EXTRACTION OF PROCESS-STRUCTURE-PROPERTY LINKAGE USING DEEP LEARNING METHODS

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ABSTRACT

The establishment of the process–structure–property linkage is essential for designing new materials with desired properties. Based on the concept, the discovery of new materials has been accelerated in the field of functional and bio- materials by combining quantum and molecular modeling tools with efficient machine learning methods. However, in the case of structural materials, even though the development of Integrated Computational Materials Engineering (ICME), it is still difficult to efficiently design new materials because of the uncertainties within models and experimental data. In the present paper, our recent development of a general methodology for extracting the linkage between hierarchical microstructure and process conditions as well as properties will be reviewed. In the proposed method, the uncertainties will be captured in the form of probability density functions using deep learning methods.

Since microstructures of typical structural materials are composed of finite kinds of dissimilar phases developing competitively with totally different physical processes, they are supposed to have different geometrical features while maintaining spatial orders. The framework, thus, has two functional components: one is for extracting geometrical features of material microstructures necessary to decompose each different microstructures, and the other is for clarifying spatial orders among the extracted characteristic components. The method was applied for generating virtual steel microstructures obtained after a certain continuous cooling process and those for desired mechanical properties. The obtained results show that the proposed methodology not only generates realistic microstructural images comparable to real experimental images but also clarifies a part of microstructures critically affecting the target property. The proposed approach has been developed to help designing the optimum welding parameters as well as structural materials with an improved weldability.

Keywords: PSPP linkage, uncertainty, deep generative models, virtual microstructure, hotspot

INTRODUCTION

Since the performance of structural materials is highly dependent on their microstructures, the materials design approach has mainly focused on optimizing microstructure to satisfy product-level performance requirements. In addition, microstructures of structural materials are usually composed of various phases developed with different kinetic processes to each other. Accordingly designing structural materials with targeted performance requires a combined strategy of bottom-up modeling and simulation

approaches which take into account the development of various levels of hierarchical material microstructures as well as their effects on the properties [1]. Especially in the case of welding process, since materials are subject to variety of temperature histories in heat affected zone (HAZ), it is expected to develop a method which can efficiently predict the microstructures and their properties in HAZ. Considering these facts, computational materials science and multiscale mechanics modeling play key roles in designing structural materials, which has brought much attention to the development of Integrated Computational Materials Engineering (ICME) in the materials community [2]. On the other hand, computational materials science and microstructural optimization based on numerical models encounter many uncertainties, such as stochasticity of processes, incomplete understanding of underlying physics, lack of complete data to quantify material microstructure, and ambiguity even in the selection of mathematical descriptors representing the hierarchical microstructures [3]. These uncertainties sometimes prevent us to apply the simple materials informatics approach, in which attention is focused mainly on data mining and providing convenient and powerful tools for designing or selecting new materials, and hence brought us difficulty in inverting process–structure and structure–property relations.

To take into account these uncertainties, the authors have developed a data-driven approach composed of two different kinds of convolution neural networks [4,5]. One is for extracting descriptors representing the hierarchical microstructure and the other for understanding the correlation between a spatial arrangement of the extracted descriptors and corresponding process parameters or mechanical properties. The present paper is a brief review of our results obtained for the several problems of extracting process–structure [4] and structure–property [5] linkages.

METHODOLOGY

EXTRACTION OF MICROSTRUCTURAL FEATURES AND THEIR ARRANGEMENTS

Metallurgists implicitly share the feeling that material microstructures are composed of finite kinds of dissimilar phases or small-scale microstructures. In addition, since individual small-scale microstructures develop competitively with completely different formation kinetics, they are supposed to have different geometrical features while maintaining certain spatial orders depending on process conditions such as cooling rate and holding temperature. Following this understanding, we demonstrated that a convolutional neural network (CNN) provides an efficient route to extract a finite number of geometrical features representing each small-scale microstructure and successfully provide an unsupervised segmentation for steel microstructures [6]. The concept was further implemented into a variational autoencoder to enable the automatic generation of virtual microstructures of steel [4]. In this framework, we adopted a vector quantized variational autoencoder (VQVAE) [7] to extract a certain number of characteristic geometrical features from micrographs of steel as well as to reveal their spatial arrangement in the microstructure.

