Mechanism for variant selection in $L1_0$-type ferromagnetic alloys under three dimensionally constrained conditions

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Anisotropies of materials originate from microscopic anisotropies of the crystal at the atomic level. The macroscopic anisotropy, however, does not necessarily emerge even if its crystal structure has anisotropy. This is primarily because the microstructure evolution of materials is often governed by thermodynamic properties other than the anisotropy. To produce anisotropic materials at the macroscopic level, applying the external field corresponding to the microscopic anisotropy should be effective. $L1_0$-type ferromagnetic alloys (FMAs) are one of those materials. $L1_0$-type FMAs transform from FCC phase, their high temperature phase, to $L1_0$ phase, their low temperature phase. Resultant microstructure would have three variants of $L1_0$ phase depending on the orientation of their c-axis. Therefore, the magnetic crystalline anisotropy of $L1_0$ phase would be cancelled out at the macroscopic level. To promote the anisotropy at the macroscopic level, a single variant structure is desired. One of the ways to obtain a single variant sample is applying external magnetic field during heat treatment. By using such method, single variant structures have been successfully obtained [1,2]. The mechanism behind it is, however, still unclear, which is an obstacle to find strategies to obtain single variant structures. Calculations of microstructure evolution have been carried out by phase-field modeling to analyze the mechanism under two-dimensionally (2D) constrained condition [3]. One of the reasons why we used 2D constrained condition is simplicity and clarity for the ease of analyses. However, the validity of the 2D constrained calculations instead of three-dimensionally (3D) constrained condition is still unclear. In general, energy can be more lowered when degree of freedom is increased, allowing microstructure evolutions to be changed. In this study, mechanisms for variant selection under 3D constrained conditions have been carried out and compared with that under 2D constrained conditions.

Initial state for calculations was set as single crystal of FCC phase with fluctuation of order parameter. Temperature was fixed at 800 K, which is under the transformation temperature. We have carried out calculations of the microstructure evolutions by phase-field modeling during and after FCC to $L1_0$ transformation in FePd, a $L1_0$-type FMA, under an external magnetic field of 6 T.

The microstructure evolution is shown in Fig. 1. Magnetically preferred variant becomes dominant when an external magnetic field of 6 T is applied. The driving force for the variant selection was calculated and shown in Fig. 2 to clarify which thermodynamic factor drives the variant selection. It is found that interface energy is dominant factor, magnetic energy is effective only at the very early stage of microstructure formation, and elastic strain energy is effective at the later stage of microstructure formation. This trend is the same as the calculations under 2D constrained condition [3]. To clarify the reason, surface features were investigated. Figure 3 shows the distribution of one variant to see surface morphology. The surface becomes planar at the latter stage of microstructure evolution, in other words, the surface becomes two-dimensional. This is presumably because there are preferred crystallographic plane to reduce elastic strain energy. This is the one of the reasons why the governing factor in 3D constrained condition is similar to that in 2D constrained condition.

In summary, we have investigated the mechanism of the variant selection of $L1_0$-type FMAs by phase-field modeling under 3D constrained condition. The results indicate that the discussion based on the calculations under 2D constrained condition is valid also on the 3D constrained condition because of the two-dimensionality of the microstructure to reduce elastic strain energy.

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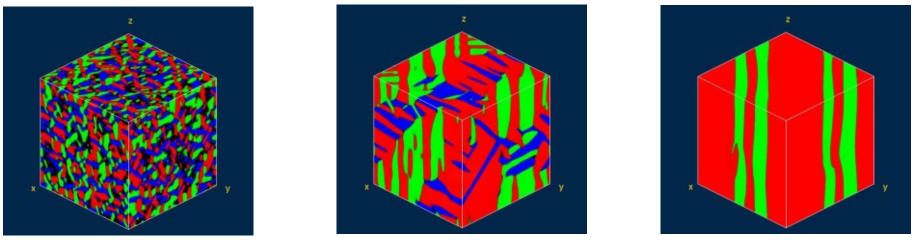

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FIG. 1. Time evolution of microstructure under an external magnetic field of 6 T. Red, green and blue regions represent the variants of $L1_0$ phase of which c-axis is along x, y and z direction, respectively.

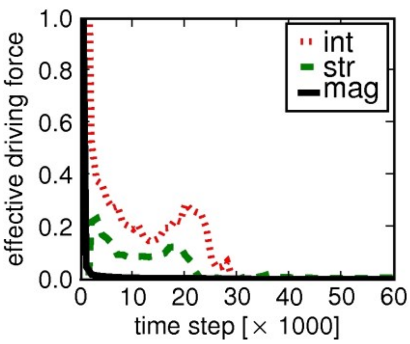

FIG. 2. Time evolution of the driving force for the variant selection. Red dotted, green broken and black solid lines represent interface, strain and magnetic contributions, respectively.

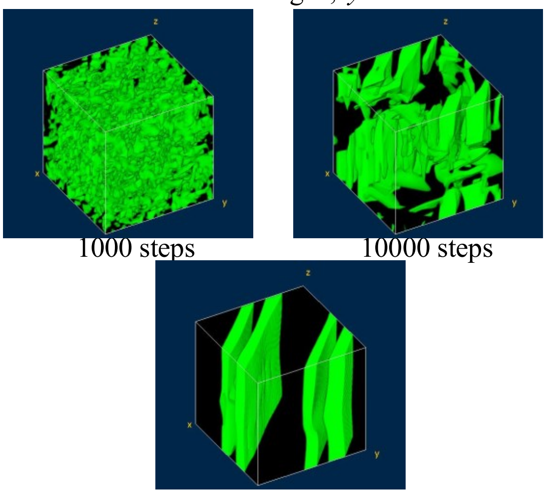

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FIG. 3. Time evolution of green region of Fig. 1.