Supplementary Materials

Advances in graph neural networks for alloy design and properties predictions: a review

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1. Supplementary information on different types of graphs

Supplementary Table 1. Different types of graphs and corresponding descriptions

Graph type	Variant Name	Description
Directed	DGP[1]	Directed graphs leverage edge direction.
Heterogeneous[2]	HAN[3]	HAN captures key relationships in heterogeneous graphs through multi-level attention mechanisms.
	MAGNN[4]	MAGNN captures rich semantic information in heterogeneous graphs through intra-metapath aggregation and interaction.
	HetGNN[5]	HetGNN enhances representation learning in heterogeneous graphs by integrating node features and structure.
	GTN[6]	GTN learns multi-hop meta-path connections to capture latent relationships in heterogeneous graphs.
	G2S[7]	G2S converts graph structures into sequences, enabling sequence-based modeling.
Dynamic	DCRNN[8]	DCRNN models spatiotemporal dependencies using diffusion convolution and recurrent neural networks.
	DGNN[9]	DGNN captures key features in dynamic relationships by adaptively updating graph structures.
Hypergraph	HGNN[10]	HGNN leverages hypergraph structures to capture high-order relationships and enhance node representations.
Signed	SGCN[11]	SGCN improves GNN efficiency and performance by sparsifying graph structures.
Large Graph	APPNP[12]	APPNP combines random walk and propagation mechanisms for efficient and accurate node representation learning.
	ProPPR[12]	ProPPR efficiently infers node relationships in graphs using constrained random walks.

2. Supplementary information on different types of graphs

Supplementary Table 2. Graph structural features stratified by different levels

Level of Graph	Attributes	Description
Nodes	Element type	The type(s) of element(s) present in the alloy.
	Atomic number[13]	The number of protons in the nucleus of the element, serving as its fundamental identifier.
	Atomic mass	The mass of the element's atoms, influencing the overall density and some mechanical properties of the materials.
	Electronegativity	The tendency of an atom to attract electrons when forming chemical bonds.
	Coordination number[16]	The number of atoms to which a given atom is directly bonded in the alloy.
	Lattice type[17]	The crystal structure (e.g., FCC, BCC) corresponding to the arrangement of atoms.
	Atomic position[18]	The spatial coordinates of each atom within the lattice.
	Density	The mass-to-volume ratio of the material (for each element, often taken as its standard/pure density).
	Melting point	The temperature at which the element transitions from a solid to a liquid phase.
	Thermal conductivity	The ability of the element (or resulting material) to conduct heat.
	Electrical conductivity	The ability of the element (or resulting material) to conduct electricity.
	Elastic modulus	The element's (or material's) resistance to elastic deformation under stress.
	Yield strength	The stress at which the element (or material) begins to plastically deform.
	Hardness	The resistance of the element (or material) to localized plastic deformation (e.g., indentation or scratching).
	Gibbs free energy[19]	A measure of the thermodynamic potential of the element,

		relevant to its stability in reactions or phase changes.
	Band structure	The electronic band characteristics (e.g., conduction and valence bands) associated with the element.
	Valence electron density	The distribution or concentration of valence electrons for a given element.
	Diffusion coefficient	The rate at which an element diffused through the alloy under given conditions.
	Metal Price[20]	The market cost of the element, affecting the economic feasibility and large-scale production considerations.
	Voronoi information[21]	Descriptors of local atomic environments, derived from Voronoi tessellation methods in materials science.
Vertices	Type of Chemical Bond Between Elements	Specifies the bond category (e.g., metallic, covalent, ionic) linking two elements.
	Bonding Energy[22]	The energy required to break or form the bond between two elements, indicating bond strength.
	Atomic Spacing[23]	The average atomic distance between two elements in the alloy.
	Atomic Exchange Energy	The energy associated with the exchange (or swapping) of atomic positions between different elements.
	Bond Angle[24]	The angle between two bonds originating from the same atom, reflecting local geometrical arrangement and stability.
Graph	Ambient Temperature	The environmental temperature affecting phase stability, diffusion behavior, and mechanical properties of the alloy.
	Applied Pressure	External pressure applied to the alloy, influencing phase transformations and mechanical behavior.
	Chemical Environment	The surrounding chemical atmosphere (e.g., inert, oxidizing), which can affect reactions such as corrosion or oxidation.
	Applied Electric Field	The strength of the electric field, which can influence

	diffusion and electrical properties in the alloy.
Applied Magnetic Field	The strength of the external magnetic field, which can affect phase transitions, domain structures, or magnetic properties of the alloy.

3. Supplementary information on different types of GNNs

Supplementary Table 3. Different kinds of GNN

GNN type	Variants	Description
Recursive GNN[13]	Gated Recursion-based Graph Neural Network (GR-GNN)[14]	Uses gated recursion to enhance node and edge information propagation within graphs.
	Deep Recurrent Graph Neural Network (DRGNN)[15]	Employs recurrent graph convolutional layers and pooling for effective graph classification, initially applied in bioinformatics datasets.
Convolutional GNN[16]	Graph Convolutional Recurrent Networks (GCRN)[17]	Combines graph convolutional layers and RNNs to capture both spatial and temporal dependencies in dynamic graph data.
	Graph Sample and Aggregation (GraphSAGE)	A scalable GNN model that aggregates features from a fixed-size neighborhood using functions such as mean, LSTM, or pooling, enabling it to handle large-scale graph datasets efficiently.
	Graph Attention Network (GAT)	Introduces attention mechanisms to GNNs, allowing each node to assign different weights to its neighbors when aggregating information.
Graph Autoencoders (GAE)[18]	Variational Graph Autoencoder (VGAE)	Extends GAE with a variational framework for probabilistic learning of node embeddings.

	GraphMAE (Masked Graph Autoencoders)[19]	A self-supervised model focusing on feature reconstruction with masked node features and a scaled cosine error function to achieve robust training.
Spatial-temporal GNN(ST-GNNs)[20]	Spatial-temporal Graph Neural Networks (ST-GNNs)	Integrates temporal convolutional networks and graph convolutions in a modular fashion, commonly used for fast traffic prediction by modeling spatial-temporal correlations.
	ASTGCN (Attention-Based Spatial-Temporal Graph Convolutional Network)[21]	Employs attention mechanisms across both spatial and temporal dimensions, enabling dynamic correlation modeling in traffic data.

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