3DMaterialGAN: Learning 3D Shape Representation from Latent Space for Materials Science Applications

Devendra K. Jangid¹, Neal R. Brodnik³, Amil Khan¹, McLean P. Echlin²
Tresa M. Pollock², Sam Daly³, B. S. Manjunath¹

¹Electrical and Computer Engineering
²Materials Department
³Mechanical Engineering
University of California, Santa Barbara
{tresap, samdaly, manj}@ucsb.edu

Abstract

In the field of computer vision, unsupervised learning for 2D object generation has advanced rapidly in the past few years. However, 3D object generation has not garnered the same attention or success as its predecessor. To facilitate novel progress at the intersection of computer vision and materials science, we propose a 3DMaterialGAN network that is capable of recognizing and synthesizing individual grains whose morphology conforms to a given 3D polycrystalline material microstructure. This Generative Adversarial Network (GAN) architecture yields complex 3D objects from probabilistic latent space vectors with no additional information from 2D rendered images. We show that this method performs comparably or better than state-of-the-art on benchmark annotated 3D datasets, while also being able to distinguish and generate objects that are not easily annotated, such as grain morphologies. The value of our algorithm is demonstrated with analysis on experimental real-world data, namely generating 3D grain structures found in a commercially relevant wrought titanium alloy, which were validated through statistical shape comparison. This framework lays the foundation for the recognition and synthesis of polycrystalline material microstructures, which are used in additive manufacturing, aerospace, and structural design applications.

1 Introduction

The ability to generate 3D objects is of interest across many different fields because of its impact on a diverse application space. Much of this stems from the potential to synthesize realizable data that can be used to solve the small dataset problem where data is expensive, or to explore the unique complexities of a dataset beyond the sum of its parts. For example, there are countless possible chair designs, but we never look at a chair and go through a checklist of designs to verify that it is one. We simply let shape dictate function. In this same respect, a generative model should be able to learn the shape of an object and its constituent components within a particular context.

Generative Models: As more comprehensive datasets like ShapeNet from Chang et al. [1] and Wu et al. [2] become available to the community, this will enable us to build better generative models to tackle the difficult problem of 3D object generation. Although there have been previous successful attempts that provide solutions to this task, the quality of the objects generated still require improvement, and many opportunities remain for the application of these models to real-world problems.

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In this paper, we develop a novel generative architecture that provides promising results for learning the shape of volumetric data. Inspired by Goodfellow et al. [3], Generative Adversarial Networks (GANs) try to generate new data based on a training data distribution. Building on this foundational idea and applying concepts from StyleGAN by Karras et al. [4] such as a non-linear mapping network and styles that control adaptive instance normalization (AdaIN), we present a novel generative network designed to produce more realistic objects that are robust to pixel-volume outliers and overfitting. This is achieved using 3D deconvolution blocks in the synthesis network, an augmented discriminator based on multiple samples (Lin et al. [5]), and a Wasserstein loss function with gradient penalty (Arjovsky et al. [6], Gulrajani et al. [7]).

Material Microstructures: The application focus of this architecture is in the field of materials science, which explores the relationships between the processing, structure, and properties of materials. The interplay between these relationships serve as means for controlling the performance of materials for different applications. This work focuses on a subset of materials known as crystalline materials. Crystalline materials are those whose atoms arrange themselves into patterns with long range order. The most common types of crystalline materials are single crystals and polycrystals. Single crystal materials are those where a single pattern of long range order is present throughout the entire structure, such as in gemstones, silicon wafers for microchips, and blades found in the hot section of turbine engines. Polycrystals, which are more prevalent, are materials composed of many connected crystals, called grains, where each grain has local long range order and unique crystal orientation. The majority of metals and ceramics used in industrial and consumer applications are polycrystalline, including those found in transportation, structural materials, consumer appliances, and aerospace.

In polycrystalline materials, much of the relationship between material processing, structure, and properties manifests through the shape, orientation, and arrangement of the constituent grains. During solidification or thermal processing, numerous grains form and grow, either through nucleation or diffusive boundary migration, until they impinge upon their grain neighbors, resulting in a fully formed polycrystalline solid. While the physics of grain formation at thermodynamic equilibrium are relatively well understood, there are many processes that can distort grain shape in a variety of ways through mechanical work, such as rolling and extrusion. Additionally, some high temperature processing, such as metal joining and additive manufacturing, results in large thermal gradients where thermodynamic equilibrium is not achievable on normal processing timescales. These extreme processing routes can lead to a variety of different grain shapes and arrangements at the microstructural level, which consequently lead to differences in material response at the property level. Different grain morphologies can produce changes in stiffness, strength, ductility, and conductivity, all of which can impact material performance in technical applications. For machine learning to be a viable tool to explore processing-structure-properties relationships in crystalline materials, a critical first step is a generative architecture that can understand grain structure.

In this paper, we make the following contributions:

1. We address the 3D object generation problem by proposing 3DMaterialGAN, a novel generative architecture that provides promising results for unsupervised learning of detailed contextual shape information.
2. Our network takes only 3D data as input and outperforms state-of-the art models on the ModelNet benchmark dataset (Wu et al. [2]) for shape classification through a feature-rich space learned by the discriminator.
3. To show generalizability and application to material science, we demonstrate the use of our network on a large scale 3D dataset of a polycrystalline titanium alloy by Hémery et al. [8], which we validate by statistical comparison of moment invariants.

