Machine learning approaches for intentional materials engineering

Yu-chen Karen Chen-Wiegart,* Norbert Huber, and Kevin G. Yager

The development of nanoporous metals and metallic composites through dealloying processes presents significant opportunities in materials engineering. However, designing multicomponent precursor alloys and establishing corresponding processing methods that yield predictable compositions and nanostructures remain a complex challenge. This article explores how machine learning (ML)-augmented computational and experimental methodologies can tackle these challenges by predicting precursor alloy compositions, final nanoporous structures, and mechanical properties, while integrating ML-enabled autonomous experimentation for material design and quantification. We highlight recent advancements in applying ML to nanostructured materials design via dealloying and discuss how techniques from other nanomaterial designs can be adapted for improved control over morphological and compositional outcomes in nanoporous and nanocomposite materials. Furthermore, we explore the role of ML in autonomous synchrotron x-ray experimentation, enabling real-time feedback between modeling and experimental setups. ML-driven approaches to microstructure characterization and mechanical property prediction are also examined, with a focus on modeling and advanced imaging techniques such as three-dimensional nanotomography. Finally, this article outlines future directions for ML-enhanced materials science, emphasizing the exploration of high-dimensional parameter spaces and the incorporation of materials kinetics into processing and property evaluation, ultimately advancing the design of nanoporous structures and materials science.

Introduction

Dealloying, as a phenomenon, refers to the selective dissolution of one or more components from an alloy.[1–3] In modern times, it has been reinvented as an innovative processing method to create nanoporous metals and metallic nanocomposites for a wide range of applications, including catalysis, sensors, actuators, batteries, fuel cells, and separation materials.[4–9] More specific applications, such as surface-enhanced Raman scattering[10,11] and radiation shielding,[12] have also been demonstrated. This is because the remaining component can self-organize into a connected network, forming an intricate, so-called "bicontinuous" nanostructure.

The term "bicontinuous" refers to two phases, each forming a continuous network, while the two phases are interlocking, as shown in **Figure 1**a. For nanoporous metals, these phases are the metal ligaments and pores, whereas for metallic nanocomposites, they consist of two different metals or alloys. Nanoporous metals can also be further infiltrated to create a broader range of composites for applications, such as artificial bones.[13,14] To initiate the selective dissolution process, a variety of solvents can be used, including aqueous solutions, ionic liquids, molten metals, molten salts, organic electrolytes, and solid metals, provided there is a driving force to remove one of the components from the precursor alloy.[15–17] For nonmetal solvents, the process can be applied under an electrochemical potential, utilizing the differing redox potentials of the elements to control the dealloying process.[18,19] Various types, shapes, and forms can be produced and integrated into the dealloying workflow, including three-dimensional (3D) printed hierarchical structures, thin films, microcrystalline or amorphous alloys, shells, and microspheres.[20,21]

Despite its potential in materials science and engineering, creating nanoporous metals and metallic nanocomposites via dealloying has often relied on intuition-driven, "trial-and-error" discovery processes. To overcome these challenges, machine learning (ML)-augmented data-driven approaches

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can be applied throughout the materials design, processing, and characterization cycle. Its potential to revolutionize the field is exciting, with impacts including materials discovery, property prediction, computational modeling, simulation enhancement, and image processing.[25]

ML-augmented materials discovery has been explored across various systems. Generally, ML applications in materials discovery have focused on predicting compositions to achieve target properties. Examples include high-entropy alloys, photovoltaic materials, thin-film metallic glasses, shape-memory alloys, energy-storage materials, and catalysts.[26–31] Promising developments in processing optimization have also emerged, such as ML for chemical vapor deposition of thin films,[32] nanoparticle synthesis control,[33] 3D printing structural design,[34] and stability assessments in solid-state synthesis.[35] Text-mined literature recipes have shown promise for areas such as battery materials, nanotubes[36,37] and metal–organic frameworks synthesis.[38,39]

This article includes three parts to cover how ML-augmented computational and experimental methods can be applied to address challenges in predicting precursor alloy compositions, nanoporous structures, and mechanical properties, while incorporating ML-driven autonomous experimentation for material design and analysis. The first section highlights recent progress in applying ML to the design of nanostructured materials through dealloying and explores how techniques from other nanomaterial designs can be adapted for better control of morphology and composition in nanoporous and nanocomposite materials. The second section focuses on characterization, discussing the role of ML in autonomous synchrotron x-ray experimentation, enabling real-time feedback between modeling and experiments. The third section then expands to understand the structure–property relationship where the ML-based approaches for microstructure characterization and mechanical property prediction are reviewed, focusing on modeling and advanced imaging techniques such as 3D nanotomography. Finally, based on the review of these three areas, the article suggests future directions for ML-enhanced materials science, emphasizing the exploration of high-dimensional parameter spaces and the integration of materials kinetics in processing and property assessments, advancing the design of nanoporous structures.

Materials discovery and design with dealloying

While a wide range of materials and structures have been created through dealloying, along with a growing list of applications, the design and development of dealloyed nanomaterials with bicontinuous structures and their derived architectures face similar challenges to those of other complex engineering materials. Most of these materials were developed through trial-and-error approaches, with slow iteration processes to improve materials properties. Key challenges include determining stable phases during dissolution and phase separation, creating specific bicontinuous morphologies with designated nanofeatures, and designing practical engineering processing protocols. The design space is vast, involving a range of engineering parameters related to the underlying physical and chemical properties of the materials and environmental conditions. On a fundamental level, the mechanisms involved are often too complex to be fully understood through experiments and computational modeling alone, as they involve various forms of mass transport processes (long-range and surface diffusion) and chemical/electrochemical reactions (Figure 1b). The key design concepts in dealloying include phase selection, morphology, and processability. These complexities, coupled with various types of dealloying processes with different dealloying agents, make it challenging to rationally design materials created through dealloying.

