Reconstruction of magnetic domain structure using the reverse Monte Carlo method with an extended Fourier image

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(Presented 4 November 2014; received 22 September 2014; accepted 4 January 2015; published online 22 April 2015)

Visualization of the magnetic domain structure is indispensable to the investigation of magnetization processes and the coercivity mechanism. It is necessary to develop a reconstruction method from the reciprocal-space image to the real-space image. For this purpose, it is necessary to solve the problem of missing phase information in the reciprocal-space image. We propose the method of extend Fourier image with mean-value padding to compensate for the phase information. We visualized the magnetic domain structure using the Reverse Monte Carlo method with simulated annealing to accelerate the calculation. With this technique, we demonstrated the restoration of the magnetic domain structure, obtained magnetization and magnetic domain width, and reproduced the characteristic form that constitutes a magnetic domain. © 2015 AIP Publishing LLC.

[<http://dx.doi.org/10.1063/1.4918955>]

I. INTRODUCTION

To develop a permanent magnet, we must find a strong substance with a coercive force, which makes it difficult for the substance to be magnetized by an external magnetic field.^{1–4} However, to elucidate the mechanism that determines the coercive force strength, we must first understand the mechanism of the magnetization process.

In 1932, Bitter⁵ first observed the magnetic domain, and since then, many magnetization analysis techniques have been developed.⁶ Unfortunately, most of these methods are only capable of obtaining a two-dimensional magnetization distribution. In contrast, the neutron beam, which is sensitive to the magnetic moment, exhibits strong transparency to magnetic materials. Therefore, small-angle neutron scattering can be used to obtain three-dimensional information on magnetic domains. Hence, the recovery of neutron diffraction data to create a real-space image is required in order to determine the mechanism of the magnetization process. In general, the relationship between the obtained diffraction data and the real-space image can be identified using a Fourier transformation or an inverse Fourier transformation. However, reconstruction from the diffraction data to the real-space image is generally difficult because of the lack of phase information in the experimental data.

In this paper, we used the Reverse Monte Carlo (RMC) method,^{7,8} which is widely applied in reflection data analysis, to visualize this magnetic domain structure. We have applied RMC with the method of extend Fourier image with mean-value padding (EFIMVP) to compensate for the phase information. It is necessary to confirm that the conversion

from the real-space image to the reciprocal-space image is exact. We obtained the reciprocal-space image by calculating the Fourier transform of the experimental magnetic domain structure. The proposition method was inspected by comparing the original magnetic domain structure and reconstructed image.

II. RMC METHOD

The restoration of the magnetic domain structure using the RMC method partially compensates for the lack of phase information provided by the Fourier transformation. Here, we explain the procedure of the RMC method. A technique of reconstructing a real image from the Fourier image, which is a reciprocal-space image, using only diffraction data has been developed.^{9,10} This is a new reconstruction technique in that it begins with the state at which phase information is completely lost.

First, an arbitrary magnetization configuration, $\mathbf{M}_g(\mathbf{q})$, is set on the lattice spin system, and the Fourier transformation of that magnetization configuration is expressed as

$$F_g(\mathbf{k}) = \int \mathbf{M}_g(\mathbf{q}) e^{i\mathbf{k}\cdot\mathbf{q}} d\mathbf{q}, \quad (1)$$

where $\mathbf{q}$ represents the coordinate on the lattice system and $\mathbf{k}$ is the wave vector of the system.

In the second step, one of the selected magnetization configurations is flipped to produce an excited state, $\mathbf{M}_e(\mathbf{q})$. According to Eq. (1), the Fourier transformation of this magnetization configuration is expressed as $F_e(\mathbf{k})$. Finally, these Fourier transformations are compared with the measured diffraction pattern, $D(\mathbf{k})$, using

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FIG. 1. Schematic diagram showing the RMC method calculation procedure.

$$\Delta F_g = \sqrt{\int [|F_g(\mathbf{k})| - |D(\mathbf{k})|]^2 d\mathbf{k}}. \quad (2)$$

Based on Eq. (2), the magnetization configuration, $M_e(\mathbf{q})$, is stored as the most likely solution when $\Delta F_e < \Delta F_g$. When the trials are completed, the RMC sequence then corresponds to the single Monte Carlo step (MCS). Repetition for many MCSs is required to obtain the statistical solution of the RMC method. This trial procedure is shown in Fig. 1, and it was conducted for complete magnetization on the lattice spin system. We generated regular patterns, an example of which is shown on the bottom right of Fig. 2. The restoration was successful. Furthermore, we restored the characteristic pattern by clipping some images obtained from the experiment and using this technique. However, the pattern position gap problem explained above remained because of the lack of phase information from the Fourier transforms.