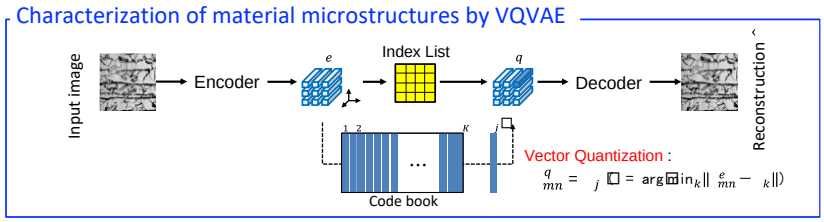

Fig. 1 Characterization of material microstructures by VQVAE

Fig.1 shows the schematic of the architecture of VQVAE. As mentioned above, VQVAE is used for the extraction of a finite number of geometrical features representing each small-scale microstructure in an unsupervised way. It is composed of a convolutional encoder and a convolutional decoder. The encoder maps input microstructure images into the corresponding spatial arrangement of characteristic microstructures (index list), and the decoder maps the extracted features back to the original microstructure images. For example, as candidates of the characteristic microstructures of steel alloys, ferrite and martensite phases or their grain boundaries can be considered. As a result, we can extract the index lists of characteristic small-scale microstructures constructing the input microstructure images. A more detailed discussion of the strategy for capturing the qualitatively different characteristic microstructures can be found in [4].

EXTRACTION OF P-S/S-P LINKAGE

The spatial arrangement of microstructures has a strong correlation with process conditions, such as cooling rate and holding temperature, and mechanical properties. A pixel convolutional neural network (PixelCNN) [8,9] was applied to reveal spatial orders of small-scale microstructures as a function of process parameters/mechanical properties.

Fig. 2 shows the schematic of the architecture of PixelCNN. PixelCNN is used for the determination of spatial correlation among extracted characteristic microstructures which is dependent on processing parameters and/or material properties **h**. PixelCNN is an autoregressive model for building the joint distribution of each component over a spatial arrangement (index list) $\boldsymbol{x} = \{x_1, x_2, \cdots, x_n\}$ as the following product of conditional distributions:

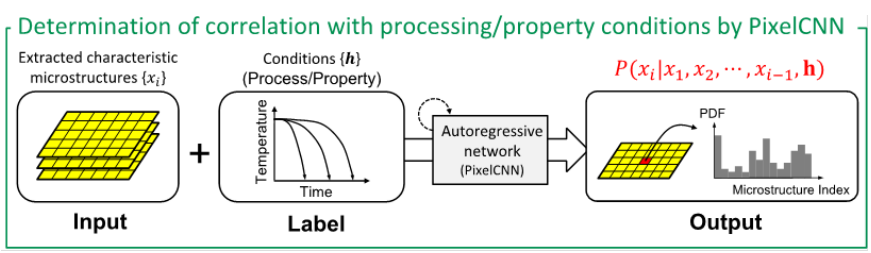

Fig. 2 Determination of spatial orders of small-scale microstructures as a function of process paramters/mechanical properties by PixelCNN

$$P(\boldsymbol{x}|\mathbf{h}) = P(x_1|\mathbf{h}) \prod_{i=2}^{n} \prod P(x_i|x_2, \cdots, x_{i-1}, \mathbf{h}), \quad (1)$$

where $\boldsymbol{x}$ represents the two-dimensional arrangement of extracted characteristic structures x_i, and $\mathbf{h}$ is the given condition. Since each x_i corresponds to some small-scale characteristic microstructure, Eq. (1) can be understood to represent a certain stochastic spatial interaction among them. This enables us to capture stochastic spatial correlation in the target material structures. This is one of the important advantages of our framework. Owing to this definition of spatial correlation, the uncertainties behind the generation of material microstructures can be considered.