2 Related Work

3D Shape Completion and Synthesis. Until recently, much of the work on 3D object generation included the retrieval of or combining of the components of the 3D object, such as the works of Chaudhuri et al. [9], Funkhouser et al. [10], Kalogerakis et al. [11]. In these cases, given a database of shapes, a probabilistic graphical model will learn the geometric and semantic relationships that will yield a stylistically compatible object. Taking this a step further, Wu et al. [2] represented geometric 3D shapes as probability distributions of binary variables on a 3D voxel grid and was able to successfully demonstrate shape completion from 2.5D depth maps. A not so similar but related
work from Choy et al. [12] proposed a network that used the ShapeNet dataset to learn a mapping from images to their underlying 3D shapes—given an input image of a plane, generate a 3D representation of a plane. This has since led to works from Zhang et al. [13], Wu et al. [14], Noguchi and Harada [15] and Nguyen-Phuoc et al. [16] which generate 3D representations from 2D images. Although these showed encouraging results, most of these methods relied on some form of supervision and lack work on the latent space to 3D object generation side. To circumvent this, Sharma et al. [17] proposed a promising autoencoder-based network to learn a deep embedding of object shapes in an unsupervised fashion, which yielded then state-of-the-art shape completion results.

3D GANs for Shapes. The most relevant works are from Wu et al. [18] and Zhu et al. [19]. The 3D-GAN network from Wu et al. [18] generates 3D objects from a low-dimensional probabilistic latent space, thus enabling the sampling of objects without a reference image or CAD models, and the exploration of the 3D object manifold. Similarly, Zhu et al. [19] propose a novel 3D GAN network, but with the small twist of using a 2D image enhancer. The enhancer network is able to effectively learn and feed the image features into the 3D model generator to synthesize high quality 3D data. While both of these networks deliver on their promise to provide a solution to the 3D model generation problem, they offer limited resolution and detail in the shapes that they generate. Our proposed network provides a solution to this challenge by generating detailed shapes without the use of additional information from 2D images. To the best of our knowledge, we achieve state-of-the-art performance on the ModelNet benchmark dataset, while also demonstrating the value of our network to solve a real-world problem in materials science.

Generation of Non-Crystalline Material Structures: Bapst et al. [20] used graph neural networks of 3D atomic arrangements to describe glasses, which have amorphous microstructures. These graphical descriptions were then used as predictive tools to explore how structure affects mobility and resultant glass properties. Additionally, Cecen et al. [21] used 3D convolutional neural networks to characterize stochastic microstructures made from filtered noise. Stochastic microstructures have also been investigated in 2D by Bostanabad et al. [22] using classification trees as well as by Li et al. [23] using GANs.

Synthetic Crystalline Microstructures: Physics-based models have been used for microstructure generation due to their high level of detail and realistic morphologies. Work by Coster et al. [24] used a Voronoi tessellation model that simulated ceramic grain boundary evolution based on equations developed by Johnson and Mehl [25], Avrami [26], and Kolmogorov [27]. Additionally, the work of Nosonovski et al. [28] combined Monte Carlo simulations and grain growth kinetics to model metal crystallization. These physics-based models show promise, but often require significant computational power as well as detailed knowledge of the energetics of the system. To avoid this knowledge and computation burden, models have also been developed to generate microstructures based on their statistics. For example, Quey et al. [29] as well as Groeber and Jackson [30] use statistical descriptors to build microstructures using tessellation and ellipsoid coarsening, respectively. Additionally, Callahan et al. [31] compared in detail microstructures generated using the approach of Groeber and Jackson [30] with experimental results. Approaches like these are computationally efficient and versatile, compared to physics-based models, but show less realistic grain morphologies and limited accuracy in local grain environment descriptions.

Machine Learning with Crystalline Microstructures: Liu et al. [32] used structural optimization to explore the microstructure space of the iron-gallium alloy Galfenol. This approach focused on techniques for optimizing grain arrangement in the Galfenol microstructure to achieve an orientation distribution that would improve desired properties. While this approach allows for extensive exploration of property space, some challenges arise because the basis of the model is theoretical, so it presents no means of verifying that the proposed microstructures can be physically realized with available processing techniques. There has, however, been progress with machine learning techniques based on experimental results. Work by DeCost et al. [33] compiled a database of 2D ultra-high-carbon steel microstructures, and then classified them based on distributions of microstructural features (DeCost et al. [34]). Additionally, in work by Iyer et al. [35], a Wasserstein GAN with gradient penalty was used to generate 2D microstructures using the database of DeCost et al. [33] as training data. More closely related to this work, Fokina et al. [36] used StyleGAN to generate various 2D microstructures, and Cang et al. [37] used a convolutional deep belief network to generate 2D microstructures of the same titanium alloy investigated in this study. While approaches like this have good experimental foundation, validation of microstructures is difficult in these 2D cases. The challenge in 2D microstructure assessment arises from the fact that unlike conventional photographs,
material micrographs are planar images of solid material, and offer little perspective-based information from which 3D appearance can be inferred. More explicitly, Torquato and Haslach Jr [38] show that for certain shape classes such as anisotropic materials, establishing 3D structure from 2D is mathematically intractable. In order for output from machine learning-based models to be fully comparable to material microstructures, generation and evaluation needs to be based in 3D space.

3 Model

In this section, we introduce the foundational idea of generative adversarial networks inspired by the StyleGAN network, followed by a formal outline of our proposed 3DMaterialGAN network.

