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REVIEW

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Applications of generative adversarial networks in materials science

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Abstract

Generative adversarial networks (GANs), as a powerful tool for inverse materials discovery, are being increasingly applied in various fields of materials science. This review provides systematic investigations on the applications of GANs from a group of different aspects. The basic principles of GANs are first introduced; then a detailed review of GANs-based studies regarding distinct scenarios across composition design, processing optimization, crystal structure search, microstructure characterization and defect detection is presented. At the end, several challenges and possible solutions are discussed and outlined. This overview highlights the efficacy of GANs in materials science, and may stimulate the further use of GANs for more intriguing achievements.

KEYWORDS

generative adversarial networks, generative models, inverse discovery, materials science

1 | INTRODUCTION

Accelerating material design, processing optimization and lifetime evaluation is the key of materials science due to an increasing demand for new materials.[1,2] The applications of machine learning to materials science, boosted by continuous advances of algorithms, as well as computing resource and size of material data repository, have led to the fourth paradigm of data-driven materials discovery. The approaches can be categorized into two main types, "forward" and "inverse".[3–7] The former focuses on the prediction of target property for unknown materials and selection of candidates guided by the predictions.[8] In contrast, the latter aims at generating target materials with desired property, instead of fully exploring the huge unknown space.[8–10] The generative models based strategy can be used in both forward and inverse materials discovery and can be more efficient because of the property-oriented essence and has attracted lots of attentions from materials community.[11,12]

A number of algorithms have been used to realize inverse discovery, including the generative adversarial networks (GANs), variational autoencoders (VAEs), flow models (Flows), and diffusion models.[13–15] Among these, the use of GANs in materials science is active and effective, especially on the microstructures.[16–22] Compared to other algorithms, GANs are able to generate more realistic high-resolution images with details and quality that surpass Flows and VAEs. Images generated by VAEs often appear blurry and their underlying representations are less interpretable.[23] Flows are powerful but they are complex to implement and difficult to be extended to high-dimensional data.[24] Diffusion models can generate high-quality images, yet they are less efficient and the inference process requires multiple network evaluations.[25] The flexibility of GANs allows researchers to adjust the model structure according to specific application requirements.[26–28] For example, Long et al. developed a GANs model that is capable of predicting stable crystal structures by optimizing the formation

energy in the latent space.[29] Li et al. used GANs to generate multi-component alloys and predict their phases.[30] There has been a few reviews outlining the application of GANs in materials science, but they mainly focus on the application on a specific material system or are combined with other generative models such as VAEs.[31–33]

This review highlights the applications of GANs in materials science across various aspects such as composition design and processing optimization, as shown in Figure 1. First, the basic concepts and common variants of GANs are presented. Next, we provide an in-depth summary of applications of GANs based on a number of typical examples from different aspects. Finally, we discuss the main challenges and provide an outlook regarding possible limitations and potentials, with emphasis on the combination of GANs with other machine learning techniques to solve complex problems in materials science.

2 | BASIC PRINCIPLES OF GANs

2.1 | Structure of GANs

GANs was first proposed by Ian Goodfellow in 2014, a deep learning model that has become an important tool in the field of machine learning.[32] The basic idea of GANs is shown in Figure 2. Two key components, the generator and the discriminator, are usually implemented through neural networks. The functions of these two networks are mapping and classification: the generator is responsible for imitating the distribution of real data to generate realistic new samples; while the discriminator acts as a binary classifier, and its main task is to distinguish generated samples from real ones. Although neural networks are often used to build these two components, other algorithms capable of mapping from input to output could also be used for this purpose.

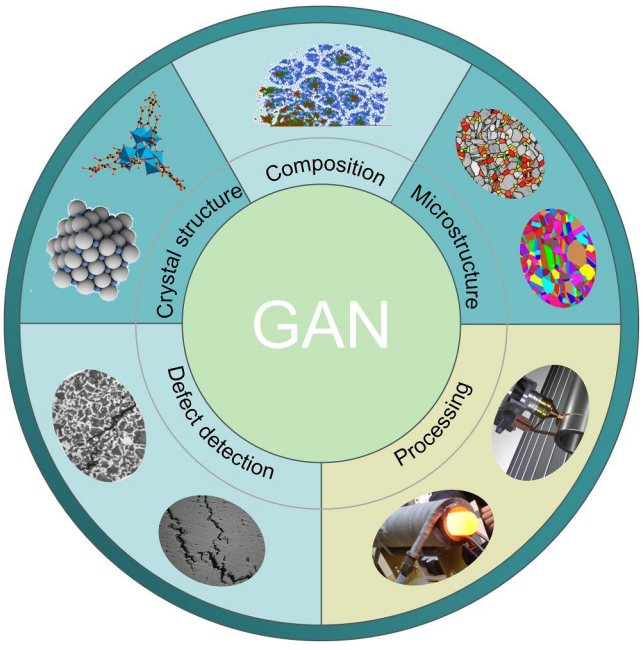

FIGURE 1 Schema showing the application of generative adversarial networks in different aspects of materials science.

2.2 | Training of GANs model

GANs is a revolutionary self-supervised or unsupervized learning technique that achieves learning goals by modeling the high-dimensional distribution of data.[32] The training of GANs involves two main parts: optimizing the discriminator D and the generator G. The training of the discriminator involves minimizing cross-entropy, and its loss function can be expressed as:

$$\mathrm{Obj}_D(\theta_D, \theta_G) = -\frac{1}{2}E_{x\sim p_{\mathrm{data}}}[\log D(x)] - \frac{1}{2}E_{z\sim p_z(z)}[\log(1 - D(g(z)))] \quad (1)$$

where x is obtained by sampling the real data distribution $p_{\mathrm{data}}(x)$, and z is obtained by sampling the prior distribution $p_z(z)$, such as Gaussian distribution. $E[\cdot]$ indicates expected value. The training data consists of two parts: one comes from the real data distribution $p_{\mathrm{data}}(x)$, and the other comes from the data distribution produced by the generator $p_g(x)$.

For the generator G, the goal is to minimize $\log(1-D(G(z)))$ so that the possibility of the generated data $G(z)$ being misjudged as real data by the discriminator is maximized. This process can be represented by the following min-max problem:

$$\min_G \max_D V(D,G) = E_{x\sim p_{\mathrm{data}}}[\log D(x)] + E_{z\sim p_z}[\log(1 - D(G(z)))] \quad (2)$$

During the training process of GANs, G is first fixed and D is optimized to improve the discrimination accuracy. Then D is fixed and G is optimized so that the data generated by G can better deceive D. This alternating process continues until the global optimal solution is reached, that is, when $p_{\mathrm{data}} = p_g$.[34]

2.3 | Variants of GANs

Traditional GANs have problems such as model collapse and unstable training. Therefore, several variants have emerged for specific purposes, which can generate more reliable samples. Here are some of the more common variants.

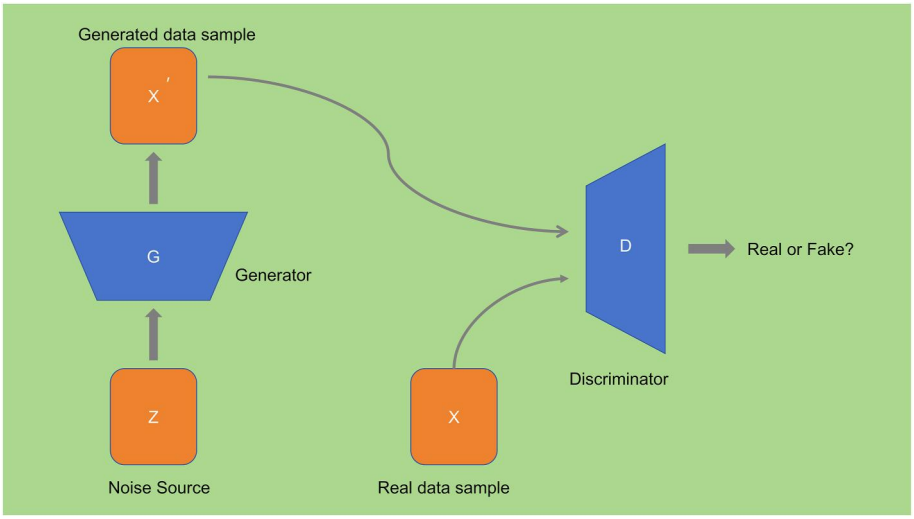

FIGURE 2 Schema to show the basic principle of generative adversarial networks.