The simple selection method of the most likely solution requires a large number of MCSs to generate a converged solution. In order to reduce the calculation time for this procedure, we incorporated simulated annealing into the RMC. Even for the case of $\Delta F_e \geq \Delta F_g$, $M_e(\mathbf{q})$ can be selected as the most likely solution under the application

of simulated annealing. The length, δF_{ge} , on the function space is defined as

$$\delta F_{ge} = \sqrt{\int [|F_g(\mathbf{k})| - |F_e(\mathbf{k})|]^2 d\mathbf{k}}, \quad (3)$$

and when the excitation probability, pv , satisfies Eq. (4), $M_e(\mathbf{q})$ can be regarded as the most likely solution of the MCS of the RMC method. This can be expressed as

$$pv \leq \exp(-\delta F_{ge} \cdot W), \quad (4)$$

where W represents an inverse temperature in the Boltzmann distribution. Thus, a smaller W allows for a large excitation probability. The value of pv is created by generating a random number between 0 and 1, although Sec. III also shows that the possibility of excitation can be adjusted by changing the value of W in the RMC calculation.

III. RESULTS AND DISCUSSION

Figure 2 demonstrates the restoration of a magnetic domain structure in which the Fourier transformation of a prepared stripe domain is regarded as a measured $D(\mathbf{k})$. The magnetization is denoted by ± 1 , and the trial magnetization distribution has 32×32 data points in a two-dimensional pattern. In order to confirm the convergence of the RMC method, the initial magnetization configuration is set to uniformity with all magnetizations equal to -1 . As shown in Fig. 2, the restored domain structure converges to the stripe domain as the number of MCSs is increased.

In order to reduce calculation time, we introduced simulated annealing into the RMC. The convergence with and without annealing is shown in Fig. 3. As expressed in Eq. (4), the acceptance probability decreases as δF_{ge} increases. For the case of small W , which indicates a higher temperature, the acceptance probability increases when the inverse temperature decreases. In contrast, the acceptance probability decreases when the inverse temperature increases when W is large. If the acceptance probability is calculated using large W when the value of δF is also large, the probability of the reversal being effective will decrease and therefore, the convergence takes time. Then, the value of δF_{ge} becomes fixed, and it does not converge. As shown in Fig. 3, δF_{ge}

FIG. 2. Magnetic domain structure and Fourier transformation for a Monte Carlo step.

FIG. 3. (a) Excitation probability, p_v , as a function of inverse temperature, W . (b) Convergence of ΔF_{ge} value to MCSs, calculated by simulated annealing.

does not converge without annealing. If the value of W is changed with MCSs, the value of ΔF_{ge} converges gradually.

In Fig. 4, the restoration of an actual domain structure has been examined, i.e., a typical magnetization configuration in the permanent magnet as a “maze domain.” The Fourier transformation of the maze domain obtained using scanning transmission X-ray microscopy¹¹ is set to $D(k)$ instead of a measured diffraction pattern, and the prepared magnetization configuration consists of 32×32 two-dimensional data. The magnetization configuration results have been partially recovered. Additionally, even the condition of $|F(k)| = |D(k)|$ is satisfied. In a real-space image, the left- and right-side parts are inverted, as shown in Fig. 4(b). The reason why a gap is produced in the obtained image is that some of the phase information for the pattern that exists all over the real space is missing from the diffraction pattern.

We next consider extending the Fourier image to compensate for the lack of phase information. The extended real space and its relationship with the Fourier image are shown in Fig. 5.

The real-space 3×3 image of Fig. 5(a) is Fourier transformed, and a reciprocal-space image of Fig. 5(c) is produced. Even if the inverse Fourier transformation of the image is performed, the original real-space image is unreconstructed. Then, the real-space image extended to 9×9 using zero padding, as shown in Fig. 5(b), is Fourier transformed. The original image can be reproduced when the inverse Fourier transform of this calculated reciprocal-space image is performed. This result shows that a real-space image of size $N \times N$ is reproducible if a method of extending

FIG. 4. Experimental domain structure obtained using scanning transmission X-ray microscopy and results of the RMC method calculation: (a) experimental domain structure and (b) domain structure calculating using RMC.