APPLICATION OF PROPOSED APPROACH

AUTOGENERATION OF STEEL MICROSTRUCTURE

Using the trained network, microstructures can be generated for given conditions such as processing parameters and/or material properties. First, we obtain the probability distribution of spatial arrangement of characteristic microstructures by giving desired conditions into the trained PixelCNN. Then, a two-dimensional spatial arrangement of microstructures sampled from the distribution can be converted into a corresponding micrograph by the trained decoder. As a result, we can construct a stochastic mapping from desired conditions into material microstructures. The detailed procedure of the autogeneration of material microstructures was given in our previous paper [4].

CONTINUOUS COOLING MICROSTRUCTURE

As an example of the applications of the proposed approach, we considered the problem of autogeneration of microstructure of low-carbon-steels obtained after a certain continuous cooling process [4]. An Fe-0.15C-1.5Mn (wt.%) low-carbon steel samples were austenitized at $1000\,℃$ and cooled at $1.0, 3.0, 10.0,$ and $30.0\,℃/s$ to room temperature. To create a training dataset, square patches (128×128 pixel) are cropped from the original microstructure images (1024×786 pixel). In total, 52 800 square images were cropped from 160 original images.

We trained VQVAE and PixelCNN presented in Figs. 1 and 2 using the training dataset. In this application, the cooling rate was given as the condition $\mathbf{h}$ to PixelCNN. As a result of training, we can obtain a stochastic mapping from the cooling rate to the corresponding microstructures. Fig. 3 shows the generated microstructures corresponding to the given cooling rates by the proposed methodology along with the sampled training images in the dataset for each cooling rate.

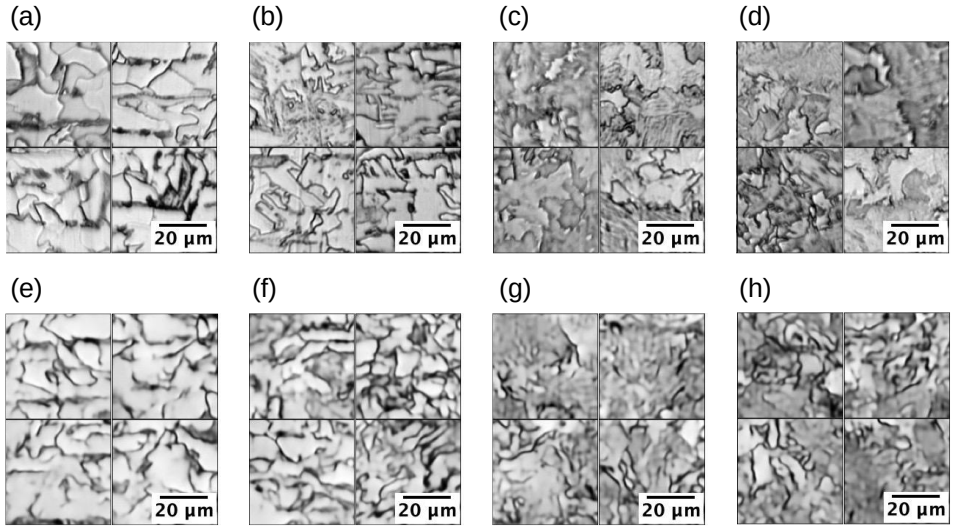

Fig. 3 Original microstructures images and generated microstructures images corresponding to the given cooling rates. Parts (a)-(b) are original microstructures for each of the four cooling rates, respectively. Parts (e)-(h) are generated microstructures for each of the four cooling rates, respectively. Each panel has four microstructure images.

These results indicate that the proposed method can produce qualitatively realistic microstructure images for each cooling rate in the sense that the generated microstructures have similar features to those observed in training microstructure images in terms of the basic topology of microstructures and a similar trend relative to the change in the cooling rate. It should be emphasized that the introduced method can generate new microstructures in the sense that the generated microstructure images are not exactly the same as the images in the training microstructure dataset. In addition, it should be noted that this method can generate an ensemble of microstructures illustrating the distribution of material microstructures for any given parameters. In this way, the uncertainty of microstructure resulting from the stochastic nature of their formation kinetics can be naturally treated, and hence help to understand the process–structure linkage.