Generative Adversarial Network (GAN): First proposed by Goodfellow et al. [3], a simple generative adversarial network consists of a generator $G$ and a discriminator $D$. The generator tries to synthesize samples that look like the training data, while the discriminator tries to determine whether a given sample is a real sample originated from the ground truth data or from the generator. The discriminator $D$ outputs a confidence value $D(x)$ of whether input $x$ is real or synthetic.

StyleGAN Network Architecture: StyleGAN, developed by Karras et al. [4], garnered widespread attention for its life-like image quality and unsupervised high-level attribute separation in the generated output. Because of these characteristics, we used StyleGAN as the base architecture for our network. Instead of passing a random noise vector $z$ to the generator, $z$ is first mapped to an intermediate latent space $W$, which is transformed into spatially invariant styles $y = (y_s, y_b)$. This is then used to control the generator through adaptive instance normalization (AdaIN) at each convolutional layer. The AdaIN is defined as:

$$
\text{AdaIN}(x_i, y) = y_{s,i} \frac{x_i - \mu(x_i)}{\sigma(x_i)} + y_{b,i}
$$

Here, $x_i$ is a feature map normalized separately, and then scaled and biased using the corresponding scalar components from style $y$.

3DMaterialGAN Network Architecture: In our 3D Material Generative Adversarial Network (3DMaterialGAN), an initial 512-dimensional latent vector $z$ is chosen through probabilistic sampling of latent space. The generator $G$ then maps this latent vector into an intermediate latent space $W$ using a mapping network of 8 fully connected layers with a LeakyReLU activation function after each layer. The output of $W$ is then converted into styles using learned affine transformation, denoted as $A$ in Figure 1 and these styles are used to control adaptive instance normalization (AdaIN) in the synthesis network. This localization of styles better preserves the fine-scale information of each object, allowing for more detailed shape capture compared to other networks (Wu et al. [18], Zhu et al. [19]). Our synthesis architecture diverges from that of StyleGAN by using blocks consisting of a 3D deconvolution passed through an AdaIN operation and ReLU activation function. The synthesis network has a total of five blocks, with the first having a constant input vector and normalization, and the fifth having a sigmoid activation function instead of a ReLU. In comparison, StyleGAN blocks use upsampling followed by two alternating convolution layers and AdaIN operations, with noise introduced after each convolution to add stochastic variation. However, in 3D, this noise was found to add instability during training, and was therefore not included in the 3DMaterialGAN network. The discriminator uses five 3D convolution layers, each with a LeakyReLU activation functions except for the last layer. The discriminator makes decisions based on multiple samples from the same class, either real or generated, as discussed by Lin et al. [5].

ShapeNet Dataset: From the ShapeNet Dataset by Chang et al. [1], six major object categories were used in the network training (car, chair, plane, guitar, sofa, rifle). Each category has a 128-sample training set. Objects are in a voxel-based format which has dimension of $64 \times 64 \times 64$.

Titanium Dataset: The material data was gathered by J. Wendorf and A. Polonsky (Hémery et al. [8]) using a method developed by Echlin et al. [39] known as the Tribeam system, which performs rapid serial sectioning using ablation with ultrashort pulse femtosecond lasers. The material of interest is a polycrystalline wrought titanium alloy containing 6.75 wt.% aluminum and 4.5 wt.% vanadium. This alloy, commonly referred to as titanium 6-aluminum 4-vanadium, or Ti 6-Al 4-V, has applications in turbine engines, aerospace, and medical prostheses. The grain information is gathered at the voxel level using electron backscatter diffraction, with each voxel having a size of $1.5 \mu m \times$
Figure 1: GENERATOR ARCHITECTURE OF 3DMATERIALGAN. A mapping network comprised of eight Fully Connected layers (FC) with Leaky ReLU activation function after each FC layer takes as input a 512 dimensional latent vector \( z \). The output is then mapped to an intermediate latent space \( W \), converted into styles using a learned affine transformation (A), and passed through an AdaIN operation for each of the five blocks in the synthesis network. Block 1 passes constant input through AdaIN and ReLU activation functions, while Blocks 2-5 are deconvolution blocks progressively grown from \( 8 \times 8 \times 8 \rightarrow 64 \times 64 \times 64 \).

Training details: Stable training was achieved by setting the learning rate for both the generator and discriminator at 0.0002, with a batch size of 16. The discriminator is updated five times for each generator update and employs the Adam optimizer described by Kingma and Ba [40] with \( \beta = 0.5 \). The output of the network is in a \( 64 \times 64 \times 64 \) dimensional space. The Wasserstein loss as described in Arjovsky et al. [6] with a gradient penalty is used for the discriminator and the generator, which are defined as follows:

\[
L_{D-Loss} = -\frac{1}{m} \sum_{i=1}^{m} D_\phi \left( x^{(i)} \right) + \frac{1}{m} \sum_{i=1}^{m} D_\phi \left( G_\theta \left( z^{(i)} \right) \right) + \frac{1}{m} \sum_{i=1}^{m} \lambda \left( \left\| \nabla \tilde{x}^{(i)} D_\phi \left( \tilde{x}^{(i)} \right) \right\|_2 - 1 \right)^2
\]

\[
L_{G-Loss} = -\frac{1}{m} \sum_{i=1}^{m} D_\phi \left( G_\theta \left( z^{(i)} \right) \right)
\]

Here, \( \tilde{x}^{(i)} \) is defined as \( \epsilon x^{(i)} + (1 - \epsilon) G_\theta \left( z^{(i)} \right) \) and \( \lambda \) is a gradient penalty coefficient. \( \epsilon \) is a uniform random variable in \([0,1]\). \( x^{(i)} \sim P_x \) is a batch from real data, \( z^{(i)} \sim p(z) \) is a batch of random noise, and \( m \) denotes batch size. \( G_\theta \) is a generator network and \( D_\phi \) is a discriminator network.