Recent developments on ML-augmented materials design in dealloying materials

This section focuses primarily on ML-augmented materials design and discovery, with relevance to dealloying materials, while other related topics will be addressed in subsequent sections. In the materials design cycle, both forward and reverse approaches are being considered. In the forward direction, processing creates structure, structure determines properties, and properties enable functionality—known as "forward predictability." In the reverse, or "designability," approach, one begins with a desired functionality that necessitates specific materials properties, structures, and processing methods to achieve the design goals. Both directions are challenging, typically requiring iterative processes to reach the desired outcome.

Specifically in dealloyed materials, data mining and automated image analysis have been applied to identify coarsening mechanisms in nanoporous gold.[40] Zhao et al. presented an ML framework for predicting dealloying systems, using combinatorial thin-film deposition and autonomous synchrotron x-ray diffraction to explore nanoarchitectured materials; **Figure 2**c illustrates the workflow.[24] However, validating these ML models and further refining them remain challenging. In follow-up work, Chung et al. attempted validation of a newly predicted system through a multimodal synchrotron x-ray characterization;[41] the work initially aimed to validate the ML model but instead discovered the significant role of the oxidation-driven process, which had not been considered in prior studies. This finding highlights the importance of oxidation in controlling nanoscale phase separation, adding a new layer of understanding to dealloying processes and suggesting additional factors for consideration in future ML models. Validation challenges, partly due to the complex parameter space, including kinetics (e.g., dealloying time and temperature), have driven recent efforts such as gradient sample creation via laser heating, showing promise in parameter exploration.[42]

Potential opportunities for developing ML-related methods in dealloying materials

- **Incorporating microstructures, morphology, and kinetics in ML-augmented design:** Materials discovery and

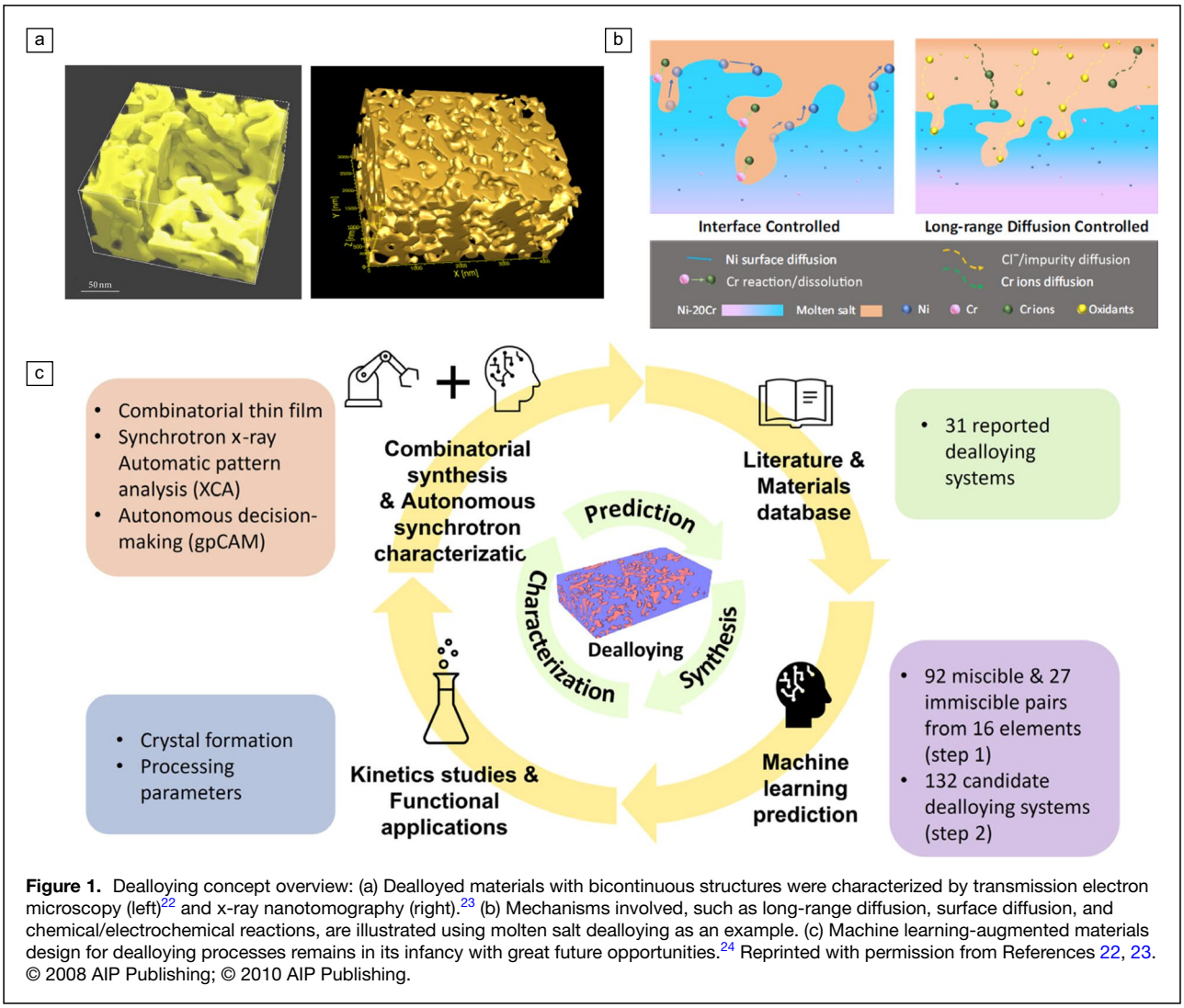

Figure 1. Dealloying concept overview: (a) Dealloyed materials with bicontinuous structures were characterized by transmission electron microscopy (left)[22] and x-ray nanotomography (right).[23] (b) Mechanisms involved, such as long-range diffusion, surface diffusion, and chemical/electrochemical reactions, are illustrated using molten salt dealloying as an example. (c) Machine learning-augmented materials design for dealloying processes remains in its infancy with great future opportunities.[24] Reprinted with permission from References 22, 23. © 2008 AIP Publishing; © 2010 AIP Publishing.

design currently focus on predicting compositions or basic forms/shapes. For dealloyed materials, it is essential to shift toward designing complex 3D microstructures with intricate morphology. Considering materials kinetics is equally important, especially for dealloying, where phase transformation or dissolution is often kinetically controlled. ML models that incorporate specific structural features and kinetics can optimize real processing conditions, advancing beyond composition alone to create functional nanomaterials.