To validate the generated microstructures quantitatively, we consider two traditional descriptors of microstructure morphology: the volume fraction and the average grain size. We calculated the ferrite volume fraction for 1000 training and 1000 generated images for each of the four cooling rates. Fig. 4 shows the box plot of the calculated ferrite volume fraction for the training images and the generated images corresponding to each cooling rate. In terms of mean values, the ferrite volume fractions of the generated images for all cooling rates are in satisfactory good agreement with those of the training images. Also, the volume fraction of ferrite in the generated images in Fig. 4 clearly shows a similar trend of variances to the observed microstructures; as the cooling rate increases, the variance of the volume fraction of ferrite also increases.

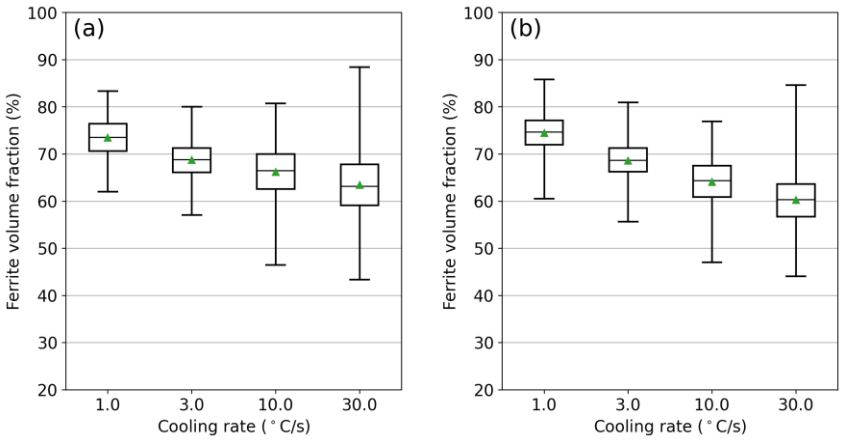

Fig. 4 Box plots of the ferrite volume fraction in (a) the microstructure patches cropped from the original images, and (b) the microstructure patches generated by the proposed methodology. The black lines and green triangles in the boxes denote median and mean values of sets of images for each cooling rates, respectively.

Next, we consider the average grain size in a micrograph. Fig. 5 shows the box plots of the local average grain sizes and their mean values as the overall averages for each patch cropped from original microstructures and the generated images. The local average grain sizes are calculated for 1000 training and 1000 generated images for each of the four cooling rates. The trend of the predicted average grain size is in good agreement with the trend of the grain size calculated using the original microstructure images. This result demonstrated that the proposed approach can also capture the trend of the traditional microstructural characteristic including their spatial variation from the given datasets.

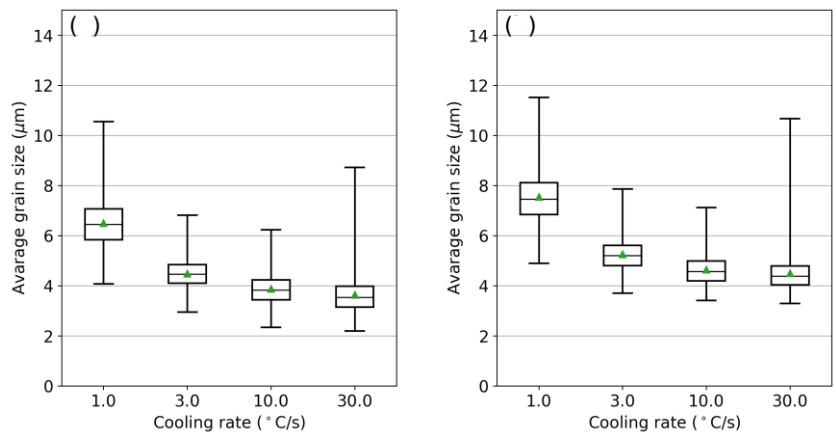

Fig. 5 Box plots oft he average grain sizes (a) in each patch cropped from the original images, and (b) in each generated microstructure patch by the proposed methodology. The

black lines and green triangles in the boxes denote median and mean values of sets of images for each cooling rates, respectively.

