 supervertices:

$$A_1 = \{D_1, D_2\}, \quad A_2 = \{D_1, D_3\}, \quad A_3 = \{D_2, D_3\}.$$

Level-4 supervertices: We form the single 4-supervertex by collecting all level-3 supervertices:

$$B = \{A_1,\ A_2,\ A_3\}.$$

Thus

$$V^{(4)} = \{B\}.$$

Level-4 superedges: Since there is only one 4-supervertex, the only nonempty 4-superedge is the singleton containing B:

$$E^{(4)} = \big\{\ \{B\}\big\}.$$

Crystal 4-SuperHyperGraph:

$$\mathrm{CSHT}^{(4)} = (V^{(4)},\ E^{(4)}) = \Big(\ \{B\},\ \{\{B\}\}\Big).$$

Here, the single 4-supervertex B encapsulates all triangular coordination motifs (level-3 clusters) in the square lattice, and the unique 4-superedge $\{B\}$ highlights the global, self-similar meta-structure at the fourth hierarchical level. This illustrates how iterated powerset constructions capture increasingly abstract, large-scale motif relationships in a crystalline environment.

Theorem 5.6 (Crystal n-SuperHyperGraph is an n-SuperHyperGraph)**.** *Every Crystal n-SuperHyperGraph* $\mathrm{CSHT}^{(n)} = (V^{(n)}, E^{(n)})$ *satisfies*

$$V^{(n)} \subseteq \mathcal{P}^n(V_0), \quad E^{(n)} \subseteq \mathcal{P}^n(V_0),$$

with incidence by membership, and hence by definition is an n-SuperHyperGraph.

Proof. By construction, both the set of n-supervertices $V^{(n)}$ and the set of n-superedges $E^{(n)}$ are subsets of $\mathcal{P}^n(V_0)$. The incidence relation $\{(v, e) : v \in V^{(n)}, e \in E^{(n)}, v \in e\}$ is exactly the membership relation required by the definition of an n-SuperHyperGraph. Therefore $\mathrm{CSHT}^{(n)}$ meets all the axioms of an n-SuperHyperGraph. □

Theorem 5.7 (Reduction to Crystal HyperGraph)**.** *If $n = 1$, then* $\mathrm{CSHT}^{(1)} = (V^{(1)}, E^{(1)})$ *coincides with the usual* Crystal HyperGraph $(V_0, \mathcal{E})$*, where*

$$V^{(1)} = V_0, \qquad E^{(1)} = \{ e_i : e_i = \{v_i\} \cup \mathcal{N}_i,\ i = 1, \ldots, N \},$$

and $\mathcal{N}_i$ is the set of k nearest neighbors of v_i. Conversely, any Crystal HyperGraph arises as $\mathrm{CSHT}^{(1)}$ *for appropriate choice of $E^{(1)}$.*

Proof. For $n = 1$, $\mathcal{P}^1(V_0) = \mathcal{P}(V_0)$. Setting $V^{(1)} = V_0$ and choosing

$$E^{(1)} = \{ e_i : \ e_i = \{v_i\} \cup \mathcal{N}_i \}$$

reproduces exactly the hyperedges of the standard Crystal HyperGraph. The incidence and all structural features then match. Conversely, any Crystal HyperGraph has vertex set V_0 and hyperedge set of this form, so it is an instance of $\mathrm{CSHT}^{(1)}$. □

Theorem 5.8 (Skeleton Consistency)**.** *Let* $\mathrm{CSHT}^{(n)} = (V^{(n)}, E^{(n)})$ *be a Crystal n-SuperHyperGraph over base atoms V_0. Define recursively for $k = n-1, n-2, \ldots, 0$:*

$$V^{(k)} = \bigcup_{S \in V^{(k+1)}} S, \qquad E^{(k)} = \{ F \subseteq V^{(k)} : F \subseteq e \text{ for some } e \in E^{(k+1)} \}.$$

Then for each k, $\mathrm{CSHT}^{(k)} = (V^{(k)}, E^{(k)})$ *is a Crystal k-SuperHyperGraph. In particular:*

- $\mathrm{CSHT}^{(1)}$ *recovers the standard Crystal HyperGraph.*
- $\mathrm{CSHT}^{(0)}$ *is the Crystal Graph.*