2.3.1 | Wasserstein GAN and gradient penalty

Wasserstein GAN (WGAN) solves the problems of mode collapse and training instability in traditional GANs by using Wasserstein distance as the loss function. Wasserstein distance can be defined as the minimum "cost" required to transfer one pile of "soil" into another pile of "soil" between two distributions, which can be expressed as:

$$W\left(p_r, p_g\right) = \inf_{\gamma \in \Pi\left(p_r, p_g\right)} \mathbb{E}_{(x,y)\sim\gamma}[\|x - y\|] \tag{3}$$

Among them, p_r is the real data distribution, p_g is the distribution of model-generated data, and $\Pi(p_r,p_g)$ is the set of all possible joint distributions $\gamma(x,y)$, whose marginal distributions are p_r and p_g respectively.

One of the key improvements of WGAN is the introduction of weight clipping to force the discriminator to meet constraints. Subsequent research proposed using gradient penalty (GP) instead of weight clipping to further improve its training stability. The purpose of GP is to constrain the gradient of the discriminator so that it does not become too steep between real data and generated data, which helps avoid overfitting and improve the generalization ability of the model. The gradient penalty can be expressed as:

$$\mathscr{L}_{GP} = \lambda(\|\nabla_{\hat{x}} D(\hat{x})\|_2 - 1)^2 \tag{4}$$

Among them, $\hat{x}$ is the interpolation between real samples and generated samples, $\nabla_{\hat{x}} D(\hat{x})$ is the gradient of the discriminator output relative to $\hat{x}$, λ is the penalty coefficient, used to control the strength of regularization.

Combining WGAN and GP results in WGAN-GP, which uses GP to replace the weight clipping in WGAN to achieve a smoother and more stable training process. This combination not only solves the problems faced by the original GAN, but also improves the diversity and authenticity of the generated samples, making GAN more reliable and effective in various application scenarios.[35]

2.3.2 | Deep convolutional generative adversarial network

Deep convolutional generative adversarial network (DCGAN) uses deep convolutional networks to improve stability and image quality and provide customized structures. In DCGAN, both the generator and the discriminator remove the pooling layer in traditional convolutional neural networks. The discriminator retains the basic architecture of CNN, while the generator uses a deconvolution layer to replace the traditional convolution layer. Both introduce a Batch Normalization layer after each level to alleviate training difficulties caused by poor initialization, speed up training, and enhance the stability of model training. In addition, all fully connected layers are replaced by 1×1 convolutional layers. In the selection of activation function, except for the output layer which uses Tanh (or Sigmoid), all other layers of the generator use ReLU. The discriminator uses LeakyReLU activation functions in all layers to prevent gradient sparsity problems.[36]

2.3.3 | Conditional generative adversarial network

Conditional generative adversarial network (cGAN) is able to generate data with specific characteristics by introducing additional conditional information to guide the generation process. The core idea of cGAN is to add conditional information to the input of the generator and discriminator, so

that the model not only learns how to generate data, but also learns how to generate data according to given conditions into an adversarial network. The objective function can be expressed as:

$$\min_G \max_D V(D,G) = \mathbb{E}_{x\sim p_{\text{data}}(x)}[\log D(x\,|\,y)] + \mathbb{E}_{z\sim p_z(z)}[\log(1-D(G(z\,|\,y)))] \quad (5)$$

Among them, x is a real data sample, z is random noise, y is condition information, $D(x|y)$ represents the discriminator's evaluation of the probability that sample x is a real sample under given conditions, $G(z|y)$ represents the data samples produced by the generator under the influence of condition y and noise z.

By introducing conditional information, cGAN can control the specific characteristics of generated data and improve the diversity and quality of data samples. These improvements provide additional guidance to the generator, allowing it to more accurately learn and mimic the target data distribution.[37]

2.3.4 | Cycle consistent generative adversarial network

Cycle consistent generative adversarial network (CycleGAN) is an innovative generative adversarial network architecture designed to handle image-to-image conversion tasks without paired training data. By introducing the concept of cycle consistency, this architecture not only ensures the reversibility of the conversion process when converting images between two different domains, but also ensures that the image converted back to the original domain retains the original information as much as possible, thereby avoiding information loss and image distortion. Specifically, CycleGAN consists of two pairs of generators and discriminators: the first pair is responsible for transforming the image from the original domain to the target domain, and the second pair performs the opposite transformation. At the same time, the two discriminators are responsible for evaluating the difference between the converted image and the real image in their respective domains. Through cycle consistency loss, CycleGAN ensures that the image can be restored to a form close to its original state after being transformed once to the target domain and then back to the original domain. This mechanism significantly reduces the difficulty of accurate inter-domain conversion without paired training samples, and greatly expands the possibilities of image generation and conversion.[38]

GANs and their variants play a key role in image completion, generated data quality control, and image conversion, providing efficient solutions for different application scenarios. Today, new variants and improvements continue to emerge, which can fully meet the application needs of different scenarios.[39–44]

3 | APPLICATION OF GANs IN MATERIAL COMPOSITION DESIGN

For composition design, one of the major challenges is exploring a vast candidate space for materials with target property. Researchers mainly relied on time-consuming and laborious experiments for a long period. Despite efforts from theory and simulation, the efficiency of design is still unsatisfactory. Recently, GANs are being used in material composition design.[45–47] They can generate new candidates from unexplored high-dimensional composition space,[48–52] thereby greatly accelerating the discovery and design of new materials.[53–55] This section summarizes the applications of GANs in material composition design.

A group of studies have demonstrated the use of GANs for the search of inorganic materials such as superconductors.[56,57] Dan et al. developed a material generative model based on WGAN.[58] This model uses inorganic materials in the ICSD database as training data and effectively generates novel materials, as shown in Figure 3. After generating 2 million samples, the model demonstrates a high novelty of 92.53%. In addition, 84.5% of these generated materials balance the charge-neutral and electronegativity. This research demonstrates the potential of GANs in learning the chemical composition rules, providing valuable guidance for the design of new inorganic materials.[59]

Zhong et al. proposed a model that combines VAEs and GANs, and applied it to the generation of superconductors with high transition temperatures (T_c), as shown in Figure 4.[60]

The model converts the superconductor's composition and its T_c label into a low-dimensional representation through an encoder, and then reconstructs the superconductor through a generator. The authenticity discriminator is used to distinguish real superconductors and reconstructed superconductors, and the T_c discriminator is used to identify the T_c value of a superconductor. They used data from the SuperCon database to train the model.[61–63] In order to maintain data balance, 2376 low-temperature superconductors (20 K < T_c < 40 K), 2313 medium-temperature superconductors (40 K ≤ T_c ≤ 77 K), and 2686 high-temperature superconductors (T_c > 77 K) were screened out in the database. The superconductors with a T_c higher than 77 K were successfully predicted. It was found that superconductors of the same type cluster together, that is, the ones with similar T_c distribute close to each other. Among the generated high-temperature superconductors, a copper-based superconductor with a maximum T_c of 129.4 K appears. The study provides new methods and potential candidates for future high-temperature superconductor design and discovery.