4 Evaluation

We evaluate our network across several areas. First, we show qualitative results of generated 3D objects from the ShapeNet dataset by Chang et al. [1]. Then, we evaluate the unsupervised learned representations from the discriminator by using them as features for 3D object classification. Lastly, quantitative results are shown on the popular benchmark ModelNet dataset from Wu et al. [2].

3D Object Generation: We train one 3DMaterialGAN for each object category using a 512 dimensional random vector which follows a normal distribution with mean 0 and variance 0.2. We compare our generated objects with Wu et al. [18], because Zhu et al. [19] used an enhancer network and additional information from 2D rendered images during training. Our network synthesizes high-resolution 3D objects (64 × 64 × 64) with detailed shape information trained from only 3D input. And to ensure that our network is not memorizing the training data, we perform nearest neighbor analysis for the synthesized objects as in Wu et al. [18]. Features were calculated from both the
generated samples and training samples to find the nearest neighbour using $\ell_2$ distance. This analysis yielded that the generated samples were not identical to its nearest neighbor.

**3D Object Classification:** To evaluate the unsupervised learned features from our network, we use the method in Wu et al. [18] to provide a means of comparison, as there is no established standard. We train our 3DMaterialGAN network on six object categories (bed, car, chair, plane, sofa, table), one object (gun) less than the analysis done by Wu et al. [18]. Each object category has 25 samples, same as Wu et al. [18], in the training set from the ShapeNet dataset.

Next, we use the ModelNet dataset from Chang et al. [1] to evaluate the unsupervised features learned by our network. The ModelNet dataset has two categories: ModelNet10 (10 classes) and ModelNet40 (40 classes). ModelNet10 has a total of 3991 training samples and 908 test samples. From this dataset, we used 100 samples from each category, totaling 1000 training samples. ModelNet40 has a total of 9843 training samples and 2468 test samples. From this dataset, we used 100 samples from each category when available, as some categories had less than 100 samples, totaling 3906 training samples. For ModelNet10 and ModelNet40, we used the entire test dataset provided, and less training samples than what Wu et al. [18] and Zhu et al. [19] used for their evaluation.

To provide a fair comparison, we used the same kernel size = {8, 4, 2} defined by both Wu et al. [18] and Zhu et al. [19], as well as the defined stride = (4, 2, 1) by Zhu et al. [19]. We calculate features from the second, third and fourth layers of the trained discriminator, which are then concatenated after applying max-pooling with the defined kernel size and stride. We then train a linear Support Vector Machine (SVM) on training features and calculate classification accuracy on the test features.

**Evaluation of Generated Grains:** Grain formation in polycrystalline microstructures is influenced by a combination of processing, thermodynamics, and statistics. Because of this, evaluation of grains cannot be easily done by visual evaluation or direct object comparison. For this reason, we use statistical distribution comparison of 3D moment invariants to assess the quality of generated results for single grains. Much like the image moments used in 2D analysis, 3D moment invariants are integration-based descriptors that numerically quantify an object based on the distribution of its solid volume. These types of invariants have been used previously by Kazhdan et al. [41] as shape descriptors for general 3D objects and in materials science by MacSleyne et al. [42] and Trenkle et al. [43] to describe the shapes of particles such as grains and inclusions. Following the approach of MacSleyne et al. [42], Cartesian moment descriptors $\mu_{pqr}$ take the form:

$$\mu_{pqr} = \int \int \int x^p y^q z^r F(r) dr$$  \hspace{1cm} (4)

where $F(r)$ is a characteristic function that has a value of one in material regions and a value of zero in void regions. In this study, because all ground-truth data is in voxel-based form, all integrations are done as Riemann sums in voxel space, rather than as continuous integrals. Following this Cartesian moment form, $\mu_{000}$ is directly equal to the volume $V$ of an object, and the centroid $(X_c, Y_c, Z_c)$ of an object can be expressed in the following form:

$$(X_c, Y_c, Z_c) = \left( \frac{\mu_{100}}{V}, \frac{\mu_{010}}{V}, \frac{\mu_{001}}{V} \right)$$ \hspace{1cm} (5)

Working from a coordinate space originating at the centroid, the non-normalized moment invariants $O_1, O_2, O_3$ are as follows:

$$O_1 = \mu_{200} + \mu_{020} + \mu_{002}$$ \hspace{1cm} (6)

$$O_2 = \mu_{200} \mu_{020} + \mu_{200} \mu_{002} + \mu_{020} \mu_{002} - \mu_{110}^2 - \mu_{101}^2 - \mu_{011}^2$$ \hspace{1cm} (7)

$$O_3 = \mu_{200} \mu_{200} \mu_{002} + 2 \mu_{110} \mu_{101} \mu_{011} - \mu_{200} \mu_{011}^2 - \mu_{020} \mu_{101}^2 - \mu_{002} \mu_{110}^2$$ \hspace{1cm} (8)

These can then be normalized to object volume to produce the moment invariants $(\Omega_1, \Omega_2, \Omega_3)$ considered in this study.

$$(\Omega_1, \Omega_2, \Omega_3) = \left( \frac{3V^{5/3}}{O_1}, \frac{3V^{10/3}}{O_2}, \frac{V^5}{O_3} \right)$$ \hspace{1cm} (9)

The distributions of these moment invariants are used to evaluate the shape quality of the generated grains. Additional analysis of 3D moment invariants can be found in MacSleyne et al. [42].
Figure 2: SHAPENET OUTPUT. Here we show a diverse range of 3D objects with detailed shape information generated by our 3DMaterialGAN network.