Proof. We proceed by downward induction. For $k = n$, the claim is true by definition. Assume $\mathrm{CSHT}^{(k+1)} = (V^{(k+1)}, E^{(k+1)})$ satisfies $V^{(k+1)} \subseteq \mathcal{P}^{k+1}(V_0)$ and $E^{(k+1)} \subseteq \mathcal{P}^{k+1}(V_0)$. Then

$$V^{(k)} = \bigcup_{S \in V^{(k+1)}} S \subseteq \bigcup_{S \in \mathcal{P}^{k+1}(V_0)} S = \mathcal{P}^k(V_0),$$

and each $F \in E^{(k)}$ is contained in some $e \in E^{(k+1)} \subseteq \mathcal{P}^{k+1}(V_0)$, so $F \subseteq \mathcal{P}^k(V_0)$. Thus $\mathrm{CSHT}^{(k)}$ meets the definition of a Crystal k-SuperHyperGraph. Applying this down to $k = 1$ and $k = 0$ yields the desired skeletons. □

Theorem 5.9 (Subedge-Induced Connectivity)**.** *In a Crystal n-SuperHyperGraph* $\mathrm{CSHT}^{(n)} = (V^{(n)}, E^{(n)})$*, each n-superedge $e \in E^{(n)}$ induces a connected subgraph in the underlying Crystal Graph on the* flat set $\mathrm{flat}(e) \subseteq V_0$ *of all base atoms appearing (possibly nested) in e.*

Proof. Let $e \in E^{(n)}$. By Skeleton Consistency (Theorem 5.8), e corresponds at level $n-1$ to a collection of $(n-1)$-supervertices whose union of base atoms is connected in the level-$(n-1)$ 2-section. Recursively descending through levels, the union of base atoms in e remains connected in the level-0 2-section, which is exactly the Crystal Graph. Therefore the induced subgraph on $\mathrm{flat}(e)$ is connected. □

6 Conclusion and Future Works

In this paper, we defined the concepts of Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs, and examined several concrete examples along with their mathematical properties.

As future work, we plan to explore extensions of these models by incorporating advanced uncertainty-handling frameworks such as Fuzzy Sets [103, 132, 133], Intuitionistic Fuzzy Sets [8–10], Vague Sets [3, 5, 54], Rough Sets [96, 97], Bipolar Fuzzy Sets [2, 135], HyperFuzzy Sets [32, 77, 122], Soft Sets [84, 87], HyperSoft Sets [?, 113], Picture Fuzzy Sets [24, 66], Neutrosophic Sets [109–111], Quadripartitioned Neutrosophic Sets [42,80,131], and Plithogenic Sets [39,46,47]. For example, we aim to explore the application of concepts from Fuzzy Sets and Fuzzy Graphs to Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs. These extensions are expected to further enhance the expressive power and practical applicability of our proposed models, particularly for capturing complex, multi-layered, and uncertain phenomena in materials science and beyond.

Furthermore, based on the above extensions of uncertainty modeling, we also hope that future research will explore the application of frameworks such as Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs through methods involving graph neural networks (GNNs) [52, 62, 67], artificial intelligence (AI) [7, 69], linear programming [72–74], and decision-making [34, 75, 85].

And as a future direction, we hope to explore extended concepts of the present paper by incorporating structures such as directed graphs [36], dynamic graphs [11, 12, 79], SemiGraphs [88, 98], bidirected graphs [14, 58, 130], and multidirected graphs [93, 94]. As demonstrated, many possibilities for further extensions and challenges remain, and we hope that future research by experts will continue to advance this field.

Data Availability

This research is purely theoretical, involving no data collection or analysis. We encourage future researchers to pursue empirical investigations to further develop and validate the concepts introduced here.

Ethical Considerations

This work does not involve any experiments or studies involving human participants or animals, and therefore no ethical approvals were required.

Conflicts of Interest

The authors confirm that there are no conflicts of interest related to the research or its publication.

Research Integrity

The authors hereby confirm that, to the best of their knowledge, this manuscript is their original work, has not been published in any other journal, and is not currently under consideration for publication elsewhere at this stage.

Disclaimer (Note on Computational Tools)

No computer-assisted proof, symbolic computation, or automated theorem proving tools (e.g., Mathematica, SageMath, Coq, etc.) were used in the development or verification of the results presented in this paper. All proofs and derivations were carried out manually and analytically by the authors.

Disclaimer (Limitations and Claims)

The theoretical concepts presented in this paper have not yet been subject to practical implementation or empirical validation. Future researchers are invited to explore these ideas in applied or experimental settings. Although every effort has been made to ensure the accuracy of the content and the proper citation of sources, unintentional errors or omissions may persist. Readers should independently verify any referenced materials.

To the best of the authors' knowledge, all mathematical statements and proofs contained herein are correct and have been thoroughly vetted. Should you identify any potential errors or ambiguities, please feel free to contact the authors for clarification.

The results presented are valid only under the specific assumptions and conditions detailed in the manuscript. Extending these findings to broader mathematical structures may require additional research. The opinions and conclusions expressed in this work are those of the authors alone and do not necessarily reflect the official positions of their affiliated institutions.

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