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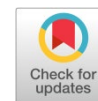
Synthesis and Sintering

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Perspective

AI-agent–enhanced knowledge graphs and memory-augmented models as a new paradigm for intelligent sintering systems



Pouria Dianati Souha *

Department of Aeronautical Engineering, Faculty of Aviation and Space Science, University of Kyrenia, Kyrenia, Mersin 10, Turkey

ABSTRACT

Sintering processes play a critical role in materials manufacturing; however, their optimization remains highly dependent on empirical knowledge, fragmented datasets, and costly experimental trials. Existing modeling and machine learning approaches often lack a unified structure for representing complex relationships among processing parameters, microstructural evolution, and final material properties. This perspective article argues that knowledge graphs can serve as a missing semantic layer for organizing sintering-related data, enabling structured representation of process–property relationships across heterogeneous databases. Furthermore, the integration of autonomous AI agents equipped with memory-augmented learning models is proposed as a promising direction for continuously constructing, updating, and reasoning over such knowledge graphs. By combining structured knowledge representation with adaptive learning and agent-based optimization, this framework has the potential to transform sintering research into a self-improving, data-driven ecosystem. This perspective highlights future research directions toward intelligent, explainable, and autonomous sintering systems for advanced materials engineering.

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KEYWORDS

Knowledge graphs
AI agents
Memory-augmented models
Sintering
Intelligent manufacturing
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1. Introduction

Sintering is a cornerstone process in materials science and manufacturing, enabling the production of metals, ceramics, and advanced composites with tailored microstructures and functional properties. The final performance of sintered materials—such as density, porosity, grain morphology, and mechanical strength—is governed by a complex interplay of processing parameters, including temperature profiles, heating and cooling rates, dwell time, and intrinsic material characteristics. Even small variations in these parameters can lead to significant changes in microstructural evolution and final material behavior [1, 2].

Despite decades of experimental investigation and theoretical modeling, the optimization of sintering processes remains largely empirical. Conventional approaches rely heavily on trial-and-error experimentation, expert intuition, and simplified physical models that

often fail to capture the high-dimensional and history-dependent nature of sintering. Although numerical simulations and machine learning techniques have been increasingly applied to assist process optimization [3–6], their impact has been limited by fragmented datasets, poor generalization across material systems, and a lack of interpretability [3, 4].

From a data-driven perspective, sintering can be viewed as a mapping from a sequence of processing conditions to final material properties. In practice, learning or modeling this function is challenging due to incomplete data, implicit domain knowledge, and the absence of a unified representation that links processing parameters, microstructural transformations, and physical constraints. Recent advances in artificial intelligence have opened new opportunities for addressing these challenges [5, 7, 8].

* Corresponding author. E-mail address: puryadianati@gmail.com (P. Dianati Souha)

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However, most existing machine learning models for sintering operate as isolated predictors, treating input variables as static features while ignoring process history, domain knowledge, and causal relationships. This perspective argues that the primary bottleneck in the digital transformation of sintering research is not the lack of algorithms, but the absence of an integrated intelligence framework. Specifically, knowledge graphs are needed to explicitly represent structured domain knowledge and process–property relationships; autonomous AI agents are required to continuously construct, validate, and update this knowledge from heterogeneous data sources; and memory-augmented learning models are essential to capture the temporal and path-dependent nature of sintering processes.

2. Mathematical formulation of the proposed paradigm

To formalize the proposed AI-driven paradigm for intelligent sintering systems, this section introduces a unified mathematical framework that integrates process history modeling, knowledge graph representation, memory-augmented prediction, and agent-based optimization. The equations are numbered sequentially to facilitate reference.

2.1. Problem setup: Process–structure–property mapping

Sintering can be fundamentally described as a dynamic mapping from a sequence of processing conditions to final material properties. Let $x_t \in \mathbb{R}^d$ denote the vector of processing parameters at time step t , including temperature, heating rate, atmosphere, and other controllable variables. The complete processing history is then defined as:

$$x_{1:T} = \{x_1, x_2, \dots, x_T\} \quad (1)$$

Let m represent material-specific attributes such as composition, particle size distribution, and initial packing characteristics, and let y denote the resulting material properties. The sintering process can be expressed as:

$$y = f(x_{1:T}, m) \quad (2)$$

where f is an unknown, nonlinear, and history-dependent function.