FIG. 5. Relationship between the extended magnetic domain structure and Fourier image.

the data to $2N \times 2N$ can be found to generate a reciprocal-space image of size $N \times N$. The Fourier images of real-space extension, both before and after, are shown in Figs. 5(c) and 5(d), with white domains indicating unknown values. As shown in Fig. 5(d), the value before extension appears alternately in the extended Fourier image. Therefore, if a computational technique for calculating these unknown values is developed, the Fourier image is extensible, as shown in Fig. 5(e).

Here, two padding methods were tested: filling the unknown section with zero and with the mean value of the adjacent elements. As an example, the stripe test pattern shown in Fig. 6(a) was examined. The Fourier transformed image of the test pattern was extended using the two methods, as described above, and the RMC process was

FIG. 6. RMC calculation result using two kinds of extended Fourier images for stripe domain structure: (a) real-space image; (b) and (c) RMC calculation result using the extended Fourier image calculated by padding with the number 0 or by taking the average of the neighborhood values, respectively.

FIG. 7. RMC calculation result using extended Fourier image for maze domain structure: (a) maze domain structure and (b) rotated clockwise by 180° .

FIG. 8. The difference between the experimental image and calculated image. (a) The difference without extended Fourier image calculation (Figs. 4(a) and 4(b)). (b) The difference with extended Fourier image with mean-value padding calculation (Figs. 7(a) and 7(b)).

conducted. The results for the zero-padding and mean-value-padding techniques are shown in Figs. 6(b) and 6(c), respectively, and some differences are apparent. It can be seen that the recovery of the image completely set to $|F(\mathbf{k})| = |D(\mathbf{k})|$ was difficult and that many trial-calculation iterations were required. Therefore, a small value of W was taken, and various possible reversals were examined in the early step, which was then repeated with different W values. It can be seen that the problem that prevents convergence has been avoided. An accurate domain structure was obtained using these methods.

The RMC result for a maze domain pattern is shown in Fig. 7(b). The original Fourier images were extended using mean-value padding, as shown in Fig. 5. Fig. 7(b) shows the obtained magnetic domain images rotated by 180° . Furthermore, the obtained images can be returned to the image shown in Fig. 7(a), and an image of the same size can be created by removing the domain (gray: 0) expanded through the extension of the Fourier image. If Fig. 7(b) is compared with Fig. 7(a), completely congruous images are not obtained, but the magnetic domain width is mostly reproduced, and the direction and length of the magnetic domain streamline are reconstructed. Moreover, it can be seen that an image gap similar to that shown in Fig. 4 does not arise, and most of the corner points of the magnetic domain are

also mostly reproduced, along with the number of turning points.

The difference between the calculated and experimental images is indicated in Fig. 8. Areas where the experimental image is different from calculated image are indicated in red. Fig. 8(a) shows the difference between Figs. 4(a) and 4(b), and Fig. 8(b) shows the difference between Figs. 7(a) and 7(b). On the right side of Fig. 8(b), the red area is small because Fig. 7(a) is mostly similar to Fig. 7(b). On the other hand, the left side of the image is filled with red, which implies that location shifts occurred while the shape of the domain is maintained. For Fig. 8(a), there are few successive patterns because Fig. 4(a) is completely different from Fig. 4(b). Therefore, we can conclude that the reconstruction method of RMC using EFIMVP accurately reproduces the features of the magnetic domain structure.

IV. SUMMARY

By using the Reverse Monte Carlo method, we restored the characteristic image of the magnetic domain structure of a non-magnetization state. In addition, we reconstructed the image of a metastable state starting from a non-magnetization state. We anticipate the possibility that the restoration accuracy of a magnetic domain structure can be further increased by setting the appropriate magnetization size and using the extended data and original Fourier transform image.

ACKNOWLEDGMENTS

This research was supported by the Japan Science and Technology Agency (JST) under Collaborative Research Based on Industrial Demand “High Performance Magnets: Towards Innovative Development of Next Generation Magnets.”

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