In addition to inorganic materials, GANs have also found applications in the design of alloys, typically in high entropy alloys due to their comprehensive mechanical and functional properties.[64–68] For example, a data ecosystem based on cGAN for the inverse design of refractory high-entropy alloys was proposed.[69] They collected 529 high-entropy alloy

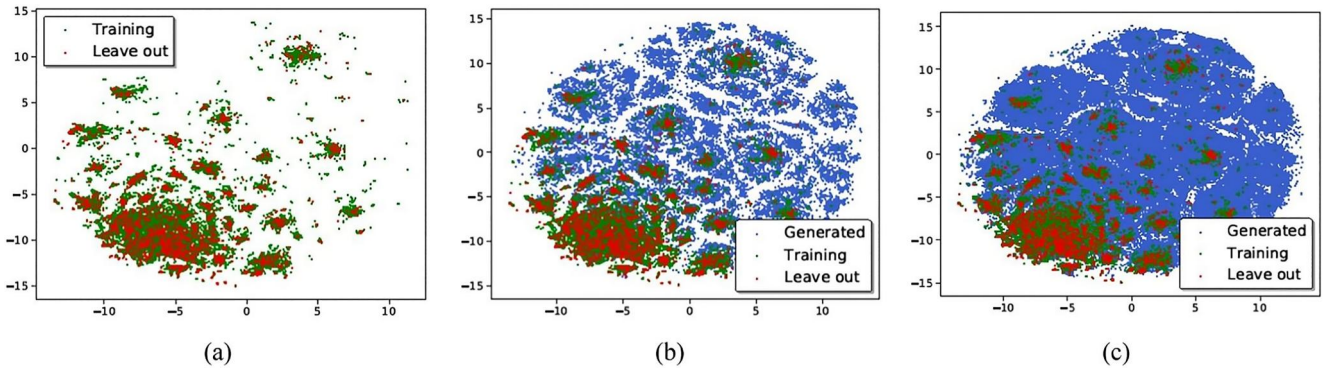

FIGURE 3 The distribution of training, leave out and generated samples visualized by using t-SNE. (a) Shows the training samples and validation samples included in ICSD, while (b) and (c) show the comparison of 50,000 and 200,000 generated samples with training and validation samples, respectively.[58] Reproduced with permission. Copyright 2020, Springer Nature.

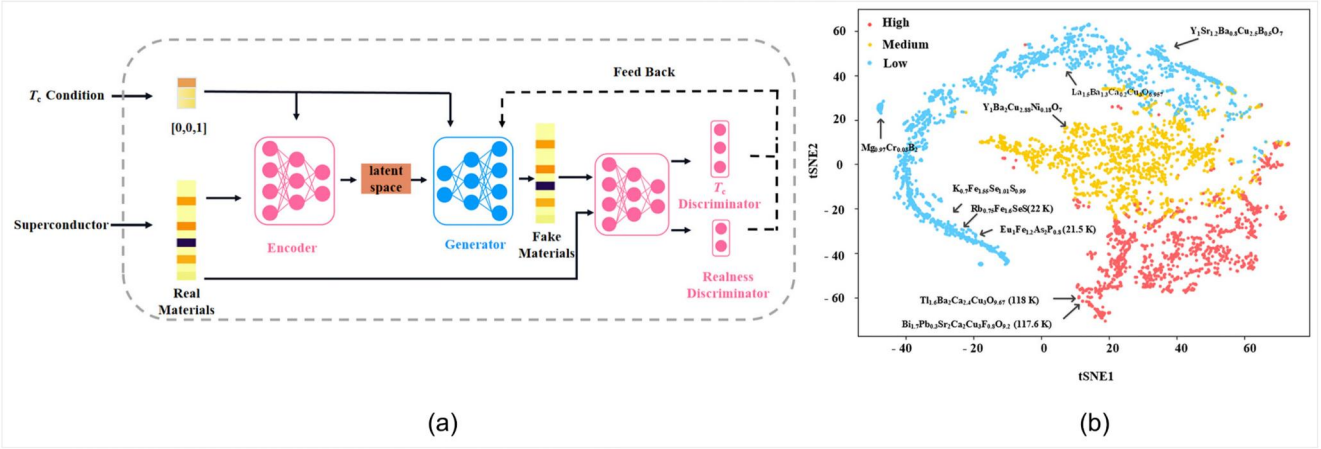

FIGURE 4 The framework for the generation of superconductors. (a) Shows the structure of the generative model, (b) shows that the superconductors form three different clusters with different T_c.[60] Reproduced with permission. Copyright 2023, American Chemical Society.

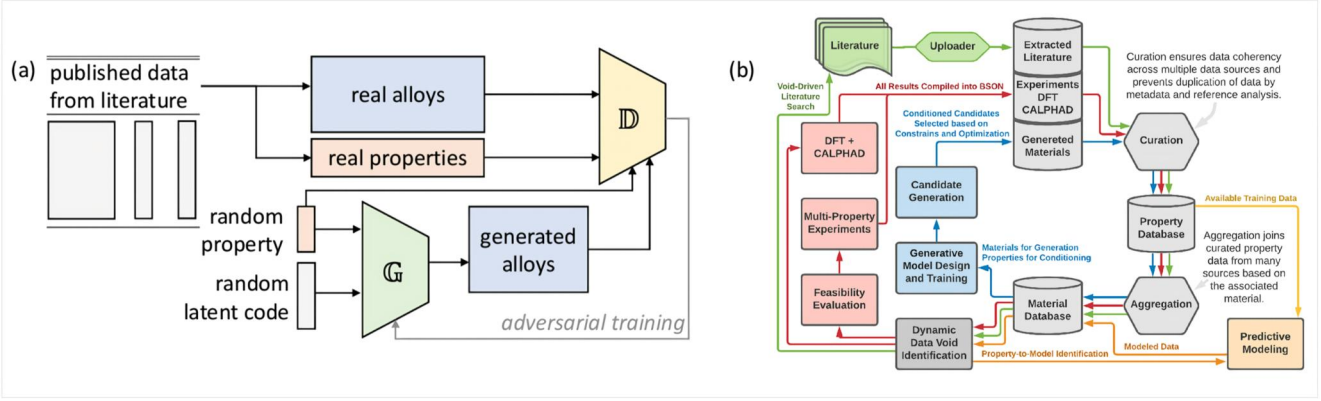

FIGURE 5 Schematic diagram of generative model for high entropy alloys based on cGAN. (a) Workflow of cGAN, (b) cGAN-based data ecosystem.[69] cGAN, conditional generative adversarial network.

compositions from the literature, and used mechanical properties such as shear modulus and fracture toughness as constraints to generate alloys with target properties. Then experiments and calculations were conducted to verify the generations which augment the database, as shown in Figure 5. This study demonstrates that GANs can capture the underlying tendency between composition and mechanical properties despite of imperfect match.[70]

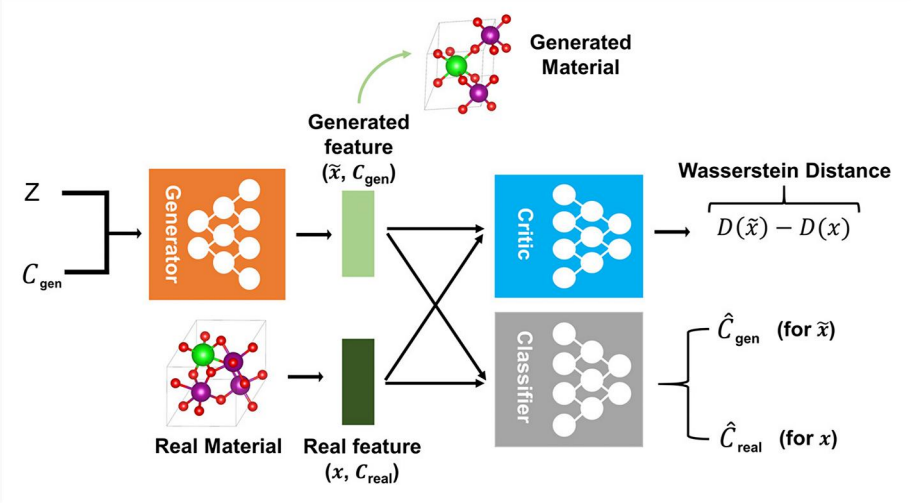

FIGURE 6 Flowchart that shows the prediction and generation of new crystal structure using conditional generative adversarial network.[74]

In summary, the use of GANs has achieved many successes in the composition design of various materials. This confirms the power of such methods and for different tasks one should select the proper variant of GANs. In addition to exploration of new compositions, GANs can also learn the underlying physics or mechanisms.[58,71,72] We envision that with the exponential increase of data, more laws and rules can be learned and extracted using GANs, which can in turn rationalize the generation of new materials.