- **Developing robust models for small data sets:** Dealloying experiments typically yield small data sets, so ML methods that work effectively with limited data are crucial. Given the variety of dealloying conditions, ensuring ML models perform consistently across different materials and environments, such as aqueous solutions, molten metals, and amorphous versus crystalline precursors, is key. Additionally, the field would benefit from coherently addressing the lack of "failed but useful" experimental data. For instance, reporting systems that do not form bicontinuous structures during dealloying can still provide valuable insights.
- **Enhancing model interpretability:** ML models should not merely rely on trial-and-error but be designed to enable hypothesis-driven autonomous search and decision-making. Interpretable ML models that incorporate underlying physical and chemical principles are crucial. Techniques such as explainable artificial intelligence (XAI) and physics-informed neural networks (PINNs) could offer deeper insights into the physical and chemical processes underpinning material formation.
- **Integrating ML-augmented experiments with computational modeling:** Integrated ML frameworks that connect experimental data with predictive models are essential, ideally enabling real-time feedback. Such frameworks could enhance the ability to design complex materials, such as those produced by dealloying, where diverse engineering processing conditions and underlying physical and chemical parameters of materials are involved.

- **Synchronizing data utilization across characterization platforms for autonomous experiments:** Autonomous experiments currently operate at various scales. In the future, driving autonomous experiments at large-scale facilities (e.g., synchrotrons and nano-centers) as well as in individual research laboratories could accelerate discovery and manufacturing for dealloying materials and beyond. Further discussion on autonomous experiments will follow in the next section.

Autonomous experimentation

Autonomous experimentation (AE) is a powerful paradigm for accelerating scientific measurements, leveraging artificial intelligence (AI)/ML to automate an entire experimental loop, notably the decision-making step.[44] AE quantitatively accelerates measurements through automation, but more importantly it qualitatively changes scientific discovery, by liberating the researcher to focus on higher-level scientific thinking, and thereby pursuing more challenging scientific problems.[44,45]

Progress in AE has been rapid. Early work focused on optimal experiment design using statistical and applied mathematical methods.[46–53] Simultaneously, experimental methods have seen improvements in combinatorial synthesis methods[54–57] and automated synthesis platforms.[58–63] The merging of advanced experimental control with instrument automation enabled autonomous loops, whereby experimental decisions are determined on-the-fly, based on the data collected to date. Decisions typically involve a combination of sample selection, synthesis/processing conditions, measurement to perform, and instrumentation parameters.[44,45,64,65]

The control algorithm is of course crucial to AE. Reinforcement learning approaches that often exploit artificial neural networks for modeling,[66,67] and Bayesian methods, which provide statistical quantification of signals and uncertainties,[68] have been pursued. Statistical methods offer the advantage of providing rigorous uncertainty quantification (important for many science applications) and making very few assumptions (allowing them to be used on new problems with minimal configuration). On the other hand, ML methods pretrained on relevant data can be more tuned and thus optimized, at the expense of generality. Among Bayesian methods, Gaussian process (GP)[69,70] modeling is popular; conceptually, a GP model trained on experimental data provides a surrogate model that fits and interpolates the data while accounting for uncertainty, and provides a corresponding uncertainty model. Both the surrogate and uncertainty models are valuable in autonomous control. In particular, a common AE approach is, on every loop, to select the region in the search-space with the highest model uncertainty. This maximizes the rate of knowledge gain. Because the GP model and uncertainty are recalculated on every loop, this adaptively samples the relevant experimental space in a way that optimally accounts for uncertainty. More sophisticated methods can also exploit the surrogate model. For instance, one can preferentially search parts of the space that maximize a quantity-of-interest, while balancing this "exploitation" optimization with "exploration" searching of the total space. As another example, one can use the gradient of the surrogate model to focus attention on parts of the parameter space with meaningful changes (e.g., boundaries in a phase diagram).

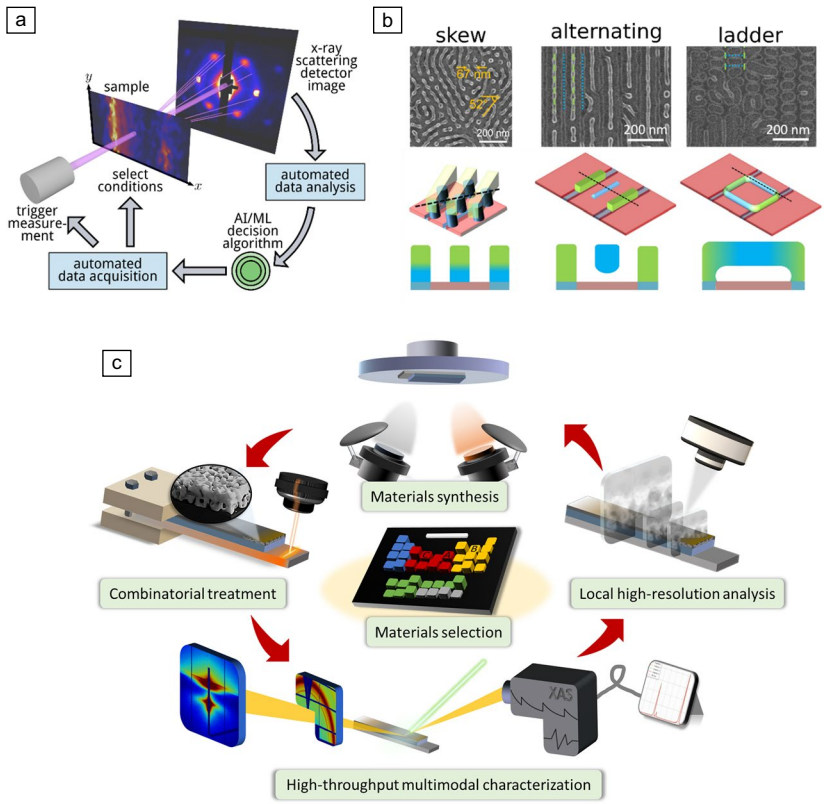

Figure 2. Autonomous experimentation: (a) Workflow for an autonomous experiment at an x-ray scattering beamline. A combinatorial sample's (x, y) coordinates are explored by an artificial intelligence/machine learning (AI/ML) algorithm. At every position, a small-angle x-ray scattering image is collected and analyzed. The algorithm builds a Bayesian model of how the selected signal varies over the exploration space, and optimally selects new high-value points for measurement. (b) Examples of three new block copolymer nanoscale morphologies discovered using this autonomous approach. Adapted with permission from Reference 43. (c) ML-driven, iterative workflow for thin-film solid-state metal dealloying: From guided selection and combinatorial synthesis, with a photothermal annealing platform for gradient heating, to high-throughput characterization and local verification. Reprinted with permission from Reference 42. © 2025 Wiley.

