Original Research Article

Unifying Grain Boundary Networks and Crystal Graphs: A Hypergraph and Superhypergraph Perspective

Abstract

A hypergraph generalizes the classical notion of a graph by allowing edges—called hyperedges—to connect more than two vertices simultaneously. A superhypergraph further extends this idea by introducing recursively nested powerset layers, thus enabling hierarchical and self-referential relationships among hyperedges. Graphs are widely used to represent networks. In this context, hypernetworks and superhypernetworks serve as the network analogues of hypergraphs and superhypergraphs, respectively. Graph theory is also applied in material sciences. In this paper, we define the concepts of Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs, and examine several concrete examples along with their mathematical properties.

Keywords: Superhypergraph, Hypergraph, Crystal graphs, HyperNetworks, SuperHyperNetworks, Grain Boundary Networks

1 Introduction

1.1 HyperGraph and SuperHyperGraph

Graph theory is a branch of mathematics that studies networks in which nodes (called vertices) are connected by links (called edges) [15, 16]. Graphs have been extensively explored and applied across a wide range of disciplines, including social sciences [57,58], chemical graph theory [22,41,88], biological networks [56],graph neural networks (GNNs) [40,46], and telecommunications [69].

Mathematical structures can often be extended to hyperstructures and superhyperstructures by employing the power set and n-th iterated powerset constructions (cf. [78–80]). These extended frameworks are particularly effective for representing hierarchical and multi-layered systems, both in theoretical contexts and practical applications. Examples of such extensions include the superhyperalgebra [39, 51, 77], superhyperfuzzy sets [37,38], and superhyperneutrosophic sets [25,74], which generalize classical algebraic, topological, and logical systems to accommodate higher-order or nested structures.

When applied to graph theory, these extensions yield two well-known generalizations: the *hypergraph* and the *superhypergraph* [21, 32, 33]. 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 [8,9,17]. A superhypergraph builds upon this by incorporating recursively nested powerset structures, allowing for hierarchical and self-referential interactions among groups of hyperedges. 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. [26, 48]).

1.2 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 [11, 12, 53, 59]. 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 [19, 65, 70]. A Crystal Graph represents atoms as nodes and interatomic bonds as edges, defined by spatial proximity within a periodic crystal lattice [61, 68, 92]. 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 [18], Dislocation Networks [5, 85], and Fracture Networks [1, 10], each providing insights into specific physical mechanisms.

1.3 Our Contribution

This subsection outlines the main contributions of the present paper. We define the concepts of Grain Boundary HyperNetworks, Grain Boundary SuperHyperNetworks, and Crystal SuperHyperGraphs, and examine several concrete examples along with their mathematical properties. Through these contributions, we hope to advance research on the Grain Boundary Network, the Crystal Graph, and graph theory more broadly, even if only modestly.

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 [81]. Intuitively, the n-th powerset is a repeated application of the powerset operation. Relevant definitions and simple examples are provided below.

Definition 2.1 (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 2.2 (Powerset)**.** [23, 66] 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:

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

Definition 2.3 (n-th Powerset)**.** (cf. [23, 81])

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.

Definition 2.4 (Classical Structure)**.** (cf. [72, 81]) 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 2.5 (Hyperoperation)**.** (cf. [64, 89–91]) 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 2.6 (Hyperstructure)**.** (cf. [23,72,81]) 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.

Definition 2.7 (SuperHyperOperations)**.** (cf. [81]) 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 2.8 (n-Superhyperstructure)**.** (cf. [24,30,81]) 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 2.9 (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 [8, 43, 44].

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 [25, 26, 34, 76].

Definition 2.10 (Hypergraph)**.** [8, 9] 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.

Definition 2.11 (n-SuperHyperGraph)**.** [75, 76]
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 2.12 (Real-World Example of a 2-SuperHyperGraph)**.** Consider the hierarchical microstructure [55, 60] 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.

Definition 2.13 (Network)**.** A *network* (or *graph*) is an ordered triple

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

where

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

If edges are *directed*, one instead writes

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

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

Definition 2.14 (Hypernetwork)**.** (cf. [4, 13, 26, 47]) A *hypernetwork* is an ordered triple

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

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);
- $w\colon \mathcal{E} \to \mathbb{R}_{\geq 0}$ 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 2.15 (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:

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

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

- For each pair $\{\mathrm{G}_i, \mathrm{G}_j\}$: the measured grain-boundary energy per unit area,

  $$w(\{\mathrm{G}_i, \mathrm{G}_j\}) = \gamma_{ij} \quad (\mathrm{J/m^2}),$$

  e.g. $\gamma_{12} = 0.60$, $\gamma_{23} = 0.55$, $\gamma_{34} = 0.62$.

- For each triple $\{G_i, G_j, G_k\}$: the triple-junction line energy per unit length,
$$w(\{G_i, G_j, G_k\}) = \tau_{ijk} \quad \text{(J/m)},$$
e.g. $\tau_{123} = 1.20$, $\tau_{234} = 1.15$.