2.2. Knowledge graph formalization

To explicitly represent domain knowledge and process–property relationships, a knowledge graph is introduced as a semantic backbone. The knowledge graph is defined as:

$$G = (V, E, R) \quad (3)$$

where V is the set of entities, E is the set of edges, and R denotes the types of relationships among entities. Knowledge is encoded in the form of relational triples:

$$(h, r, t) \in T \quad (4)$$

where h and t represent head and tail entities, respectively, and $r \in R$ denotes the relation type. For computational reasoning, entities and relations are embedded into a vector space. Relational consistency is encouraged through:

$$h + r \approx t \quad (5)$$

The embedding parameters are optimized by minimizing a margin-based ranking loss:

$$L_{KG} = \sum_{(h,r,t) \in T} \max(0, \gamma + d(h + r, t) - d(h' + r, t')) \quad (6)$$

where γ is the margin hyperparameter in the ranking loss function.

2.3. Memory-augmented predictive model

To capture the history-dependent nature of sintering, a memory-augmented predictive model is employed. Let h_t denote the latent state of the model at time t . The state evolution is defined as:

$$h_t = f_\theta(h_{t-1}, x_t) \quad (7)$$

The final prediction of material properties integrates the terminal latent state with knowledge graph embeddings:

$$\hat{y} = g_\phi(h_T, z_{KG}) \quad (8)$$

where z_{KG} is a knowledge-informed representation derived from the graph embeddings. Supervised learning is guided by a standard regression loss:

$$L_{pred} = \|y - \hat{y}\|^2 \quad (9)$$

2.4. Agent policy and optimization objective

An autonomous AI agent proposes sintering strategies. At time t , the agent observes a state s_t and selects an action a_t according to a policy:

$$a_t \sim \pi_\theta(a_t | s_t, G) \quad (10)$$

The objective of the agent is to maximize the expected cumulative reward:

$$J(\pi) = E \left[\sum_{t=1}^T \beta^{t-1} r_t \right] \quad (11)$$

where β is the discount factor ($0 < \beta \leq 1$) for future rewards, and r_t is the reward at time t .

Policy parameters are updated using a policy gradient formulation:

$$\nabla_\theta J(\pi_\theta) = E[\nabla_\theta \log \pi_\theta(a_t | s_t) \hat{A}_t] \quad (12)$$

Here, s_t denotes the observed system state and A_t the advantage estimate.

A multi-objective optimization formulation accounts for competing objectives: $\min_p [w_1(1 - \rho) + w_2 \text{porosity} + w_3 \text{cost} - w_4 \text{strength}]$, where ρ denotes relative density.

2.5. Application to realistic sintering scenarios

While the mathematical formulation provides a theoretical basis, its practical value is best illustrated through specific material systems. Sintering involves distinct mechanisms—such as surface diffusion, grain boundary diffusion, and volume diffusion—that dominate at different stages of the thermal cycle. Fig. 1 illustrates these mechanisms in a visual format.

Consider the case of alumina (Al_2O_3) ceramic sintering. Achieving full density while suppressing grain growth is a classic optimization challenge. At intermediate temperatures (e.g., 1200 °C), surface diffusion contributes to neck growth without densification. As temperatures exceed 1400 °C, grain boundary diffusion and volume diffusion become active, driving shrinkage. An AI agent, utilizing the formulation in multi-objective optimization problem, would balance the conflicting objectives of maximizing density (ρ) while minimizing grain size (represented implicitly in the "strength" term). The knowledge graph would constrain the search space by encoding the known activation energies for these diffusion mechanisms, preventing the agent from proposing physically implausible rapid heating rates that would lead to thermal shock or entrapped porosity.

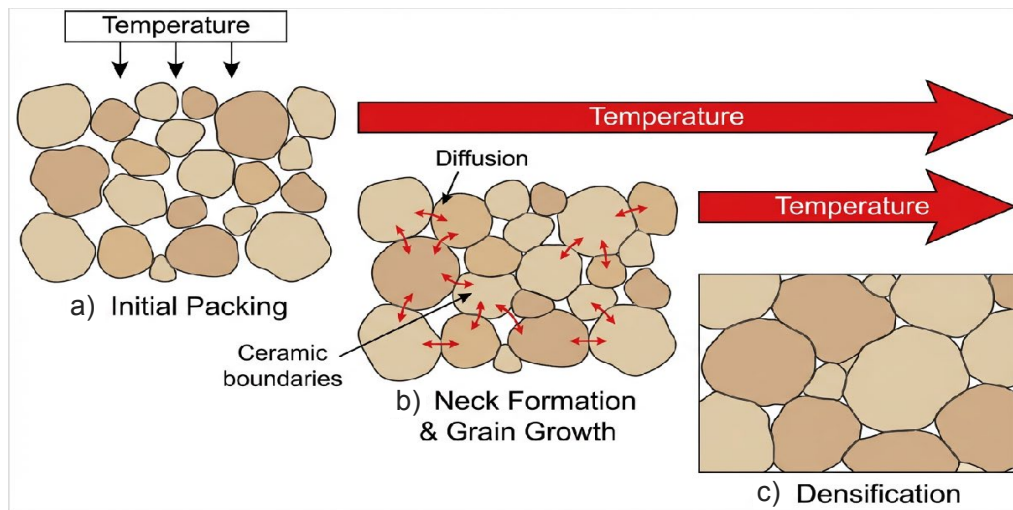


Fig. 1. Conceptual visualization of sintering evolution: a) initial particle packing with voids, b) intermediate stage showing neck formation driven by surface and grain boundary diffusion, and c) final densified structure with grain growth.