Autonomous experimentation with synchrotron x-ray scattering

Autonomous experimentation has been applied productively to synchrotron x-ray scattering.[71–75] In x-ray scattering or diffraction, a collimated x-ray beam is directed through a sample of interest. The far-field scattering pattern, collected on an area detector, provides detailed information about atomic/molecular scale ordering (for wide-angle scattering) and nano-/mesoscale ordering (for small-angle scattering), including size/shape of entities, packing motifs, unit-cell dimensions, grain size, and orientation distribution. The rapid, nondestructive measurement of x-ray scattering makes it amenable to a variety of AE schemes. AE was used for imaging heterogeneous materials (e.g., nanoparticle thin films),[69,76] wherein the new (x, y) imaging coordinate can be selected adaptively; in conjunction with combinatorial synthesis,[43] wherein measurements in the combinatorial space are selected; and to control real-time/*in situ* material processing,[75] wherein synthesis/processing conditions can be tuned during material formation/transformation. Figure 2a illustrates the workflow for autonomous experiments.

As an instructive example, consider AE exploration of self-assembled morphologies in block copolymers. Although belonging to a different category of materials, the various nanoscale morphologies of block copolymers and their associated self-assembly processes could be intriguing cases for future AE studies of dealloying, as their morphology not only resembles, but also involves a spontaneous self-organizing process. Block copolymers are polymer chains where chemical incompatibility of different chain regions drives toward phase separation, which is frustrated by the covalent links of the polymer backbone; the result is local phase separation, regulated by chain length and architecture and thus the spontaneous formation of a nanoscale morphology.[77,78] This ordering can be responsive to local conditions[79,80] (so-called directed self-assembly), such as chemical templates patterned onto the substrate.[81,82] In studying blends of different block copolymers, Yager et al. discovered unexpected coexistence phases[83,84] whose ordering was responsive to chemical templates.[85] However, the large number of control parameters, such as polymer blend composition, chemical template pitch, and duty cycle, makes it challenging to explore this responsive ordering. Noack, Doerk et al. used autonomous x-ray scattering to search through combinatorial samples[43,69] using a GP control method with a succession of objective functions designed to explore broadly, then focus on regions with strong scattering intensity, and finally focus on regions with unexpected ordering. This process was able to rediscover previously known motifs, as well as uncover several previously unknown nanoscale morphologies that form owing to the local repartitioning of block copolymer chains in response to the chemical pattern. This demonstrates the power of AE to efficiently explore experimental problems, and to discover new materials.

AE methods have recently been applied to solid-state metal dealloying. Automated crystallographic classification[86] was combined with Bayesian control[69] to explore combinatorial samples. More recently, a photothermal annealing platform was used to create temperature gradients on thin-film samples to explore a continuous thermal space, allowing observation of dealloying transitions and the resulting nanostructures of interest (See Figure 2c).[42] Ongoing efforts include combining autonomous x-ray scattering with GP control with this photothermal annealing platform in order to study metal dealloying processes in real time during thermal annealing; wherein the AE algorithm selects temperatures for study, within a steady-state thermal gradient, during the annealing. The parameter spaces for metal dealloying, high-entropy alloys,[87] and other multicomponent inorganic systems are ideal candidates for study by AE, as the associated combinatorial spaces are too vast to explore using exhaustive searches or other naive exploration methods. The simultaneous evolution of phases and nanoscale morphology in these systems also makes them particularly compelling cases to study using a combination of wide-angle x-ray scattering (WAXS) and small-angle x-ray scattering (SAXS). WAXS, with its sensitivity to different phases through crystalline structure identification, complements SAXS, which can probe distinct nanoscale morphologies.

Autonomous experimentations for dealloying materials and beyond

An interesting avenue for future AE studies is to develop "interdisciplinary learning" schemes, wherein a model trained on one class of materials is used to direct experiments in a different class of materials. This is most obviously useful among closely related materials, for example, the GP parameter-space modeling performed for one set of alloys is likely to be a reasonable prior when beginning studies of a new class of alloys (e.g., with partially overlapping compositions). More ambitiously, one can imagine performing transfer learning across disparate classes of materials that exhibit some kind of analogies. Famously, Pierre-Gilles de Gennes was able to make progress in soft material physics by drawing rigorous analogies to alignment of magnetic domains.[88] The dealloying process gives rise to a locally phase-separated nanomorphology, which exhibits some conceptual similarities to phase separation in polymer blends and block copolymers, as previously discussed, shown in Figure 2b. It would thus be exciting to train an ML model on block copolymer ordering, and then use it as a prior to guide exploration of dealloying problems. Such transfer learning would likely benefit from a set of learnable parameters describing the unknown mapping between the spaces. In addition to providing a reasonable prior to guide initial data collection, such an approach would hold the promise of uncovering (were it to exist) deep and quantitative analogies between different domains.

Even more ambitiously, this interdisciplinary learning approach would lay the groundwork for integration among the studied domains. Continuing our thought experiment, one can imagine a hybrid metal/polymer nanomaterial exploiting both

dealloying and polymer self-assembly, and thereby exploiting multiple aspects of a trained ML model. For instance, allowing block copolymer self-assembly to proceed is in line within the 3D confinement volume obtained from dealloying (after removal of one of the phases) would be an interesting case of hierarchical assembly.