5 Results

ModelNet Benchmark Results: With fewer training samples than Wu et al. [18] and Zhu et al. [19], we achieve 92.29% accuracy on the ModelNet10 dataset and 85.08% accuracy on the ModelNet40 dataset. Given the graph in Figure 4 and Figure A1 in the supplementary material from Wu et al. [18], if we use a comparable training set size, we achieve a 2.29% improvement on ModelNet10 and a 3.78% improvement on ModelNet40 dataset. Furthermore, Zhu et al. [19] uses all available training samples as well as additional rendered 2D images for both datasets, compared to our use of both fewer training samples and only 3D input.

| Method                        | Supervised | ModelNet10 (%) | ModelNet40 (%) |
|-------------------------------|------------|----------------|----------------|
| 3D ShapeNets (Wu et al. [2])  | Yes        | 83.54          | 77.32          |
| VoxNet (Maturana and Scherer [44]) | Yes       | 92.00          | 83.00          |
| Geometry Image (Sinha et al. [45]) | Yes       | 88.40          | 83.90          |
| PointNet (Qi et al. [46])     | Yes        | 77.60          | -              |
| GIFT (Bai et al. [47])        | Yes        | 92.35          | 83.10          |
| FusionNet (Hegde and Zadeh [48]) | Yes       | 93.11          | 90.80          |
| SPH (Kobbelt et al. [49])     | No         | 79.79          | 68.23          |
| LFD (Chen et al. [50])        | No         | 79.87          | 75.47          |
| VConv-DAE (Sharma et al. [17]) | No         | 80.50          | 75.50          |
| 3D-GAN (Wu et al. [18])       | No         | 91.00          | 83.30          |
| 3D-GAN ([18]) (≈ 100 samples) | No         | 90.00          | 81.30          |
| Ours (3DMaterialGAN) (100 samples) | No       | **92.29**      | **85.08**      |

Grain Generation Results: Representative volumes of grains generated using the 3DMaterialGAN are shown in Figure 3. Unlike the benchmark results, which are shown as contour displays, these figures are shown in voxel form, which matches the representation of the ground-truth data. It should be noted that some generation artifacts were present in 64 × 64 × 64 volume containing these grains, with the most common of these artifacts being voxels of solid volume at random locations in the void. Some examples of these artifacts can be seen in the contour images of the benchmark set shown in Figure 2. In the case of grain volumes shown in Figure 3 only the largest connected volume is shown. These representative volumes show shapes that would be reasonably expected of grains in an equiaxed polycrystalline metal like wrought Ti 6-Al 4-V, but these representative volumes alone are insufficient verification of generated grain quality.

The distributions of the 3D moment invariants (Ω₁, Ω₂, Ω₃) evaluated in this study are shown in Figure 4. The ground truth dataset contained 84,215 grains and the 3DMaterialGAN generated a total
Figure 3: **EXAMPLE OF SINGLE GRAINS**. Voxel size is 1.5 µm × 1.5 µm × 1.5 µm. For generated grains, only largest connected component is shown.

Figure 4: Histogram of moment invariants (Ω₁, Ω₂, Ω₃) for grains. Vertical lines indicate the mean.

of 150,000 grains. For each of the three invariants, less than 0.2% of the grains had values that were either infinite or nonphysical across both the ground truth and generated sets. In observed cases, this resulted from very small grain structures that were linear or planar in nature, which led to extremely large errors in Riemann summation during calculation of the invariants. Due to their nonphysicality, these values were omitted from the statistical distribution comparisons.

The ground-truth mean (μₑ) and standard deviation (σₑ) are compared with the generated mean (μₑ) and standard deviation (σₑ) in the insets of Figure 4. These values show a trend of differences between the real and generated data, with the generated data consistently exhibiting lower mean values and larger standard deviations. Comparison of the distribution shapes in Figure 4 reveals the cause to be that the generated data has a range of moment invariants values in the region close to zero not seen in the real dataset. These values are likely due to the previously mentioned generator noise. Although the generator noise was not displayed in Figure 3 for visual clarity, this noise was still included in the moment invariant calculation, which was performed on raw network output to minimize bias in quantitative comparison. This distinction is critical because, as Figure 5 shows, some of the grains are relatively small in volume compared to the 64 × 64 × 64 voxel region in which they were generated. Thus, generator artifacts located far away from the grain itself can cause significant shifts in the centroid location that is used to establish the coordinate basis for the calculation of the moment invariants, creating distortions in the data. Beyond this effect, the overall shape and position of the main peaks for both distributions are very similar, indicating that the 3DMaterialGAN network is producing data that is similar to the ground truth data without directly replicating it.