In stainless steel (e.g., 316L) powder metallurgy, the problem extends to atmosphere control. The variable x_t in Eq. 1 must include partial pressure of hydrogen or vacuum levels to manage oxide reduction. The memory-augmented model (Eq. 7) is particularly critical here, as the removal of binders at lower temperatures (300–500 °C) dictates the final carbon content and corrosion resistance. If the heating rate is too high during debinding, defects form that cannot be healed later. The memory state h_t captures this history, allowing the model to predict failure even if the final sintering temperature is correct.

3. Knowledge graphs as the missing layer in sintering research

Sintering research produces a large volume of heterogeneous and distributed knowledge. Knowledge graphs provide a principled solution by offering a structured, semantic, and machine-interpretable representation of domain knowledge. Unlike conventional tabular databases, knowledge graphs explicitly encode entities and their relationships, allowing complex dependencies to be represented in a unified framework.

3.1. Ontology design for sintering knowledge

At the core of a sintering knowledge graph lies a domain-specific ontology that defines the fundamental concepts and their relationships. A minimal ontology for sintering includes material system, processing parameters, microstructural features, and physical mechanisms. Fig. 2 illustrates this structure.

3.2. Constraint-aware reasoning

A key advantage of knowledge graphs is their ability to support logical reasoning. Constraint satisfaction can be expressed as:

$$C(G) = 0 \quad (13)$$

where C represents a set of physical constraints (e.g., monotonic density increase with time). By enforcing such constraints, reasoning becomes physically grounded.

4. AI agents for autonomous knowledge construction

In the proposed paradigm, an autonomous AI agent operates as a goal-driven system that interacts with data sources, the knowledge graph G , and constraints. The agent iteratively improves the knowledge graph by extracting new entities/relations and validating them.

4.1. Algorithm and workflow

The agent operates in a continuous loop, formalized as an algorithm that combines information extraction with constraint-aware validation. Fig. 3 depicts this autonomous workflow.

4.2. Knowledge graph-guided active learning

AI agents can actively guide data acquisition. We propose a strategy where the agent selects an action a to maximize information gain [9, 10]:

$$a^* = \operatorname{argmax}_a I(y; a | D) \quad (14)$$

This formulation allows the system to prioritize experiments that resolve uncertainty in the knowledge graph or process model.

5. Memory-augmented models for sintering intelligence

Sintering is inherently history-dependent. Conventional static models limit predictive accuracy by ignoring temporal trajectories. Memory-augmented models (Eq. 7) address this by maintaining a latent state h_t that evolves with the process. Attention mechanisms can further enhance this by selectively weighting critical process stages, such as the onset of rapid shrinkage or the peak temperature dwell.

6. Toward a self-optimizing sintering ecosystem

The integration of knowledge graphs, autonomous AI agents, and memory-augmented predictive models leads to a self-optimizing ecosystem. Unlike offline tuning, this framework enables adaptive