The future of autonomous methods for physical science is exciting, as both control algorithms and automated platforms increase in sophistication. Parallel advancements in generative AI, such as the training of large language models (LLMs), could soon become integrated into these efforts. While LLMs are often thought of as text-generators such as chatbots,[89] they can also be used as the decision locus for AI agents that execute sophisticated workflows in response to imprecise objectives. Efforts to use LLMs for instrument control are already underway.[90–92] These LLMs can also be incorporated into autonomous synthesis and processing laboratories,[93] and further coupled with the AE of characterization. Overall, AI agents hold enormous promise as a higher-level abstraction built on top of existing AE instruments,[94] allowing researchers to phrase their scientific goals more naturally, and relying on the AI to translate this into concrete experimental objectives and AE execution plans.

Experimentally informed micromechanical modeling of nanoporous metals

ML has been increasingly utilized to support microstructure characterization and predict mechanical properties.[95,96] A successful ML model typically requires a comprehensive understanding of existing knowledge, expertise in translating this knowledge into meaningful input features, an effective ML architecture, and robust validation of the trained model. Despite the rapid growth in publications incorporating ML methods in recent years, there is limited literature specifically addressing nanoporous metals. Richert and Huber[97] provide an overview of deriving structural descriptors from imaging data and discuss perspectives for data-driven development of structure–property relationships. A physics-based ML approach with sophisticated feature engineering can incorporate existing knowledge, enabling reasonable training accuracy even with sparse data.

Although commonly used for predicting Young's modulus and strength, the Gibson–Ashby (GA) scaling laws do not fully capture the relevant physics of dealloying-made nanoporous metals.[98] Based on numerical simulations using leveled wave structures with varying solid fractions, Soyarslan et al. proposed rewriting the GA scaling law as a Roberts–Garboczi scaling law: $E^*/E_{\mathcal{B}} = C_2[\left[\phi_{\mathcal{B}} - \phi_{\mathcal{B}}^P\right]/[1 - \phi_{\mathcal{B}}^P]]^m$, which showed good agreement with available literature data for samples in their initial state before coarsening. This approach uses a one-to-one relationship between solid fraction (φ) and scaled genus (g), along with a percolation threshold ($\phi_{\mathcal{B}}^P \simeq 0.159$) at which the structure loses connectivity.[99] Samples with $\varphi \lesssim 0.3$ show a decrease in connectivity density at constant solid fraction, which has similar impact on the Young's modulus.[100,101] Hence, a more general form of the GA scaling law is required (e.g., of the form $E = \hat{E}_0(\varphi)\hat{E}_c(\zeta)$).[102] This multiplicative decomposition of the dependency of Young's modulus E allows for decoupling the effects of solid fraction, modeled by $\widehat{E}_0$, and the connectivity represented by $\widehat{E}_c(\zeta)$, providing a more general framework. It is in line with a GA scaling law, where the leading constant $C_Y = (g/g_0)^m$ depends on the scaled genus density. Xiang et al. proposed a $g^{4/3}$ relationship based on strength and Young's modulus data of dealloyed porous $Fe_{0.80}Cr_{0.20}$.[103] Sohn et al.[104] found a g^2 scaling law to be fundamental for predicting the load-bearing solid fraction property based on leveled wave model and finite element simulation data. Although all these approaches considered a decay in stiffness with ongoing reduction in connectivity due to coarsening, it became evident that differences in the underlying microstructure lead to different structure–property relationships. Detailed statistical analysis revealed differences in ligament cross sections and free ligament lengths by comparing artificial microstructures and tomography data from experiments.[105] Therefore, for a predictive ML model, a more detailed description and representation of microstructural details at the local scale are needed, emphasizing the importance of high-resolution tomography and reliable segmentation of larger experimental data sets.

Mechanical properties under uniaxial loading conditions

Workflows for property prediction using ML are illustrated in **Figure 3**. The starting point is structural data obtained from experiments or computer generation. Uncertainties in the segmentation of image data, as discussed elsewhere,[106] can lead to unacceptable biases in the prediction of mechanical properties. To improve segmentation, Sardhara et al. presented a convolutional neural network (CNN) to reconstruct nanoporous structures from focused ion beam (FIB) tomography images using synthetic training data.[107] They produced data similar to experimental images by blurring the synthetic data and adding noise. Additional depth information was included to compensate for uncertainty by presenting a group of three adjacent slices to the CNN. Similar issues arise in subsequent image processing steps, depending on the chosen algorithm for ligament thickness computation.[108] Voxel resolution and the choice of thickness algorithm were found to introduce significant biases.[109] Therefore, ML offers powerful tools for correcting thickness information in postprocessing steps, as demonstrated for parabolic-shaped ligaments.[109]

By integrating existing knowledge through feature engineering in a physics-based approach, an ML model can significantly improve its prediction accuracy, robustness, and generalization capability. Such models can achieve reliable results, also when only a relatively small amount of training data are available, which is often the case for data sets available for nanoporous metals. The key question is whether all this information, available in the voxelized structure

representation, can be directly used to predict macroscopic stiffness via a deep learning approach. In this scenario, the absence of a physics-based foundation must be compensated by a substantially larger data set. Liu et al.[112] demonstrated this approach using a 3D CNN trained and validated on 4186 microstructures, labeled with mechanical stiffness data from finite element simulations. Compared to the scaling law proposed by Soyarslan et al.,[99] the well-trained CNN architecture reduced the prediction error from 17.22 to 0.53, clearly illustrating the potential of deep learning to provide highly reliable and robust predictions of effective stiffness for given microstructures. Additionally, by comparing neuron maps with Gaussian curvature maps, it was shown that the CNN learned hierarchical features of the input microstructures, such as edges, corners, and surfaces (see **Figure 4**a). These learned hierarchical features can, in principle, be transferred to study other materials, such as composite materials or porous nanomembranes, thereby accelerating research on structure–property linkages for various materials.[112] In terms of intentional materials engineering, the work by Wang et al.[113] uses a CNN to predict and tune the structure generation for establishing a desired elastic anisotropy. In this work, the CNN was used to speed up the structure generation for optimization (Figure 4b). Here, the prediction of the anisotropic elasticity tensor was realized via a fast Fourier transform approach that is accurate as well as computationally efficient.