4 | APPLICATION OF GANs IN MATERIAL CRYSTAL STRUCTURE PREDICTION

GANs not only perform well in exploring the material composition space, but also show excellent performance in predicting the crystal structure of materials.[73] Compared to traditional crystal structure prediction and optimization methods such as evolution algorithms, GANs can be more efficient due to the strong generation ability under constraints including certain property. This section will focus on the application of GANs in predicting and searching for a new crystal structures of materials to meet the requirement.

To explore the vast chemical space of photoanode materials, a cGAN was used to generate new crystal structures of the Mg−Mn−O ternary system, as shown in Figure 6.[74] The model takes random Gaussian noise and one-hot encoding synthetic vectors as input, and uses this information to generate 2D material representations that meet specific composition conditions. They use Wasserstein distance to optimize the generation process to ensure that the generated materials have high fidelity. At the same time, they ensure the structural consistency of the generated materials through arrangement invariance, ensuring that the generated materials both meet the composition conditions and are of high quality. Of the 3300 materials generated, 368 were predicted to be metastable with formation energies less than 200 meV/atom. Among them, 35 are considered synthesizable because of their formation energies below 80 meV/atom. In particular, $MgMn_4O_8$ is more stable than the polymorphic materials in the initial database. They then successfully screened 23 new stable compounds by considering the pourbaix stability and the band gaps. This study demonstrates the ability of GANs to quickly discover stable compounds that may be missed by using traditional methods.

Similarly, to rapidly design stable Bi-Se binary compounds, Long et al. developed an inverse model for crystal structure search with a constrained crystal DCGAN (CCDCGAN), as shown in Figure 7.[75] With the developed model they generated a series of possible crystal structures, some of them show good thermodynamic stability. Specifically, 89.9% of the 2832 generated structures have negative formation energies, 1233 are metastable, and 58 are stable.

A physics guided crystal structure generation model (PGCGM) was developed, as shown in Figure 8.[76] PGCGM integrates four key parts: the discriminator, the generator, the self-enhancement module and the atomic distance matrix/loss calculation module, and achieves the generation and identification of crystal structures through the combination of machine learning technology and physical principles. The core of the model is to use affine matrix and space group symmetry information to ensure the structural accuracy and symmetry of the generated crystal material. The generator is responsible for generating fake crystal structures, while the discriminator is used to distinguish real and fake materials. The two are integrated into the training process through an affine matrix to enhance the authenticity and symmetry of the generated materials. The self-enhancement module improves the generalization ability of the model by increasing the diversity of training samples, especially for rare space groups. Physically guided loss calculations further ensure the accuracy of the physical and chemical properties of the generated materials, such as controlling the reasonable

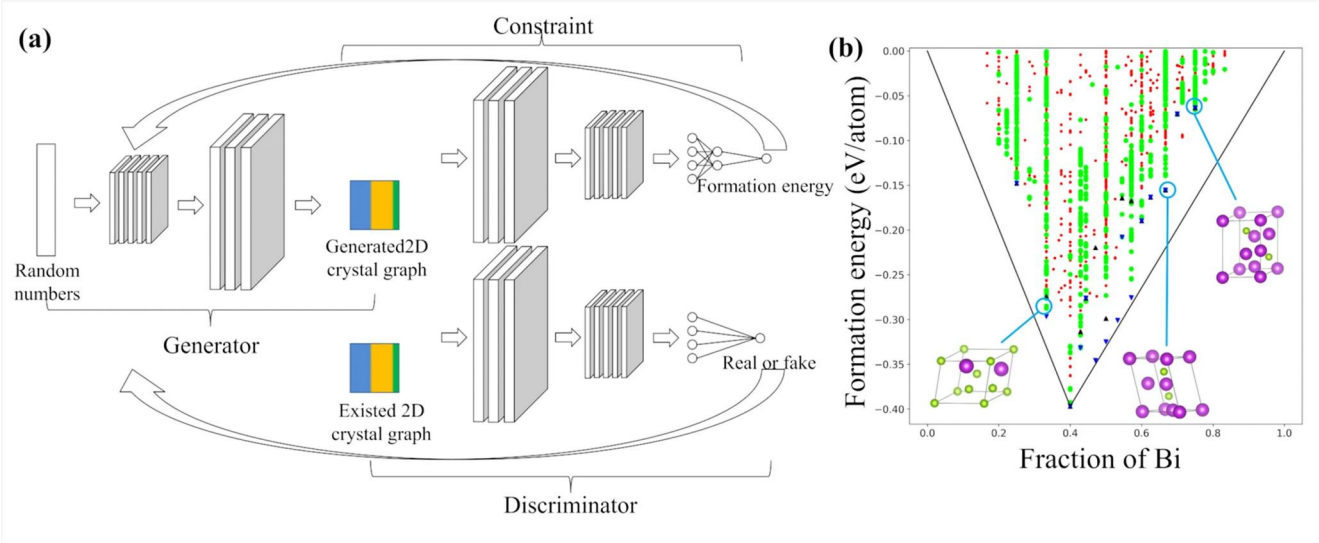

FIGURE 7 (a) Basic idea of the CCDCGAN model, (b) The formation energy of generated structures with CCDCGAN, where red points are the structures in the database, green circles are the generated structures, blue triangles represent the experimental validated phases, and black triangles indicate the Bi-Se phases in the Bi-Se database. The highlights by circles are crystal structures of interest, that is, Bi_2Se_4, Bi_4Se_2 and Bi_6Se_2.[75] Reproduced with permission. Copyright 2021, Springer Nature. CCDCGAN, constrained crystal DCGAN.