MECHANICAL PROPERTIES

As a second example, we applied the proposed methodology to the problem of clarifying a hotspot critically affecting the target property [5]. The sample problem is the structure optimization of artificial dual-phase steels composed of the soft phase (ferrite) and hard phase (martensite). The prepared dual-phase microstructures can be divided into four major categories: laminated microstructures, microstructures composed of rectangle- and ellipse-shaped martensite/ferrite grains, and random microstructures. The size of microstructure images is also 128×128 pixel and the total number of prepared microstructures is 3824. As an example of a target material property, the fracture strain was selected since fracture behavior is strongly related to the geometry and distribution of the constituent phases. The fracture strain is the elongation of materials at rupture estimated using the Gurson–Tvergaard–Needleman (GTN) model [10]. Using this dataset, we investigate whether the machine learning framework can identify a part of material microstructures that strongly affects a target property in a similar way that human experts can predict based on their experiences.

To identify a critical part of microstructures, we consider calculating a gradient of material microstructures with respect to the fracture strain based on the mapping obtained by our methodology in the same way as shown in the previous section. This assumes that human experts unconsciously consider the *sensitivity* of material microstructures to a slight change in target property. If the machine learning framework correctly captures the physical correlation between the geometry of the material microstructures and the fracture strain, the gradient calculated based on the correlation is expected to correspond to the areas that highly affect the determination of the fracture strain even without giving the physical mechanism itself.

Fig. 6 shows the comparison of the parts of microstructures critically affecting the fracture strain obtained by the physical model and our machine learning framework. Figs. 6 (a) and (b) illustrate the crucial parts of the microstructures composed of relatively long and narrow rectangle-shaped martensite grains. We can see an acceptable agreement between the results of the physical and machine learning methods in terms of the overall distribution of crucial areas which are shown in red in the colormaps. Figs. 6 (c) and (d) show the results for the microstructures composed of similarly shaped martensite grains. In Fig. 6 (c), the rectangle-shaped martensite grains are irregularly arranged, and some martensite grains are close to each other, whereas, in Fig. 6 (d), circular martensite grains are almost regularly arranged. In both Figs. 6 (c) and (d), the machine learning framework identifies the crucial parts that are predicted by the physical model. As mentioned above, the hotspots are in the regions where martensite grains are close to each other.

For incompletely laminated structures such as that shown in Fig. 6 (a) the martensite layers are suggested to expand to achieve a higher fracture strain. Similarly, we can see in Fig. 6 (c) that it is suggested to fill a small gap between martensite grains. Together with the fact that eliminating tiny holes that could cause hotspots and reaching *completely* laminated structures markedly improve their fracture strains [5,11], these results imply

that the framework recognizes the potential of laminated structures to achieve a higher fracture strain in a similar way that human researchers reach an intuition on complete laminate structures as a result of the consideration of reducing the occurrence of hotspots.