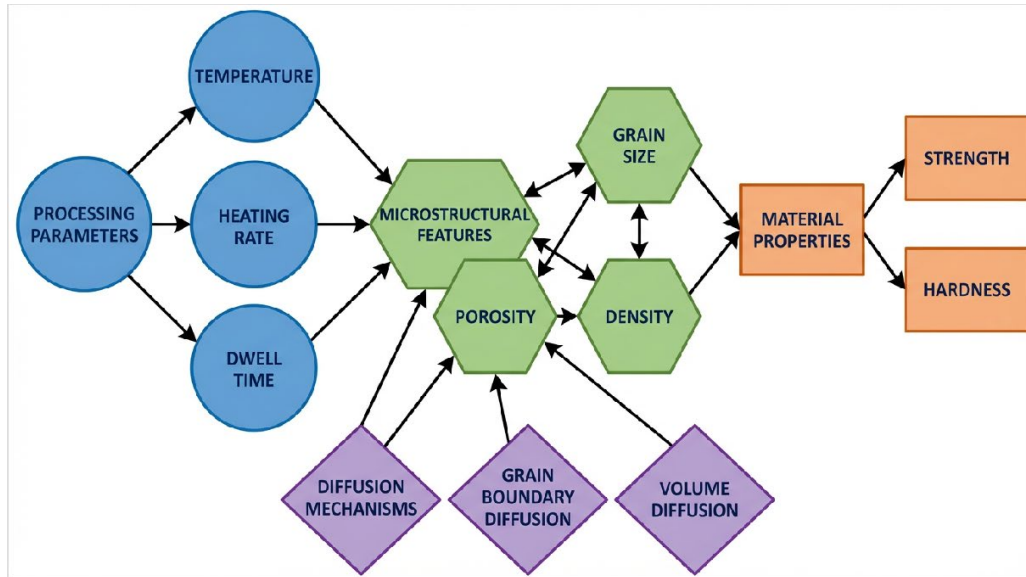


Fig. 2. Schematic representation of the sintering knowledge graph ontology. Blue circles represent processing parameters (T, time, rate), green hexagons represent microstructural features (grain size, porosity), and orange rectangles denote final properties (strength, hardness), all connected via semantic relationships.

refinement. The closed-loop optimization objective (multi-objective optimization problem) is dynamically updated as the agent learns, and Bayesian optimization provides data-efficient exploration of the parameter space. This paradigm shifts materials processing from human-driven trial-and-error to autonomous, intelligent precision engineering.

7. Future directions

Future research should focus on developing large-scale, community-

driven sintering knowledge graphs to improve data reuse. Additionally, advancing AI agents capable of direct interaction with high-fidelity simulations and experimental equipment (digital twins) will be crucial. Standardization of ontologies will facilitate interoperability between different research groups and AI systems.

8. Conclusions

This perspective has presented a unified framework for intelligent sintering systems. By formalizing sintering as a sequence-dependent

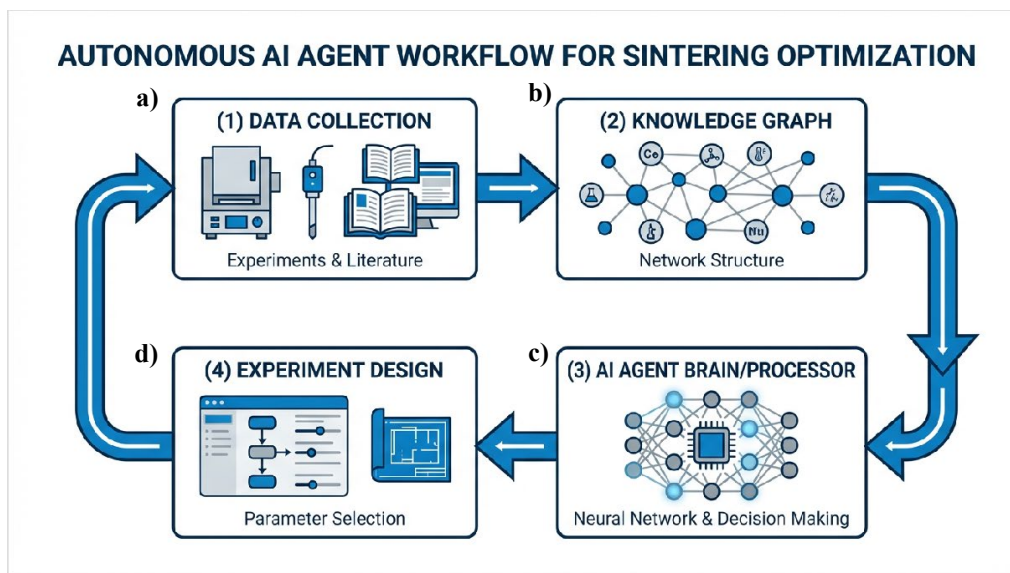


Fig. 3. Conceptual architecture of the autonomous AI agent. The system operates in a closed loop: a) data collection from experiments/literature, b) integration into the knowledge graph, c) reasoning via the AI agent "brain", and d) intelligent experiment design which feeds back into data collection.

mapping and leveraging knowledge graphs for structured representation, we can overcome the limitations of fragmented data. Autonomous agents and memory-augmented models provide the necessary dynamic reasoning capabilities. Together, these components form the foundation for a self-improving sintering ecosystem that promises to accelerate materials discovery and process optimization.

CRediT authorship contribution statement

Pouria Dianati Souha: Conceptualization, Methodology, Formal Analysis, Investigation, Writing – original draft, Writing – review & editing, Visualization, Validation.

Data availability

The data underlying this article will be shared on reasonable request to the corresponding author.

Declaration of competing interest

The author declares no competing interests.

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Declaration of Ai and Ai-assisted technologies in the writing process

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