Prediction of microstructure formation during heating in low-carbon steels using machine learning

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The mechanical properties of heat-treated low-carbon steels are affected by the volume fraction of ferrite and austenite phases during heating. Therefore, it is important to clarify the factors of austenite formation and to predict the microstructure under various heat-treatment conditions. The prediction, such as the JMAK equation, requires many parameters and uses image information of the microstructure to decide parameters. In machine learning, GAN (Generative Adversarial Networks) architecture has been developed to generate new images. The generation of the microstructure image has been investigated using the architecture. In this study, the austenitization behavior of low-carbon steel with a composition of Fe-0.2 mass% C was experimentally investigated. Moreover, the microstructure formation during heating was predicted by the GAN architecture. Fe-0.2 mass% C steel was melted in a vacuum melting furnace. The ingot was heat-treated and hot-rolled, and cold-rolled specimens with a thickness of 1.2 mm were prepared. The specimens were heated at 1000 °C and then water quenched. In addition, the specimens were heated to temperatures ranging from 699°C to 1002°C, then water-quenched to hold the microstructure during heating. Microstructure images of specimens at various temperatures were taken using the SEM (Scanning electron microscope), and these were trained to create the generator using the WGAN (Wasserstein GAN-GP) technique. Before heating, the specimen consisted of the martensite microstructure. Cementite particles precipitated in the martensite matrix for the specimen heated to 731°C. Furthermore, austenite was formed at temperatures above 736°C and grew into the martensite matrix with increasing temperature. Finally, austenite transformation was completed above 840°C. According to the predictions of the microstructure above 730°C, the two-phase microstructure consisting of bright and dark regions was generated. The bright and dark regions correspond to austenite and martensite microstructures during heating, respectively. Bright regions widened as temperature increased. Moreover, the lath-like microstructure was reproduced above 840°C. Therefore, the GAN architecture generated microstructures at various temperatures during heating, and the microstructures reproduced the microscopic observation.

Keywords: *Generative Adversarial Networks, microstructure simulation, austenite formation, low-carbon steel*

1. Introduction

The low-carbon steel is heated to the ferrite/austenite two-phase or the austenite single-phase temperature range. The mechanical properties of heat-treated low-carbon steel are affected by the volume fraction of ferrite and austenite phases during heating, as well as by the austenite grain size. Therefore, it is important to clarify the metallurgical factors that contribute to austenite formation and to predict the formation process. The austenite formation and growth from low-carbon martensite with dispersed cementite have been simulated, and the volume fraction of each phase and austenite grain size during heating have been predicted [1)]. Moreover, microstructural features during heating, such as austenite morphology and spatial distribution, are predicted by the phase-field method [2)]. Parameters are required for these predictions, and the parameters are obtained from the micrograph information of the investigated steel. On the other hand, in the field of machine learning, techniques to generate demanded images, such as GANs (Generative Adversarial Networks), have been developed [3,4)]. In this study, the austenitization behavior during continuous heating was investigated using the low-carbon steel with Fe-0.2mass% C alloy, and the microstructure formation during heating was predicted by the GANs technique. Thus, we examined the possibility of applying generative AI to steel science.

2. Experimental Procedure

The alloy (Fe-0.2mass%C) was vacuum induction melted using high-purity materials. The ingot was heated and forged to a hot-rolling slab 30 mm in thickness, 160 mm in width, and 100 mm in length. Then, the slab was heated at 1250 °C for 1800 s and hot-rolled at a temperature above 900 °C to form a plate, 5 mm in thickness. The hot-rolled plate was machined to remove scale and cold-rolled to a plate, 1.2 mm in thickness. The cold-rolled plates were annealed at 1000 °C for 60 s and then water-cooled to prepare heat-treatment specimens with a martensitic structure. The samples were heated at a temperature range between 699 °C and 1002 °C at a heating rate of 100 °C/s and then water cooled to freeze the microstructures. The microstructure of the cross-section was observed by SEM in the specimen. The metallographic images taken by SEM were learned by the WGAN (Wasserstein GAN-GP) technique, and metallographic images at various temperatures were generated.

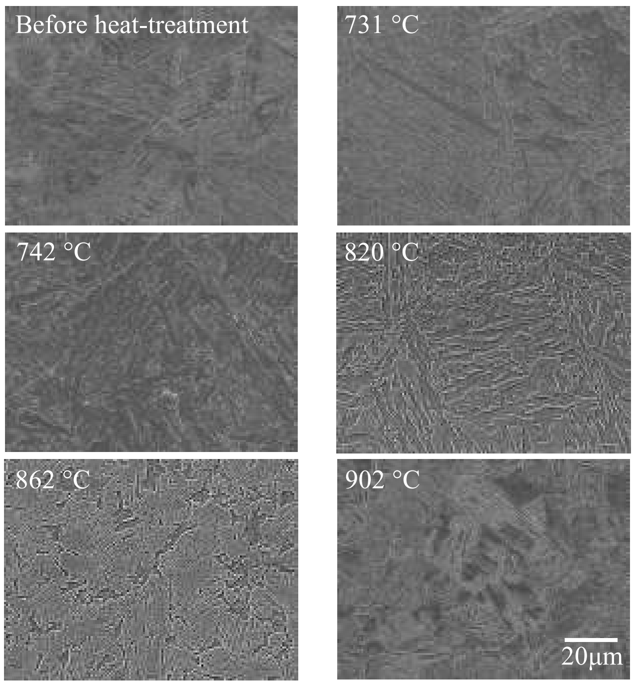

Figure 1 SEM images of Fe-0.2mass%C alloy before and after heat-treatment at various temperatures.