6 Conclusion

**Summary:** This work presents 3DMaterialGAN, a network designed for use on crystalline material microstructures that can recognize and synthesize high-resolution 3D objects from latent space vectors without any supplemental 2D input. We demonstrate the capabilities of this network on the ModelNet benchmark dataset, as well as on an experimental 3D material dataset of Ti 6-Al 4-V. On the benchmark dataset, the 3DMaterialGAN yields more reliable discriminator classification with exposure to fewer objects, which highlights the quality of discriminator feature recognition in
the network. When working with experimental data, the effects of generator noise produce some variations in moment invariant distribution, but the 3DMaterialGAN network is still able to produce results morphologically similar to the ground truth without being a direct replication.

**Broader Impact:** In the context of impact on the scientific world at large, this work has several implications centered in materials research and development. Since the 1990s, there have been several large-scale initiatives, including the Materials Genome Initiative (MGI) developed in the United States under the Obama Administration (National Science and Technology Council (US) [51]), with focus to improve the efficiency of the materials development process. Therefore, many applications across numerous industries rely on metal alloys and ceramic compositions that are over 50 or even 100 years old. Development of new materials that are suitable for a wide range of processing approaches and applications is an effort that costs an enormous amount of time, capital, and manpower. A major contributor to this cost is the enormous price of iteration: any new material composition must be evaluated under all performance scenarios of interest, and this must be done enough times to ensure the evaluation results are representative of all potential processing variabilities. Turbine materials must withstand the environment of an engine, and biomedical implants must suitable for a lifetime of use inside the body. Evaluations of these materials must be robust enough to be representative for thousands or even millions of manufacturing iterations. The magnitude of this development cost means that any progress made towards reducing it presents the potential for significant technical advances in applications like power generation, transportation, construction, consumer products, aerospace, and defense.

This work is the first step in teaching a neural network to understand the crystalline microstructure of a titanium alloy in full detail, backed by experimental verification. If a network can understand the morphology of titanium grains and how those grains are arranged with respect to one another for different processing conditions, it has the potential to generate new titanium microstructures for evaluation that are representative of a given processing condition, which reduces the cost of iteration needed for building a representative description of the titanium alloy. With enough information, the network may be able to predict how changes in processing conditions affect the titanium microstructure without performing any new experimental evaluations. Even this singular problem is a major challenge, but this work helps establish an approach through which this challenge might be overcome.

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References

[1] Angel X Chang, Thomas Funkhouser, Leonidas Guibas, Pat Hanrahan, Qixing Huang, Zimo Li, Silvio Savarese, Manolis Savva, Shuran Song, Hao Su, et al. Shapenet: An information-rich 3d model repository. *arXiv preprint arXiv:1512.03012*, 2015.

[2] Zhirong Wu, Shuran Song, Aditya Khosla, Yu Fisher, Linguang Zhang, Xiaou Tang, and Jianxiong Xiao. 3D ShapeNets: A Deep Representation for Volumetric Shapes. Technical report, 2015. URL http://3dshapenets.cs.princeton.edu.

[3] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 27*, pages 2672–2680, Curran Associates, Inc., 2014. URL http://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf.

[4] Tero Karras, Samuli Laine, and Timo Aila. A style-based generator architecture for generative adversarial networks. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 4401–4410, 2019.

[5] Zinan Lin, Ashish Khetan, Giulia Fanti, and Sewoong Oh. Pacgan: The power of two samples in generative adversarial networks. In *Advances in neural information processing systems*, pages 1498–1507, 2018.
[6] Martin Arjovsky, Soumith Chintala, and Léon Bottou. Wasserstein gan. *arXiv preprint arXiv:1701.07875*, 2017.

[7] Ishaan Gulrajani, Faruk Ahmed, Martín Arjovsky, Vincent Dumoulin, and Aaron C. Courville. Improved training of wasserstein gans. *CoRR*, abs/1704.00028, 2017. URL: http://arxiv.org/abs/1704.00028.

[8] S. Hémery, A. Naït-Ali, M. Guéguen, J. Wendorf, A. T. Polonsky, M. P. Echlin, J. C. Stinville, T. M. Pollock, and P. Villechaise. A 3D analysis of the onset of slip activity in relation to the degree of micro-texture in Ti–6Al–4V. *Acta Materialia*, 181:36–48, dec 2019. ISSN 13596454. doi: 10.1016/j.actamat.2019.09.028.

[9] Siddhartha Chaudhuri, Evangelos Kalogerakis, Leonidas Guibas, and Vladlen Koltun. Probabilistic reasoning for assembly-based 3D modeling. *ACM Transactions on Graphics*, 30(4):1, jul 2011. ISSN 07300301. doi: 10.1145/1964921.1964930. URL: http://portal.acm.org/citation.cfm?doid=1964921.1964930.

[10] Thomas Funkhouser, Michael Kazhdan, Philip Shilane, Patrick Min, William Kiefer, Ayellet Tal, Szymon Rusinkiewicz, and David Dobkin. Modeling by example. *ACM Transactions on Graphics (TOG)*, 31(4):1–11, 2012.

[11] Evangelos Kalogerakis, Siddhartha Chaudhuri, Daphne Koller, and Vladlen Koltun. A probabilistic model for component-based shape synthesis. *ACM Transactions on Graphics (TOG)*, 31(4):1–11, 2012.

[12] Christopher B Choy, Danfei Xu, JunYoung Gwak, Kevin Chen, and Silvio Savarese. 3d-r2n2: A unified approach for single and multi-view 3d object reconstruction. In *European conference on computer vision*, pages 628–644. Springer, 2016.