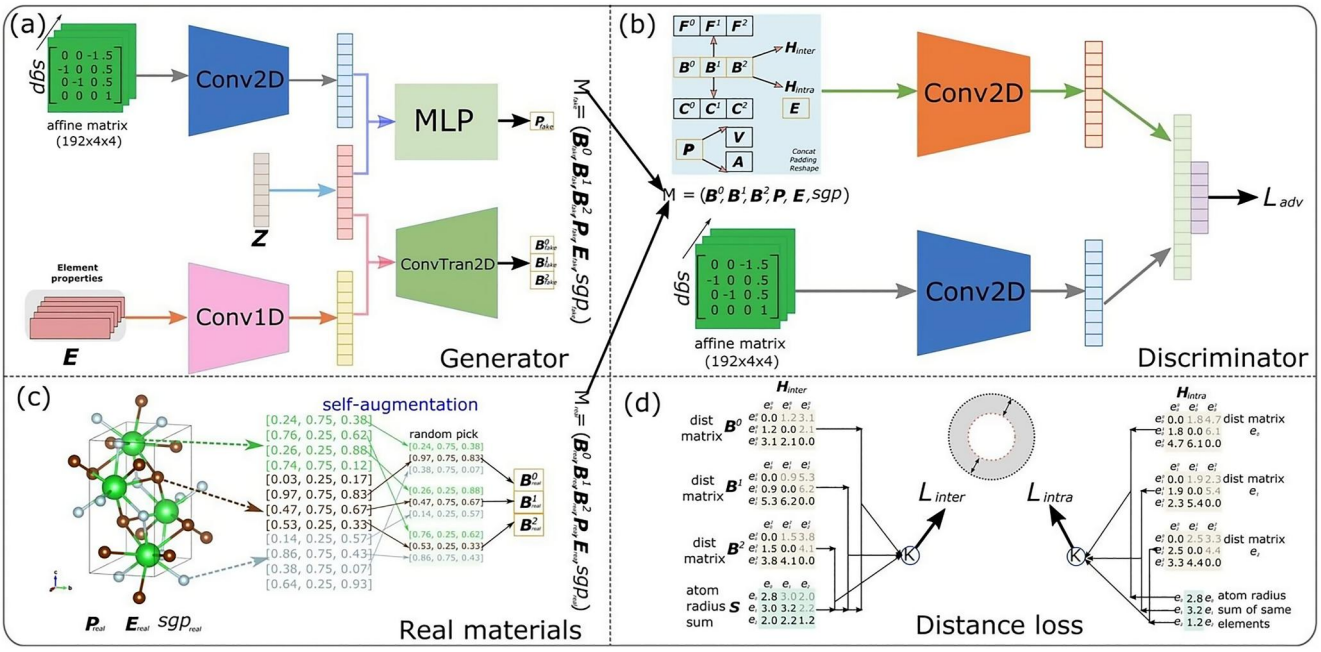

FIGURE 8 (a) Generator creates atomic structures from input data, (b) the discriminator evaluates whether the structure is accurate using two types of data: an affine matrix and a matrix of atomic positions and parameters, (c) the accuracy of the assessment can be improved by diversifying atomic position and spatial information, (d) the discriminator checks the distance between atoms to determine whether the generated structure matches the actual one.[76] Reproduced with permission. Copyright 2023, Springer Nature.

distance between atoms through the atomic distance matrix to avoid the generation of physically unfeasible structures. In addition, the use of WGAN-GP method and data enhancement technology not only improves the stability of model training, but also optimizes the quality of generated materials, allowing the model to efficiently generate crystal structures that meet specific physical and chemical property requirements. This model generates crystal structures with high structural diversity and symmetry and is verified by density functional theory calculations, significantly improving the effectiveness of the generation. The results showed that out of 2000 materials, 1869 were successfully optimized. After removing six materials with formation energies greater than 10 eV from the optimized materials, 39.6% of them showed negative formation energies, indicating that they may be synthetic. This study demonstrates

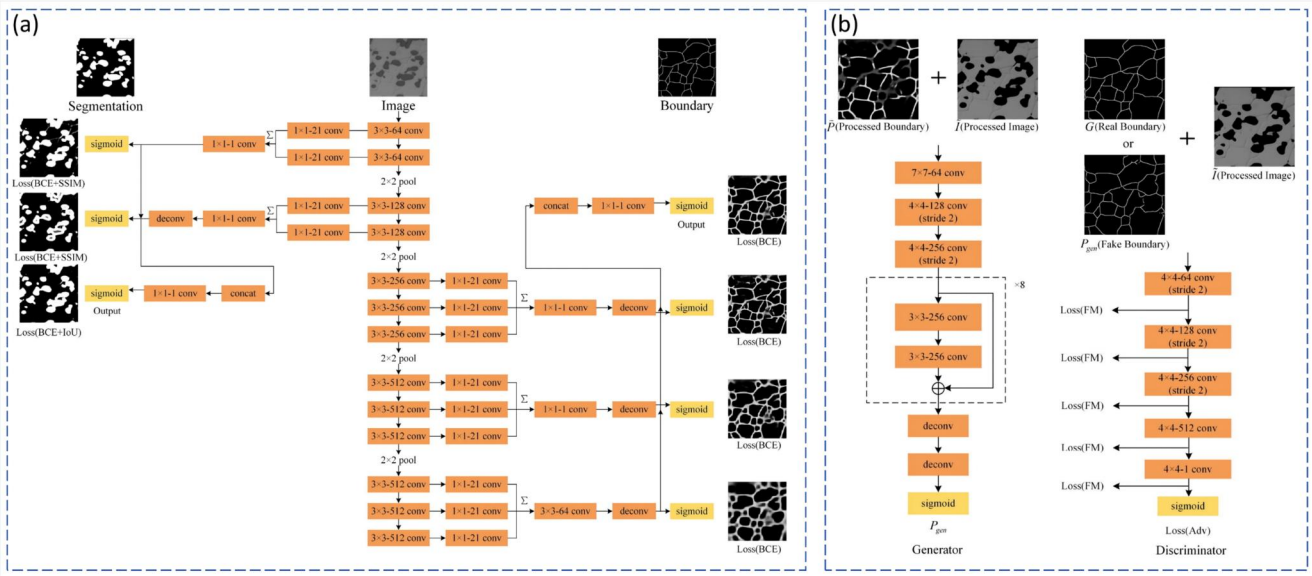

FIGURE 9 (a) Multi-task learning network structure; (b) generative adversarial networks structure for boundary fine-tuning.[82] Reproduced with permission. Copyright 2020, Elsevier.

the effectiveness of deep learning and GANs in the inverse design of crystal structures with symmetry constraints.

In conclusion, GANs as relatively new tools in crystal structure prediction and search, have proven more efficient than traditional strategies. By considering constraints such as composition condition or formation energy, the generative efficiency can be further improved. It has also shown that the involvement of physics like symmetry and group theory can also enhance the generation. Therefore, materials and physical knowledge deserve more attention when constructing GANs for crystal structure optimization in the future.

5 | APPLICATION OF GANs IN MATERIAL MICROSTRUCTURE

Traditional materials microstructure characterization and reconstruction usually rely on experiments and simulations that are time-consuming and costly. Generative models such as GANs, which are popular in image recognition, are being increasingly used to handle the materials images such as microstructures. The methods can effectively learn the information encoded in the images and then generate new images.[77–81] In addition, one can relate the learned representation to property of interest. This section outlines how GANs can be used in the characterization, reconstruction and generation of materials images.

Combination of multi-task learning and GANs was used to effectively analyze and extract microstructures information, as shown in Figure 9.[82] They used a data set of 120 microscopic images of heat-treated Al-12.7Si-0.7Mg direct-cooled cast alloy, which are acquired by optical microscopy characterized by silicon particles and aluminum matrix. They first utilized a convolutional architecture based on multi-task learning for preliminary detection and segmentation of microscopic images, and then used GANs to clean the hidden grain boundaries covered by the second phase. In addition, they designed a quantitative analysis module to extract indicators such as the number, size and eccentricity of aluminum grains. In terms of performance evaluation, the designed algorithm achieved an accuracy of 96.65% in the silicon particle segmentation task, and achieved a precision of 92.65% and a recall rate of 91.90% in the grain boundary detection task. These quantitative results demonstrate the method's excellent performance on two tasks, providing materials scientists with an effective analytical tool.

In addition, GANs were used to reconstruct material microstructure images.[83] They used three different types of GANs models: DCGAN, CycleGAN and super-resolution GAN (SRGAN) to perform image generation, image-to-image conversion, and microstructure image quality augmentation, respectively.[84,85] DCGAN was used to generate microstructure images from parametric descriptors, while CycleGAN was used to convert microstructure images between optical microscopy and scanning electron microscopy, and SRGAN was used to convert low-resolution microstructure images into high-resolution images. The data they used for training includes 386 microstructural images of dual-phase steel and 987 optical microscopy and scanning electron microscopy images as well. The results show that microstructure images generated by DCGAN and CycleGAN are very realistic and almost indistinguishable from real images, as shown in Figure 10. In addition, the high quality microstructural images generated by SRGAN can be used as input for finite element analysis.