Plasticity under multiaxial loading conditions as a consequence of hierarchy

When considering plastic deformation behavior under uniaxial loading, the situation is similar to that of elasticity. As demonstrated in several studies,[100,102] similar scaling laws exist, allowing elasticity and plasticity to be connected via a one-to-one relationship. This makes plasticity seemingly straightforward once the structure–property relationship for elastic properties is established. Additionally, due to the random nature of the network structure, the yield behavior can be assumed to be isotropic, eliminating the need to consider anisotropy when predicting yield strength. However, when large deformations are applied, the deformation mechanisms of porous materials change significantly depending on the loading direction. Notable differences between tension and compression lead to tension–compression asymmetry in plastic flow, including ligament stretching during tension and the establishment of internal contacts up to pore compaction during compression, as observed in simulations.[116,117] Beyond these specific observations, there is limited literature addressing these aspects on a more general level.

The inelastic deformation of open-cell foams was investigated using periodic representative volume elements in the

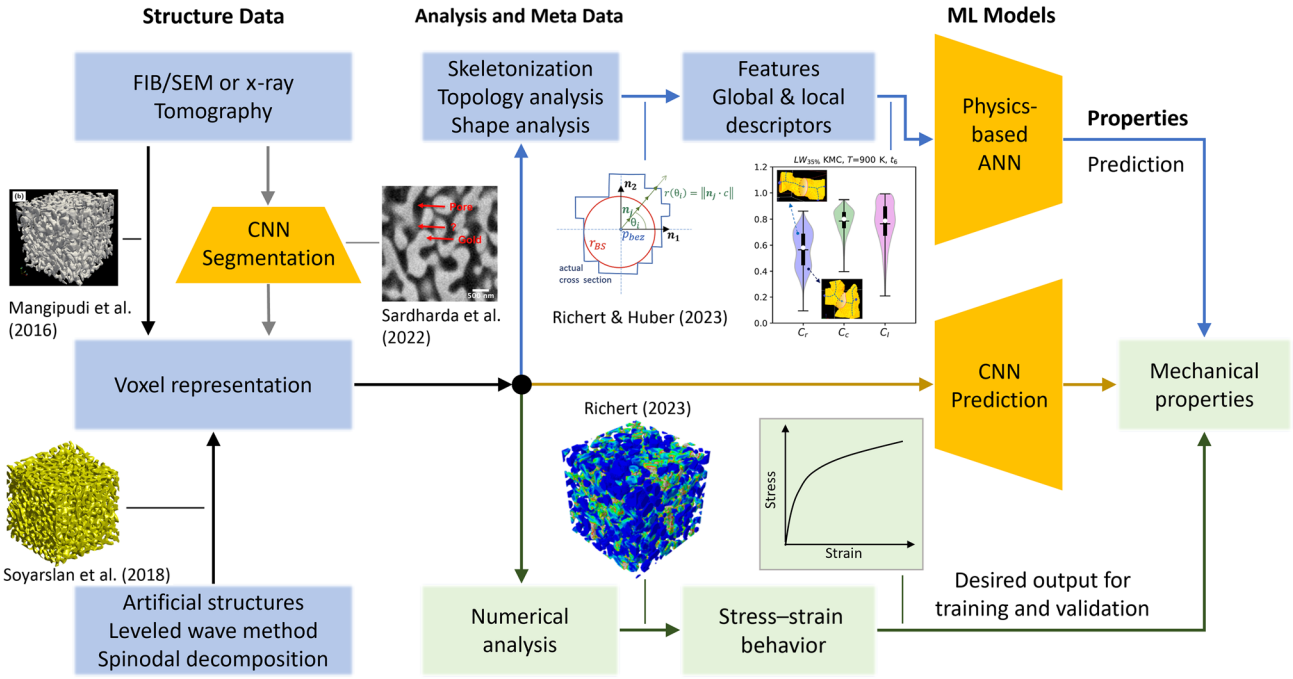

Figure 3. Workflow for data-driven prediction of mechanical properties. Structure data can be obtained from imaging or computational methods for structure generation (left). A carefully segmented set of voxel data forms the core of the property prediction, providing input for mechanical simulations, morphological analysis as input for a physics-based artificial neural network (ANN) (blue) or, alternatively, direct feeding into a convolutional neural network (CNN) (golden) for the prediction of mechanical properties (green). FIB, focused ion beam; LW, leveled wave; KMC, kinetic Monte Carlo; SEM, scanning electron microscopy; ML, machine learning. Components of the figures are adapted from References 99, 105, 107, 110, and 111. Reprinted with permission from References 99, 105, 110. © 2018 Elsevier; © 2023 Elsevier; © 2016 Elsevier.

form of 2D and 3D Kelvin cells to provide training data for neural networks and implementation as a user material routine in ABAQUS.[118] Initial yield surfaces exhibited significant tension–compression anisotropy and complex shapes that are not easily described by common phenomenological models for anisotropic plasticity. The authors demonstrated that both the initial yield surfaces and their evolution during plastic deformation could be predicted with a trained artificial neural network (ANN) for proportional loadings and small deformations. Their implementation in ABAQUS showed that computational effort could be reduced by a factor of more than 10,000 compared to a discretely resolved foam structure, with nearly identical solution quality. Several ML models for predicting yield surfaces under multiaxial loading with arbitrary combinations of normal and shear components where compared in Reference 114. Yield surfaces were predicted for different representative volume elements (RVEs) (diamond cell, Kelvin cell) and at two plastic strain levels (1% and 10%). Comparing the performance of a data-driven ANN, a hybrid ANN combined with the Deshpande–Fleck model and a support vector machine (SVM) model revealed that for 3D and 6D stress spaces, the SVM provided the best results, allowing for good generalization and extrapolation, likely due to its convex nature (Figure 4c). Surprisingly, the hybrid approach did not outperform the data-driven ANN, mainly because the required corrections to the Deshpande–Fleck model were too large for the 6D case, offering little advantage.