[13] Xiuming Zhang, Zhoutong Zhang, Chengkai Zhang, Joshua B. Tenenbaum, William T. Freeman, and Jiajun Wu. Learning to reconstruct shapes from unseen classes. In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, NIPS’18, page 2263–2274, Red Hook, NY, USA, 2018. Curran Associates Inc.

[14] Jiajun Wu, Yifan Wang, Tianfan Xue, Xingyuan Sun, Bill Freeman, and Josh Tenenbaum. Marrnet: 3d shape reconstruction via 2.5d sketches. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 540–550. Curran Associates, Inc., 2017. URL: http://papers.nips.cc/paper/6657-marrnet-3d-shape-reconstruction-via-25d-sketches.pdf.

[15] Atsuhiro Noguchi and Tatsuya Harada. Rgbd-gan: Unsupervised 3d representation learning from natural image datasets via rgbd image synthesis. *arXiv preprint arXiv:1909.12573*, 2019.

[16] Thu Nguyen-Phuoc, Chuan Li, Lucas Theis, Christian Richardt, and Yong-Liang Yang. Hologan: Unsupervised learning of 3d representations from natural images. In *Proceedings of the IEEE International Conference on Computer Vision*, pages 7588–7597, 2019.

[17] Abhishek Sharma, Oliver Grau, and Mario Fritz. Vconv-dae: Deep volumetric shape learning without object labels. In *European Conference on Computer Vision*, pages 236–250. Springer, 2016.

[18] Jiajun Wu, Chengkai Zhang, Tianfan Xue, Bill Freeman, and Josh Tenenbaum. Learning a probabilistic latent space of object shapes via 3d generative-adversarial modeling. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, *Advances in Neural Information Processing Systems 29*, pages 82–90. Curran Associates, Inc., 2016. URL: http://papers.nips.cc/paper/6096-learning-a-probabilistic-latent-space-of-object-shapes-via-3d-generative-adversarial-modeling.pdf.

[19] Jing Zhu, Jin Xie, and Yi Fang. Learning adversarial 3d model generation with 2d image enhancer, 2018. URL: https://www.aaai.org/ocs/index.php/AAAI/AAAI18/paper/view/16064.

[20] Victor Bapst, T. Keck, A. Grabska-Barwińska, C. Donner, Ekin Cubuk, Samuel Schoenholz, A. Obika, A. Nelson, T. Back, D. Hassabis, and P. Kohli. Unveiling the predictive power of static structure in glassy systems. *Nature Physics*, 16:448–454, 04 2020. doi: 10.1038/s41567-020-0842-8.

[21] Ahmet Cecen, Hanjun Dai, Yuksel C. Yabansu, Surya R. Kalidindi, and Le Song. Material structure-property linkages using three-dimensional convolutional neural networks. *Acta Materialia*, 146:76–84, mar 2018. ISSN 13596454. doi: 10.1016/j.actamat.2017.11.053.

[22] Ramin Bostanabad, Anh Tuan Bui, Wei Xie, Daniel W. Apley, and Wei Chen. Stochastic microstructure characterization and reconstruction via supervised learning. *Acta Materialia*, 103:89–102, jan 2016. ISSN 13596454. doi: 10.1016/j.actamat.2015.09.044.
[23] Xiaolin Li, Zijiang Yang, I Catherine Brinson, Alok Choudhary, Ankit Agrawal, and Wei Chen. A deep adversarial learning methodology for designing microstructural material systems. In ASME 2018 international design engineering technical conferences and computers and information in engineering, 2018.

[24] Michel Coster, Xavier Arnould, Jean-Louis Chemant, Abder El Moataz, and Thierry Chartier. A Microstructural Model by Space Tessellation for a Sintered Ceramic: Cerine. *Image Analysis & Stereology*, 24(2):105, may 2005. ISSN 1580-3139. doi: 10.5566/ias.v24.p105-116.

[25] William Johnson and Robert Mehl. Reaction kinetics in processes of nucleation and growth. *Transactions of the Metallurgical Society of AIME*, 135:416–442, 1939.

[26] Melvin Avrami. Kinetics of phase change. I general theory. *The Journal of Chemical Physics*, 7(12): 1103–1112, 1939.

[27] Andrei Nikolaevich Kolmogorov. A statistical theory for the recrystallization of metals. *Izvestiya Rossiiskoi Akademii Nauk. Seriya Matematicheskaya*, 1937.

[28] Michael Nosonovsky, Xiangyi Zhang, and Sven K Esche. Related content Scaling of Monte Carlo simulations of grain growth in metals. *Modelling and Simulation in Materials Science and Engineering*, 17:1–13, 2009. doi: 10.1088/0965-0393/17/2/025004.

[29] Romain Quey, PR Dawson, and Fabrice Barbe. Large-scale 3d random polycrystals for the finite element method: Generation, meshing and remeshing. *Computer Methods in Applied Mechanics and Engineering*, 200(17-20):1729–1745, 2011.

[30] Michael A. Groeber and Michael A. Jackson. DREAM.3D: A Digital Representation Environment for the Analysis of Microstructure in 3D. *Integrating Materials and Manufacturing Innovation*, 3(1):56–72, dec 2014. ISSN 21939772. doi: 10.1186/2193-9772-3-5.

[31] P. G. Callahan, M. Groeber, and M. De Graef. Towards a quantitative comparison between experimental and synthetic grain structures. *Acta Materialia*, 111:242–252, jun 2016. ISSN 13596454. doi: 10.1016/j.actamat.2016.03.078.