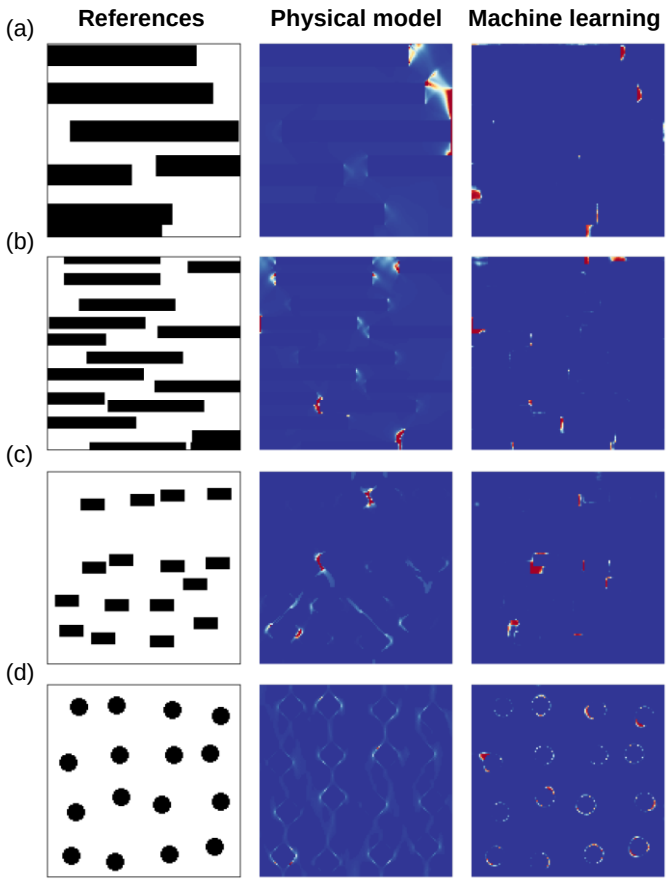

Fig. 6 Comparison of derivative of microstructures with respect tot he fracture strain obtained using deep learning framework with the distributions of void volume fractions calculated on the basis of physical model. The left, middle, and right column in (a)-(d) correspond tot he reference microstructures, the volid distributions by the physical model, and the derivative by the deep learning mframework, respectively.

From the above results, we can conclude that our framework can identify the areas that critically affect a target property without human prior knowledge.

CONCLUSION

In the present paper, our recent development of a general methodology for extracting the linkage between hierarchical microstructure and process conditions as well as

properties was reviewed. In the proposed method, the uncertainties are captured in the form of probability density functions using deep learning methods. The method was applied for generating virtual steel microstructures obtained after a certain continuous cooling process and those for desired mechanical properties. The obtained results show that the proposed methodology not only captures the stochastic nature of the real microstructure but also helps to clarify a part of microstructures critically affecting the target property

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References

[1] G. B. OLSON: 'Computational design of hierarchically structured materials', *Science*, 277, 1237-42, 1997.

[2] T. M. POLLOCK, J. E. ALLISON, D. G. BACKMAN, M. C. BOYCE, M. GERSH, E. A. HOLM ET AL.: 'Integrated computational materials engineering: A transformational discipline for improved competitiveness and national security', National Materials Advisory Board, NAE, *National Academies Press*, 2008, Report Number: ISBN-10: 0-309-11999-5.

[3] J. H. PANCHAL, S. R. KALIDINDI, D. L. MCDOWELL: 'Key computational modeling issues in Integrated Computational Materials Engineering', *Computer-Aided Design*, 45, 4-25, 2013.

[4] S. NOGUCHI, J. INOUE: 'Stochastic characterization and reconstruction of material microstructures for establishment of process-structure-property linkage using the deep generative model', *Physical Review E*, 104, 025302, 2021.

[5] S. NOGUCHI, H. WANG, J. INOUE: 'Identification of microstructures critically affecting material properties using machine learning framework based on metallurgists' thinking process', *Scientific Reports*, http://doi.org/10.1038/s41598-022-17614-0.

[6] H. KIM, J. INOUE, T. KASUYA: 'Unsupervised microstructure segmentation by mimicking metallurgists' approach to pattern recognition', *Scientific Reports*, 10, 17835, 2020.

[7] A. VAN OORD, O. VINYALS, K. KAVUKCUOGLU: 'Neural discrete representation learning', In: *Neural Information Processing System Conference*, 2017.

[8] A. VAN OORD, N. KALCHBRENNER, K. KAVUKCUOGLU: 'Pixel recurrent neural networks', In: *International Conference on Machine Learning*, 2016.

[9] A. VAN OORD, N. KALCHBRENNER, L. ESPEHOLT, O. VINYALS, A. GRAEVS: 'Conditional image generation with pisxelcnn decoders', In: *Neural Information Processing System Conference*, 2016.

[10] V. TVERGAARD, A. NEEDLEMAN: 'Analysis of the cup-cone fracture in a round tensile bar', *Acta Meterialia*, 32, 157-169, 1984.

[11] T. KOSEKI, J. INOUE, S. NAMBU: 'Development of multilayer steels for improved combinations of high strength and high ductility', *Materials Transactions*, 55, 227-237, 2014.