As a 3D extension of an efficient hybrid scale-bridging approach, Malik et al.[115] proposed using a representative volume element realized as a 3D open-cell Weaire–Phelan structure in a periodic arrangement of $2 \times 2 \times 2$ unit cells. Various macroscopic loading paths were applied in a stress-controlled manner. The trained ANN demonstrated that elastic–plastic stress–strain responses could be predicted with high efficiency and precision for arbitrary loading directions and histories, including partial unloading (Figure 4d). This approach has been used to simulate hierarchical nanoporous metals consisting of multiple levels of hierarchy.[119] Hierarchy implies that multiaxial loading becomes an issue at the lower hierarchy levels, even when the upper level is loaded uniaxially, as is commonly the case. Depending on the specific location of a material point and its interaction with its homogeneously deforming neighborhood, the lower-level porous structure will experience multiaxial loading. Due to the random nature of the material, all possible combinations of shear and normal strains can occur. Because the plastic deformation behavior of porous metals shows a strong dependence on multiaxial loading history,[115] numerical prediction of hierarchical nanoporous metals requires fully resolved models of all hierarchy levels, leading to computationally demanding simulations. Implementing an ANN surrogate model in a multiscale simulation would significantly speed up the process, bringing simulation times closer to those of nanoporous metals with a single hierarchy level.

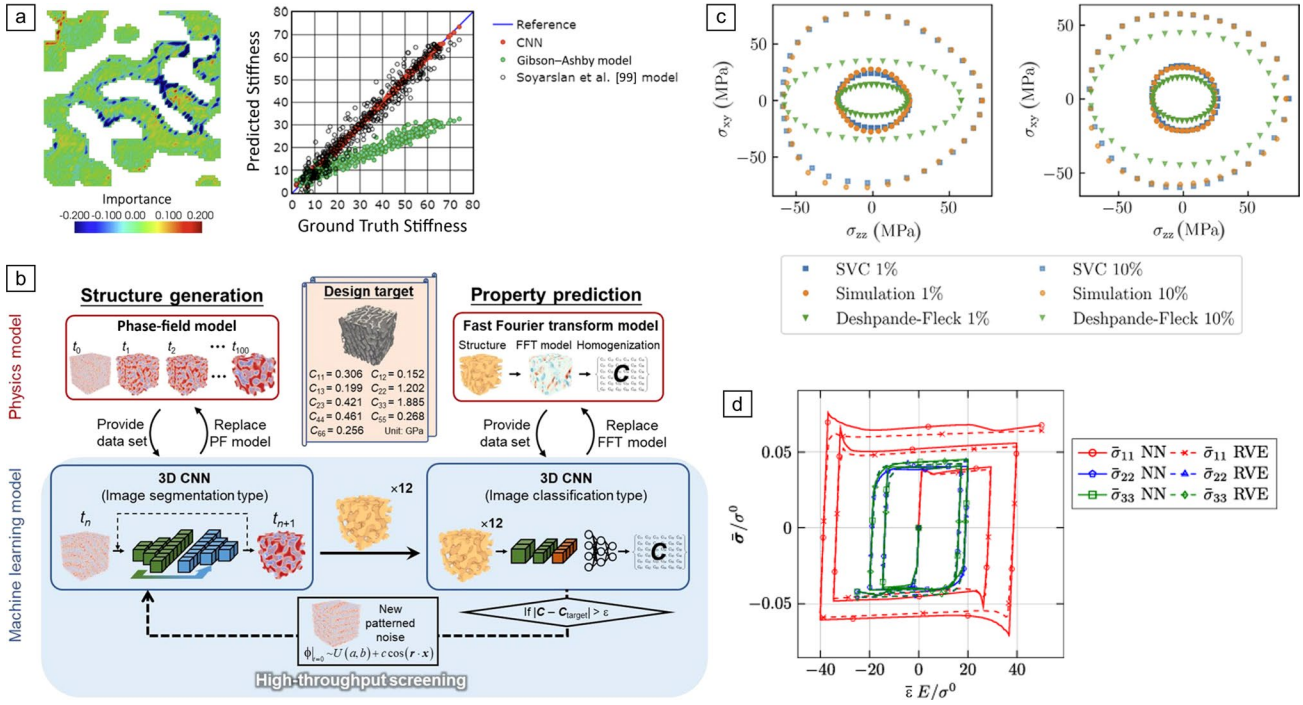

Figure 4. Prediction of various mechanical properties and elastic–plastic deformation behavior of open-pore metallic foams for uniaxial and multiaxial loading: (a) Macroscopic elastic modulus via convolutional neural network (CNN).[112] (b) Anisotropic porosity and elastic stiffness tensor via CNN and fast Fourier transform (FFT).[113] PF, phase field; NN, neural network; RVE, representative volume element. (c) Anisotropic yield surface for multiaxial loading predicted by support vector classification (SVC) and artificial neural network (ANN).[114] (d) Loading history-dependent stress–strain behavior predicted by ANN.[115] Reprinted with permission from References 112,114. © 2022 Elsevier, © 2023 Elsevier.

Most ML models in the literature are developed by groups that generate their databases through computer simulations. Experimental data sets remain scarce and are often small enough to be analyzed using conventional visualization and fitting methods. However, these data sets are typically too small for effective machine learning, particularly for modeling relationships in intentional materials engineering. To collect data from across the community and make them available for this purpose, efforts should focus on the following directions:

- Provide data sets with proper metadata descriptions, ideally along with an ontology to ensure semantic interoperability and machine readability,[120,121] to establish the process–structure–properties chain (or its elements, where necessary) using ML models.
- Develop methods for extracting data from unstructured sources, mainly literature, where data are provided without semantic interoperability and machine readability.[122]
- In the long term, combine both approaches to establish a common database on nanoporous metals that can be data mined for specific problems. This approach could be extended by using deep learning models to guide materials synthesis, targeting desired structures and properties,[123] without requiring too many intermediate steps that demand specialized expertise.