In this hypernetwork:

- 2-node hyperedges $\{G_i, G_j\}$ represent individual grain boundaries.
- 3-node hyperedges $\{G_i, G_j, G_k\}$ 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 2.16 (n-SuperHypernetwork)**.** [26] 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 2.17 (2-SuperHypernetwork in Polycrystalline Microstructure)**.** A polycrystalline microstructure consists of numerous small crystals or grains, each with different orientations, separated by grain boundaries (cf. [67, 71, 83]). Consider a polycrystalline alloy whose microstructure consists of five grains:
$$V_0 = \{G_1, G_2, G_3, G_4, G_5\}.$$
First iterated powerset (grain-boundary pairs):
$$\mathcal{P}^1(V_0) \supseteq \{\{G_1, G_2\}, \{G_2, G_3\}, \{G_3, G_4\}, \{G_4, G_5\}\}.$$
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:
$$V = \{v_1, v_2\} \subseteq \mathcal{P}^2(V_0),$$
$$v_1 = \{\{G_1, G_2\}, \{G_2, G_3\}\},$$
$$v_2 = \{\{G_3, G_4\}, \{G_4, G_5\}\},$$
and
$$\mathcal{E} = \{e_1\} \subseteq \mathcal{P}^2(V_0), \qquad e_1 = \{v_1, v_2\},$$
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 $\{G_i, G_j\}$ 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 [19, 65, 70]. If we were to define it mathematically, it could be expressed as follows.

Definition 2.18 (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 2.19 (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. [45, 96]). Consider a 2D polycrystalline domain Ω partitioned into three wedge-shaped grains meeting at the origin:

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

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

$$\mathbf{n}_{12} = (\cos 120^\circ, \sin 120^\circ),$$

$$\mathbf{n}_{23} = (\cos 240^\circ, \sin 240^\circ),$$

$$\mathbf{n}_{13} = (\cos 0^\circ, \sin 0^\circ).$$

Thus the Grain Boundary Network is

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

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

2.5 Crystal Hypergraph

A Crystal Graph represents atoms as nodes and interatomic bonds as edges based on spatial proximity within a periodic crystal lattice [61, 68, 92]. If we were to define it mathematically, it could be expressed as follows.

Definition 2.20 (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

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

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 2.21 (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 $\|\mathbf{r}_j - \mathbf{r}_i\| = 1 \le r_c$ are included (with $\mathbf{R} = \mathbf{0}$ in Λ). Each edge (v_i, v_j) carries the feature

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

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. [50]). If we were to define it mathematically, it could be expressed as follows.

Definition 2.22 (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 $\mathcal{N}_i = \{v_{i_1}, \dots, v_{i_k}\}$ of the k closest neighbors (including periodic images). The *crystal hypergraph* is the hypergraph

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

where the hyperedge set

$$\mathcal{E} = \left\{ e_i : i = 1, \dots, N \right\}, \quad e_i = \{v_i\} \cup \mathcal{N}_i$$

connects each central atom v_i with its k-nearest neighbors. Each hyperedge e_i is equipped with a feature vector $\mathbf{h}_{e_i} = [\, d_{i,i_1}, \dots, d_{i,i_k}, \alpha_{i,i_1,i_2}, \dots]$ 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 2.23 (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 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.

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

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

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

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

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.

Theorem 3.3 (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 3.4 (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. □

Definition 3.5 (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

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

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 3.6 (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:

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

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 3.7 (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 3.8 (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 3.9 (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. □

4 Result: Crystal n-SuperHypergraph

A Crystal n-SuperHypergraph models atomic structures using nested powersets, capturing hierarchical groupings of atoms and their multi-level interactions.

Definition 4.1 (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 4.2 (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 4.3 (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

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

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

Theorem 4.4 (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 4.5 (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*

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

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

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

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 4.7 (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 4.6), 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. □

5 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 [94,95], Intuitionistic Fuzzy Sets [6,7], Vague Sets [3,42], Rough Sets [62,63], Bipolar Fuzzy Sets [2], HyperFuzzy Sets [20,52,84], Picture Fuzzy Sets [14,49], Hesitant Fuzzy Sets [86,87], Neutrosophic Sets [73,82], Quadripartitioned Neutrosophic Sets [31,54,93], HyperPlithogenic Sets [27–29], and Plithogenic Sets [25,35,36].

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.

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 Approval

As this research is entirely theoretical in nature and does not involve human participants or animal subjects, no ethical approval is required.

Conflicts of Interest

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

Disclaimer

This work presents theoretical concepts that have not yet undergone practical testing or validation. Future researchers are encouraged to apply and assess these ideas in empirical contexts. While every effort has been made to ensure accuracy and appropriate referencing, unintentional errors or omissions may still exist. Readers are advised to verify referenced materials on their own. The views and conclusions expressed here are the authors' own and do not necessarily reflect those of their affiliated organizations.

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