[32] Ruoqian Liu, Abhishek Kumar, Zhengzhang Chen, Ankit Agrawal, Veera Sundararaghavan, and Alok Choudhary. A predictive machine learning approach for microstructure optimization and materials design. *Nature Scientific Reports*, 5(1):1–12, jun 2015. ISSN 20452322. doi: 10.1038/srep11551.

[33] Brian L. DeCost, Matthew D. Hecht, Toby Francis, Bryan A. Webler, Yoosuf N. Picard, and Elizabeth A. Holm. UHCSDB: UltraHigh Carbon Steel Micrograph DataBase. *Integrating Materials and Manufacturing Innovation*, 6(2):197–205, jun 2017. ISSN 2193-9764. doi: 10.1007/s40192-017-0097-0.

[34] Brian L. DeCost, Toby Francis, and Elizabeth A. Holm. Exploring the microstructure manifold: Image texture representations applied to ultrahigh carbon steel microstructures. *Acta Materialia*, 133:30–40, jul 2017. ISSN 13596454. doi: 10.1016/j.actamat.2017.05.014.

[35] Akshay Iyer, Biswadip Dey, Arindam Dasgupta, Wei Chen, and Amit Chakraborty. A Conditional Generative Model for Predicting Material Microstructures from Processing Methods. Technical report, 2019.

[36] Daria Fokina, Ekaterina Muravelova, George Ovchinnikov, and Ivan Oseledets. Microstructure synthesis using style-based generative adversarial networks. *Physical Review E*, 101(4):043308, apr 2020. ISSN 24700053. doi: 10.1103/PhysRevE.101.043308.

[37] Ruijin Cang, Yaopengxiao Xu, Shaohua Chen, Yongming Liu, Yang Jiao, and Max Yi Ren. Microstructure Representation and Reconstruction of Heterogeneous Materials Via Deep Belief Network for Computational Material Design. *Journal of Mechanical Design, Transactions of the ASME*, 139(7), jul 2017. ISSN 10500472. doi: 10.1115/1.4036649.

[38] Salvatore Torquato and HW Haslach Jr. Random heterogeneous materials: microstructure and macroscopic properties. *Applied Mechanics Reviews*, 55(4):B62–B63, 2002.

[39] McLean P. Echlin, Marcus Straw, Steven Randolph, Jorge Filevich, and Tresa M. Pollock. The TriBeam system: Femtosecond laser ablation in situ SEM. *Materials Characterization*, 100:1–12, February 2015. doi: 10.1016/j.matchar.2014.10.023. URL [https://doi.org/10.1016/j.matchar.2014.10.023](https://doi.org/10.1016/j.matchar.2014.10.023)

[40] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
[41] Michael Kazhdan, Thomas Funkhouser, and Szymon Rusinkiewicz. Rotation Invariant Spherical Harmonic Representation of 3D Shape Descriptors. Technical report, 2003.

[42] J P MacSleyne, J P Simmons, and M De Graef. On the use of moment invariants for the automated analysis of 3D particle shapes. *Modelling and Simulation in Materials Science and Engineering*, 16(4):045008, apr 2008. ISSN 0965-0393. doi: 10.1088/0965-0393/16/4/045008.

[43] A. Trenkle, M. Syha, W. Rheinheimer, P. G. Callahan, L. Nguyen, W. Ludwig, W. Lenthe, M. P. Echlin, T. M. Pollock, D. Weygand, M. Graef, M. J. Hoffmann, and P. Gumbsch. Nondestructive evaluation of 3D microstructure evolution in strontium titanate. *Journal of Applied Crystallography*, 53(2):349–359, apr 2020. ISSN 16005767. doi: 10.1107/S160057672000093X.

[44] D. Maturana and S. Scherer. Voxnet: A 3d convolutional neural network for real-time object recognition. In *2015 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, pages 922–928, Sep. 2015. doi: 10.1109/IROS.2015.7353481.

[45] Ayan Sinha, Jing Bai, and Karthik Ramani. Deep learning 3d shape surfaces using geometry images. In *ECCV*. 2016.

[46] Charles R Qi, Hao Su, Kaichun Mo, and Leonidas J Guibas. Pointnet: Deep learning on point sets for 3d classification and segmentation. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 652–660, 2017.

[47] Song Bai, Xiang Bai, Zhichao Zhou, Zhaoxiang Zhang, and Longin Jan Latecki. Gift: A real-time and scalable 3d shape search engine. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 5023–5032, 2016.

[48] Vishakh Hegde and Reza Zadeh. Fusionnet: 3d object classification using multiple data representations. *arXiv preprint arXiv:1607.05695*, 2016.

[49] Leif Kobbelt, P. Schröder, Michael Kazhdan, Thomas Funkhouser, and Szymon Rusinkiewicz. Rotation invariant spherical harmonic representation of 3d shape descriptors. *Proc 2003 Eurographics*, vol. 43, 07 2003.

[50] Ding-Yun Chen, Xiao-Pei Tian, Yu-Te Shen, and Ming Ouhyoung. On visual similarity based 3d model retrieval. In *Computer graphics forum*, volume 22, pages 223–232. Wiley Online Library, 2003.

[51] National Science and Technology Council (US). *Materials genome initiative for global competitiveness*. Executive Office of the President, National Science and Technology Council, 2011.