3. Result and Discussion

Microstructure images before and after heating to various temperatures are shown in Figure 1. The samples possessed a lath-like martensite microstructure before heat-treatment. Cementite particles precipitated in the martensite matrix at 731 °C. When the temperature reached 736°C, austenite was formed in the matrix like the microstructure heated at 742°C. With increasing temperature, the austenite developed and the microstructure at 876 °C was a single austenite phase.

Generative SEM images at various iterations are shown in Figure 2. The size of the generative image was 128 pixels in height and 128 pixels in width. PyTorch, a deep learning library, was used to build the simulator of microstructure. Initial images were determined by three-dimensional random numbers. As can be seen, with increasing the number of iterations, the generated images reproduced the microstructure.

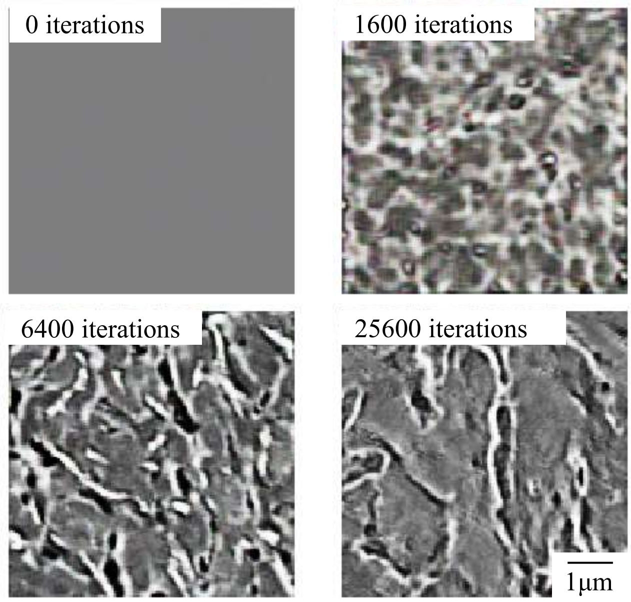

Figure 2 Generative SEM images at various iterations

The microstructures observed by SEM and simulated by the WGAN technique are shown in Figure 3 (a) and (b), respectively. The microstructure during heating was predicted by fixing the random number and varying the temperature. The SEM microstructure shows a two-phase contrast, with the light and dark areas corresponding to austenite and martensite, respectively.

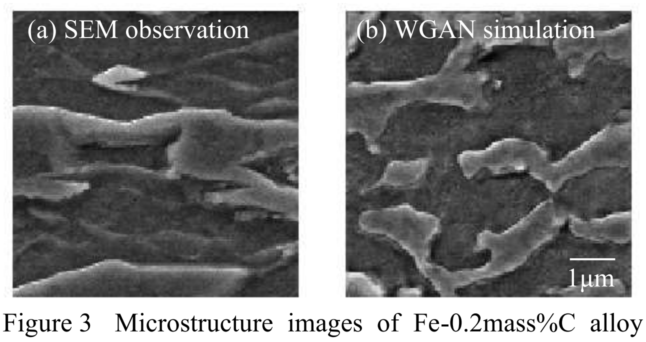

Figure 3 Microstructure images of Fe-0.2mass%C alloy heated at 782 °C by (a) SEM observation and (b) WGAN simulation.

The variation of the second phase volume fraction in temperature is shown in Figure 4. The results of SEM measurements are plotted, the WGAN predictions are shown as solid lines, and the phase equilibrium calculations using Thermo-Calc TCFE10 are shown as dotted lines. The SEM observations show that the formation of austenite at each temperature does not reach phase equilibrium. At temperatures below 811 °C, the WGAN predictions agree with the SEM measurements. However, at temperatures above 820 °C, the two results diverge.

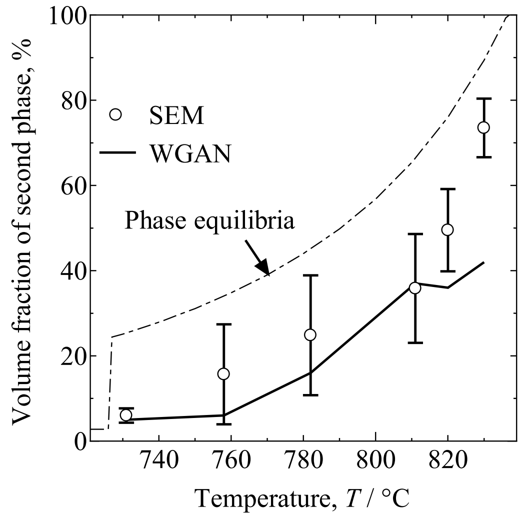

Figure 4 Variation of second phase volume fraction in temperature.

4. Conclusion

The austenitization behavior of low-carbon steel with Fe-0.2 mass % C alloy under continuous heating was investigated, and microstructure formation during heating was predicted by GANs. The WGAN technique could represent the microstructure of the low-carbon steel. Contrasts due to the formation of ferrite and austenite two-phase microstructures during heating also appeared in the images generated by the WGAN technique. By adjusting the random number, the technique could predict the continuous change of microstructure during heating.

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References

1) M. Enomoto and K. Hayashi, Metall. Trans. A, 51 (2020), 618-630.
2) H. Azizi-Alizamini and M, Militzer, J. Mater. Res, 101 (2010) 534-41.
3) I. J. Goodfellow, J. Pouget-Abadie, M. Mirza, Bing Xu, D. Warde-Farley, S. Ozair, A. Courville and Y. Bengio, Technical report, arXiv: 1406.2661.
4) J-W. Lee, N. Goo, W. Park, M. Pyo and K-S. Sohn, Engineering reports, 3 (2021), e12274.