In addition to 2D images, several studies have focused on 3D microstructures. For example, Nguyen et al. employed

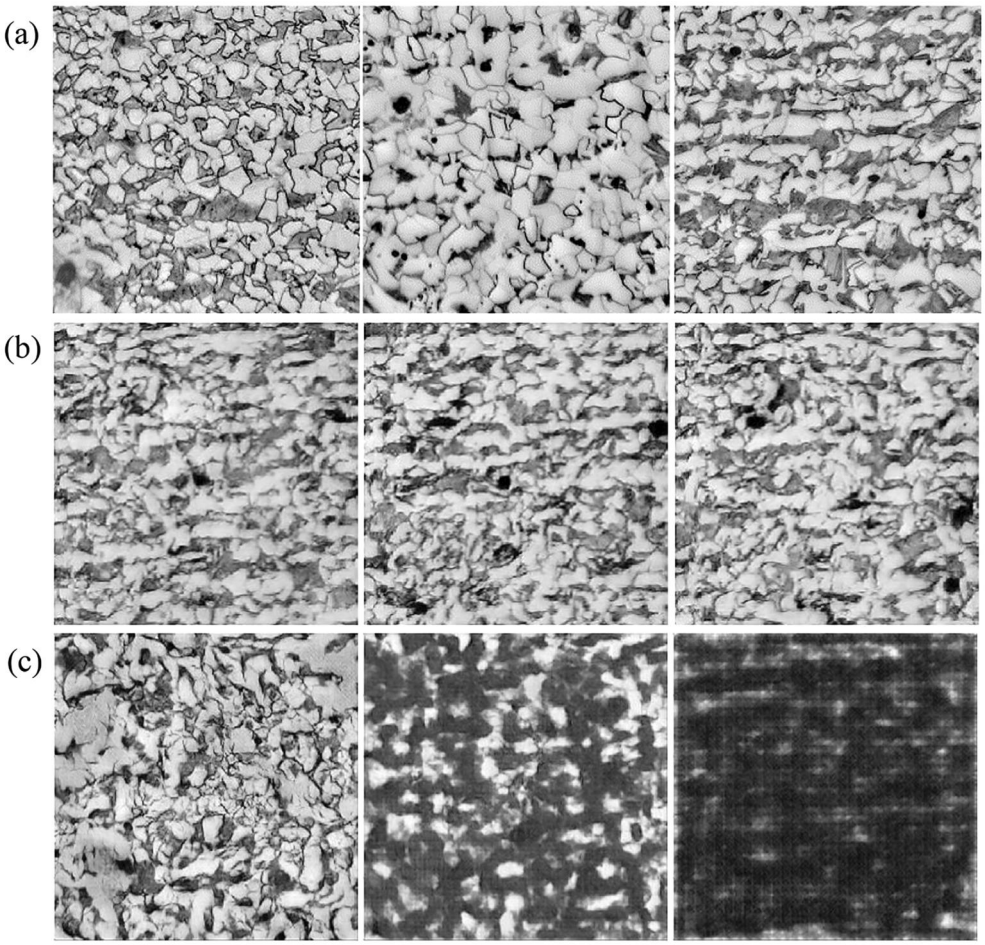

FIGURE 10 Comparison between real and generated micrographs of dual phase steel. (a) Real micrographs, (b) DCGAN generated micrographs, (c) micrographs generated by DCGAN model trained with additional noise.[83] Reproduced with permission. Copyright 2022, John Wiley and Sons. DCGAN, deep convolutional generative adversarial network.

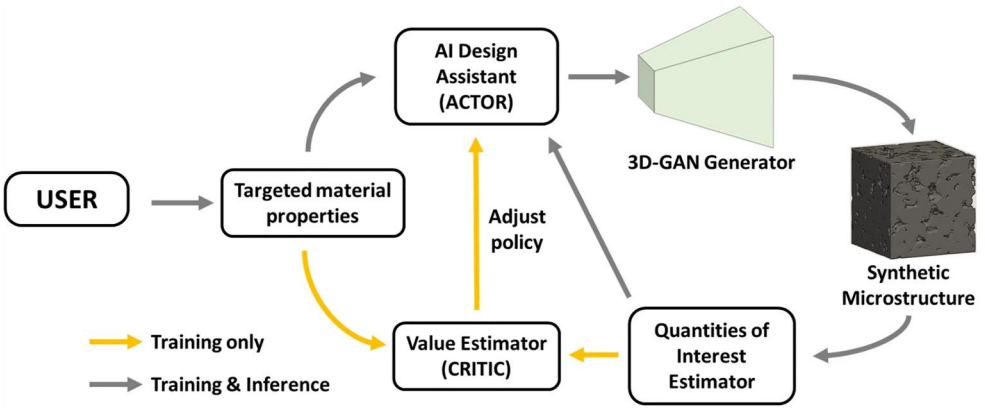

FIGURE 11 Schema of GAN-RL model framework for porous media microstructure design.[86] Reproduced with permission. Copyright 2022, Springer Nature.

GANs and reinforcement learning (RL) to synthesize porous media microstructures with specific physical properties, as shown in Figure 11.[86] The model adjusts the input parameters of the 3D-GAN via an artificial intelligence design assistant (actor network) with the aim of generating 3D synthetic microstructures with specific target physical properties. The process involves physical analysis of the microstructure using OpenPNM, an open source software package for pore network modeling, and evaluates the physical quantities of interest (QoI) of the synthesized 3D

microstructure, such as porosity, specific surface area, effective permeability, etc. The Actor-Critic (AC) model is used for iterative optimization, in which the actor network generates morphological parameters, and the critic network is responsible for evaluating the conformity of the generated microstructure. The entire system is iteratively optimized under the framework of reinforcement learning. The training process is divided into two stages: first, the training of 3D-GAN on real microstructure images, and secondly, the training of AC models to solve the inverse microstructure design problem. With this design, the model not only learns to generate microstructures that match the target QoI, but also optimizes its performance in a continuous feedback loop, effectively combining deep learning with physical modeling to achieve accurate microstructure design.

To conclude, GANs have demonstrated their ability in the characterization, reconstruction and generation of material microstructures. Besides, they can enhance the resolution of microstructures. The use of GANs not only simplifies the processing of microstructure images but also generates amounts of image data that can be utilized in other fields such as simulations.

6 | APPLICATION OF GANs IN MATERIAL PROCESSING

Processing is an important part in materials fabrication and largely affects the property. GANs have demonstrated a unique role in material processing, especially in the optimization of processing parameters.[87–90] This section summarizes recent applications of GANs in this field.

In the directed energy deposition process, in order to reduce the number of experiments, a cGAN technique was employed to predict and generate the surface morphology of Ti-6Al-4V alloys.[91] They first produced 80 samples with different surface morphologies by changing the laser power, powder feeding rate and scanning speed, and used the process parameters as labels for the image samples. Using these image samples to train the cGAN model, the surface topography can be predicted based on the given processing parameters, as shown in Figure 12. As a result, this strategy can not only help improve surface quality quickly by controlling the processing parameters, but also effectively reduce experiments required, thus providing new solutions in additive manufacturing.

In addition, GANs have also been adopted in the optimization of rolling such as ring rolling where ovality is a key indicator of ring quality. Traditional predictions of ovality mainly rely on experience and simplified computational models with less accuracy and reliability. Fahle et al. utilized semi-supervised learning and GANs to optimize the Radial Axial Ring Rolling (RARR) process, as shown in Figure 13.[92] The model used a dataset of 3670 samples (including 1256 labeled real samples and 2414 unlabeled samples), and achieved a notable increase in prediction accuracy to 88.84% that surpasses traditional methods. This improvement was largely due to the integration of semi-supervised learning with random Gaussian noise. The key was the use of cGAN to create synthetic multivariate time series data that is essential for simulating various time-dependent aspects of the RARR process. They also used a GANs variant, the Classifier Generative Adversarial Network, but found it is less effective in generating reliable RARR data. This highlights cGAN's superior ability in generating synthetic multivariate time series data.