Conclusion and outlook

ML approaches hold the promise to accelerate the transition of fundamental research to scalable manufacturing by addressing the inherent complexities in designing and controlling the properties of advanced materials such as dealloying. By using ML-augmented computational and experimental methods, ML methods can be incorporated into the materials design loop with an enhanced understanding of processing-structure–property–functionality relationship in nanoporous metals and composites created by dealloying. This can enable a better prediction of materials compositions and processing conditions for targeted microstructures and macroscopic structural design, achieving tailored properties and functionalities, including but not limited to the mechanical properties as illustrated in this article. This predictive capability has a potential to significantly reduce the time and energy currently taken in the traditional trial-and-error materials design cycles, streamlining the design process to reach targeted outcomes for designing nanomaterials more efficiently.

ML-enabled autonomous experimentation can allow real-time feedback between modeling and experimental data, as seen with techniques such as synchrotron x-ray experimentation and autonomous synthesis laboratories. This real-time integration of an AI agent in the decision-making experimental control enables dynamic adjustments, advancing both microstructure characterization and property prediction. By exploring high-dimensional parameter spaces and incorporating materials thermodynamics and kinetics into ML models, the AI agent can ultimately search for processing conditions at scale, enabling faster and more precise scaling of complex materials systems from laboratory-based studies to large-scale manufacturing. Moreover, ML can assist with the analysis of complex data sets from x-ray microscopy and tomography by performing tasks like noise reduction, 3D reconstruction, feature recognition, image segmentation, and property prediction based on images. Advanced capabilities, such as multimodal data fusion, 4D time-series analysis, sparse data recovery, and resolution enhancement (super resolution enabled by deep learning), show promise and also require further development and research. These tools enable detailed insights into structural and morphological characteristics essential for practical applications in the nanoporous metals and composites created by dealloying.

ML approaches can help to establish structure–property relationships that reach beyond the capabilities of scaling laws, which are commonly limited to a few global descriptors, such as solid fraction and scaled genus density. They allow us to include much more detailed and quantitative 3D microstructure information, which at the same time emphasizes the requirement of an unbiased segmentation as a solid basis for extracting local features. This quantitative assessment serves for deriving engineered features as inputs for physics-based neural networks. At this level of detail, the experimental database is still scarce. So far, applications are limited within groups and their own data sets, usually of the same kind. A sound validation and demonstration of the applicability of ML methods trained with larger computer-generated data sets with experimental data sets need to be addressed in the future. Therefore, open data sets from 3D and 4D imaging as well as from computer-generated 3D microstructures are needed, ideally along with their properties and further metadata provided in an interoperable and machine-readable data format. Beyond the Young's modulus, the prediction of the stress–strain behavior shows great potential for the development of ML methods, especially toward hierarchical nanoporous materials. This is a direction of research that cannot adequately be addressed by any other method, due to the multiaxial and non-radial loading that is induced by the upper level to the lower level of hierarchy.

While ML-augmented methods show promise for designing nanoarchitectured materials, including through dealloying processes for nanoporous metals and metallic composites, implementing a comprehensive approach that spans the entire design loop remains unrealized. This loop would include selecting an alloy system, setting dealloying processing parameters, characterizing structure and properties of dealloyed materials, and then providing feedback to refine the initial dealloying material system and processing conditions to achieve the desired nanostructure and properties. Currently, only individual components of each step are in place or under study, with preliminary efforts underway to develop proof-of-concept design workflows. Significant challenges remain, such as in integrating ML-enhanced predictions for nanostructures and incorporating advanced characterization techniques, including x-ray tomography and transmission electron microscopy, to facilitate

a feedback-driven design cycle in materials development. Despite these hurdles, the prospect of enabling a closed-loop design process presents substantial opportunities for advancing research and technological innovation within the dealloying community, as well as incorporating a broader range of processes and functional applications. Another crucial aspect is the ongoing acquisition of scientific knowledge, particularly in the underlying thermodynamics and kinetics, which are essential for advancing this field. This context brings us to share our perspective on the outlook for future development:

AI/ML methods hold enormous promise for improving scientific discovery. At the same time, there are pitfalls, including researchers becoming over-reliant on automation they do not understand, the replacement of interpretable theory with black-box approximators, the biasing of research outcomes or models, and the extinguishing of creativity and serendipity. The ultimate goal in science is not raw data collection, reproduction of existing understanding nor even predictive power of methods, but rather intelligible insights that humans can use to advance understanding and pursue goals. AI/ML, if properly integrated into research, is not in conflict with this aim. For instance, treating research as a purely productivity-maximizing enterprise can lead to building full-automated workflows that eliminate the need for human researchers. However, this would diminish much of the true value of research. By contrast, AI methods that seek to empower the researcher—sometimes called intelligence augmentation—keep humans in charge of high-level decisions and maintain the focus on interpretable discovery. Additionally, outlining materials design workflow and setting experiments compatible with ML-augmentation often require deeper consideration of the hypotheses being tested, the specific design goals, and the costs involved, potentially enriching the research process. Moreover, properly deploying these methods can help to reduce the number of parameters to be measured to a small number of relevant inputs, mitigate experimental biases or outliers (by making them explicit), reveal systematic differences in data from different sources, discover new physical laws (e.g., via interpretable machine learning), or create new opportunities for serendipity (by lowering the barrier to exploration and playful science). Overall, AI/ML methods can excel at modeling and interpreting vast complexities and high-dimensional data, enabling deeper insights that would be challenging to achieve manually. While they build upon existing information, they have the potential to enhance discovery by accelerating processes, uncovering hidden patterns, and freeing humans to focus on creative thinking and high-level scientific exploration.

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Author contributions

All co-authors collaboratively developed the concept of the review paper. Y.K.C.-W. led the sections covering the Introduction and Materials Discovery and Design through Dealloying, as well as the integration of different sections. K.G.Y. led the section on Autonomous Experimentation and related concepts. N.H. led the section on Experimentally Informed Micromechanical Modeling of Nanoporous Metals and related concepts.

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Conflict of interest

The authors declare no conflict of interest.

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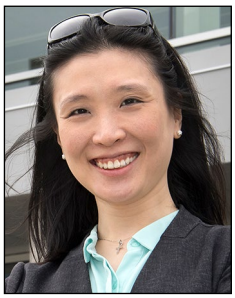

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