To conclude, GANs play an important role in the field of material processing, especially when many parameters should be considered simultaneously. Besides straightly using the processing parameters as input for surrogate models, one can envision that integrating GANs with theory-based simulations can further accelerate and rationalize the processing of materials. In addition, GANs can also automate the optimization of processing and advanced equipment and software can be expected in the near future.

7 | APPLICATION OF GANs IN DEFECT DETECTION

Defects such as crack and their evolution determine the service lifetime of materials, and GANs are becoming an important tool for detecting such defects. By using advanced GANs models, researchers can more accurately detect defects and thereby evaluate the reliability of components. This section will focus on how GANs were used in the detection of material defects.[93–97]

To automatically detect defects in composite materials, a IRT-GAN model based on GANs and infrared thermography (IRT) was developed.[98] It uses a multi-head fusion strategy to analyze infrared thermal image data and then identifies the defects. They created a large dataset of images containing distinct defects to train the model. Experimental results show that IRT-GAN exhibits over 90% accuracy in identifying defects of different types, sizes and depths, confirming the efficacy in automatic defect detection. Additionally, such method was also applied in fiber-reinforced polymers, Cheng et al. proposed a defect-aware GANs framework called Dual-IRT-GAN and used it to perform both super-resolution and defect detection tasks in infrared thermal imaging, as shown in Figure 14.[99–103] Dual-IRT-GAN employs four main network components, each optimized for the specific task of infrared image processing. The super-resolution network (SRnet) is based on the residual in residual dense block (RRDB) structure, inherits the architecture of ESR-GAN, and is specifically designed to improve the resolution of infrared images. By learning the mapping from low resolution to high resolution, it generates High-resolution images with rich texture details. Defect segmentation network (SEGnet), following the design principles of U-net, achieves accurate segmentation of defect areas in infrared images through the structure of the encoder and decoder and jump connections. Two discriminators, DSR and DSEG, evaluate the authenticity of images and segmentation maps generated

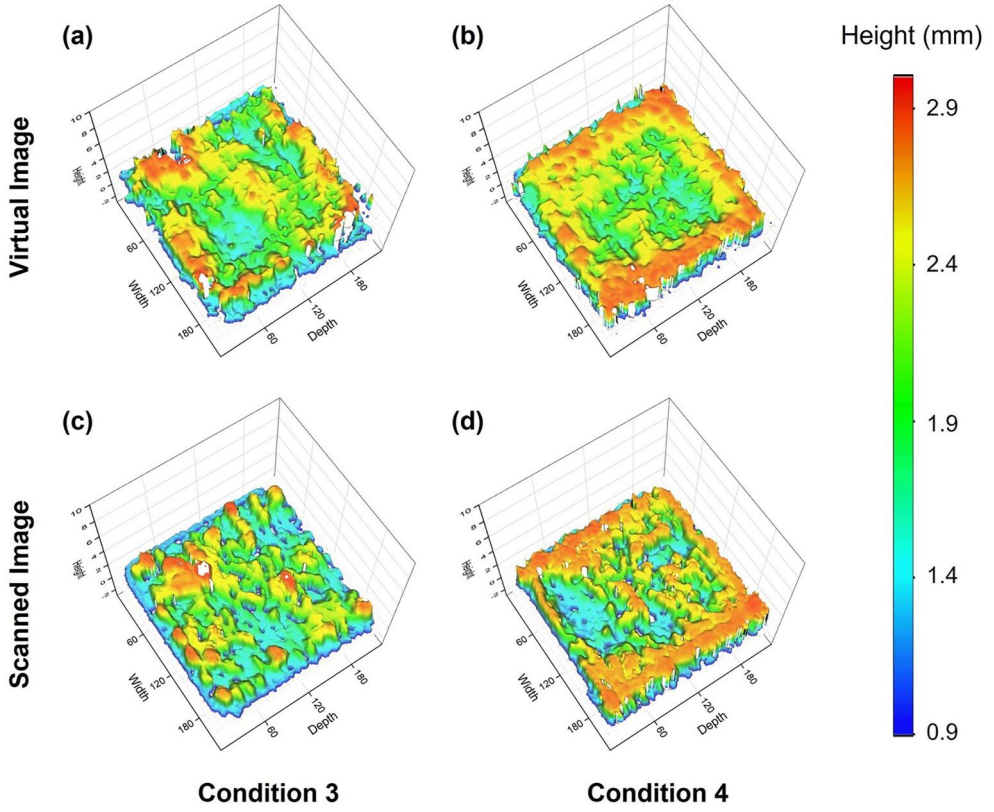

FIGURE 12 Comparison between generated surface and experimentally scanned surface, color bar represents surface roughness.[91] Reproduced with permission. Copyright 2022, Elsevier.

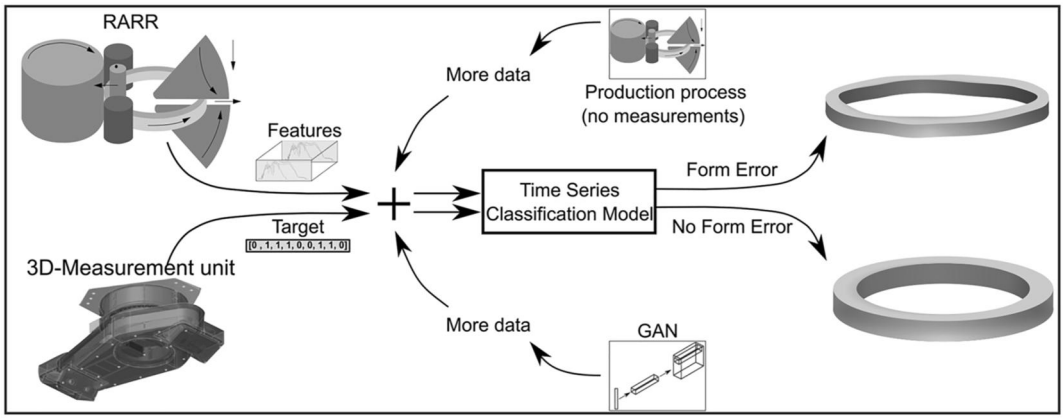

FIGURE 13 Schematic diagram showing the workflow for prediction of orality during ring rolling.[92] Reproduced with permission. Copyright 2021, Springer Nature.

by SRnet and SEGnet respectively. They adopt the *U*-net architecture and spectral normalization technology to not only focus on local textures, but also consider global structures, thereby striking a balance between local details and global consistency. In addition, the model introduces a defect cross-attention module, a cross-attention mechanism based on CBAM. This mechanism guides SRnet to focus on enhancing the texture of defective areas during the reconstruction process by fusing the segmentation results of SEGnet with the feature maps of SRnet, improving visibility of defects. During the training process, by combining content loss, perceptual loss and adversarial loss, the model can accurately reconstruct images at the pixel level, while ensuring that the generated images are perceptually similar to real images, further improving the realism of the generated images through adversarial learning. Overall, the Dual-IRT-GAN model enhances the visibility of defective areas through the fusion of deep learning and image processing

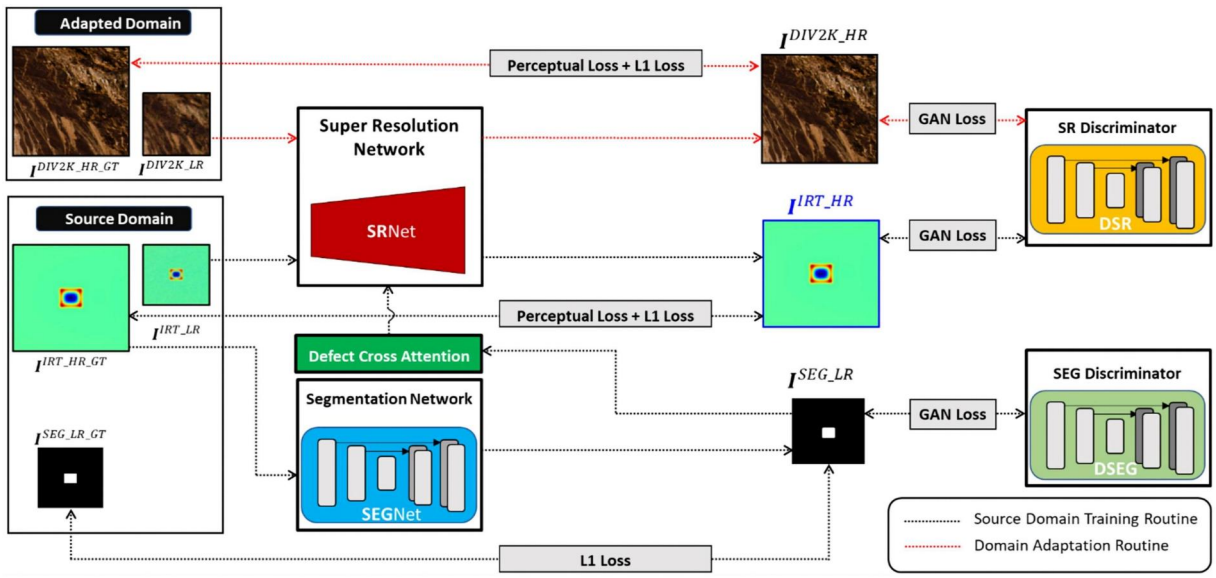

FIGURE 14 Overview of the Dual-IRT-GAN framework for defect detection in infrared thermal imaging.[99] Reproduced with permission. Copyright 2022, Elsevier.

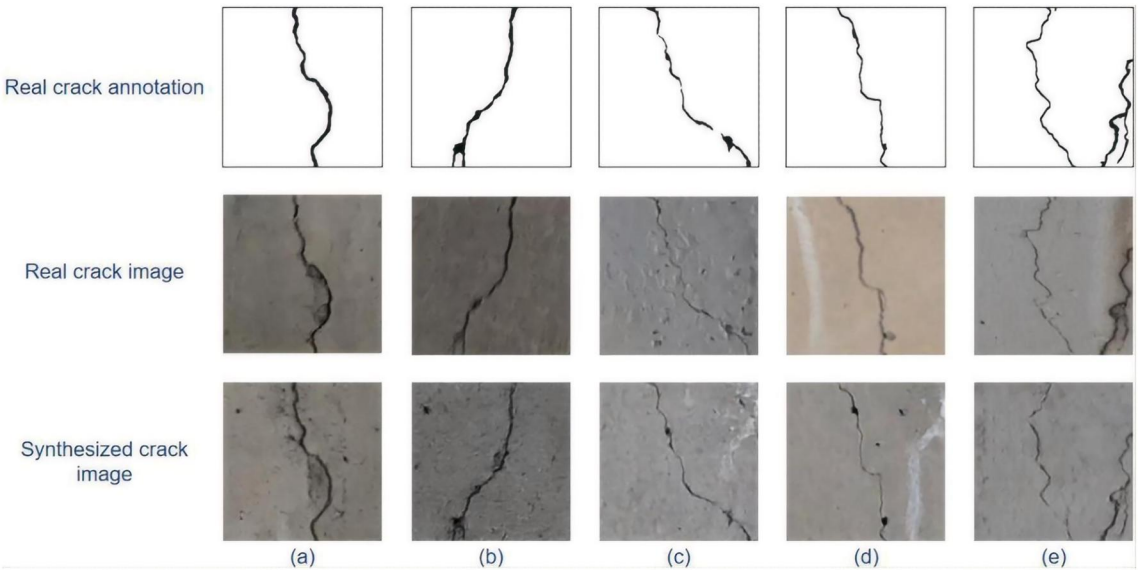

FIGURE 15 Comparison of different concrete crack images, including manually labeled, real and synthetic crack images. (a) and (e) images with spots, (b) images with wrinkles, (c) and (d) images with calcifications.[110] Reproduced with permission. Copyright 2023, Elsevier.

technology. The model was trained on numerically generated thermography datasets of composite materials with various defect types, sizes and depths. The inference performance was demonstrated on multiple experimental thermography datasets.[104,105]

Crack detection also plays a key role in assessing the safety of bridge structures. Since structural cracks on bridges in service exist in various geometric forms and are accompanied by various noise patterns, a large number of different types of crack images are needed to learn crack characteristics and noise patterns to achieve accurate detection.[106–109] However, the lack of crack images has been an obstacle to improving the performance of deep learning-based crack detection methods. Jin et al. proposed a method based on GANs to build a synthetic crack image dataset with pixel-level annotations, which provides an alternative to traditional data augmentation methods.[110] They used a dataset of 7800 images to train a DCGAN model and generated synthetic crack annotations, and used the Pixel2Pixel model to generate the corresponding synthetic crack. Figure 15 compares the real and synthetic crack images. It is seen that a deep neural network (DNN) trained on these synthetic images achieves a mean intersection-over-union ratio (MeanIoU) of 74.34%, comparable to the DNN model trained on real images. In addition, the fine-tuning model for real images assisted by the pertaining one with synthetic crack images

works better than the model that was trained on a dataset by directly mixing synthetic and real crack images. This work provides a guideline for the establishment of a GAN-based crack image dataset and the assessment of image quality for training crack detection models.

Overall, by using GANs models researchers are able to identify and detect materials defects of different types, sizes and depths. Boosted by the increasing amounts of available data, GANs can further improve the recognition accuracy for defects. In the future, GANs are expected to enable automated and precise tools for defect detection in materials science.

8 | CONCLUSION AND OUTLOOK

In summary, GANs have been applied widely in different aspects of materials science and facilitated the progress of composition design, processing optimization, structure recognition and generation, and defect detection as well. Despite many efforts and achievements, this field is still in its infant stage and a number of challenges need to be solved. Here, we outline several challenges and suggest possible solutions.

First, a dataset of large size is often required to train robust GANs. However, for experiments and high-fidelity simulations, available data is quite limited and will hinder the direct application of GANs. A few examples have trained GANs using such limited data by data augmentation (e.g., image rotation and cropping). This sometimes works, however, such kind of data augmentation in essence does not improve the information of initial data and it is not necessary to obtain robust GANs-based models. Bayesian methods using uncertainty associated with model prediction have been proven suitable for small data in materials design. Thus, it is expected that the integration of such methods or concepts to GANs can mitigate the issues with small data.

Second, the data generated by GANs, including both compositions and micrographs, are often very similar to the training data. In reality, one expects that the generation should be distinct to the existences so that they may lead to new discoveries or understandings. Hence, it is required to further improve the balance between model fitting and generation diversity. Several possible strategies deserve to be considered: first, the integration of GANs with VAEs may be useful considering the randomness in the continuous latent space of the latter. Second, the tailoring of the loss function by using prior knowledge, as well as the fusion of multimodal data to enhance the model generalization ability. To validate the generation, the most strong method is always the synthesis and characterization, regardless of its time-consuming and laborious essence.[111–113]

At the end, to date the applications of GANs in materials science are mainly data-driven. Nonetheless, there are a number of mature experiences and theories such as thermodynamics and kinetics that have assisted the development of materials research over many decades. Thus, it is natural to imagine how to combine these two paradigms effectively, which will not only improve the interpretability of GANs but also accelerate the discovery of new materials further.

AUTHOR CONTRIBUTIONS

Yuan Jiang: Investigation, methodology, writing. **Xiang Yang**: Methodology, writing. **Ruihao Yuan**: Supervision, conceptualization, editing, methodology. **Jinshan Li**: Conceptualization.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

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