Phase Field Analysis of the Mechanism of Variant Selection in FePd

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FePd exhibits high magnetocrystalline anisotropy, which is preferred by materials for magnetic storage media [1]. Its high-temperature and low-temperature phases respectively exhibit FCC and $L1_0$ type structures. Of these, the $L1_0$ phase has high magnetic anisotropy. One of the ways to obtain single-variant $L1_0$-FePd having high magnetic anisotropy is to apply external magnetic field to FCC-FePd matrix during the heat treatment process. In contrast, multi-variant FePd, which has lower magnetic anisotropy, would form under no external field. Though a number of studies have reported that single-variant FePd can be obtained by applying external field, such as magnetic field [2, 3] or external stress [4], the mechanism of formation of single-variant FePd is still unclear and, therefore, there are few guidelines to improve the process. One of the aims of this study is to reveal this mechanism behind this process and propose better strategies to obtain single-variant FePd.

One of the obstacles to reveal the mechanism is the difficulty of in-situ measurement. Hence, Phase Field calculation has been carried out, enabling us to analyze the time evolution of microstructure. In our model, chemical, gradient, magnetic and strain energy were taken into account. Temperature is fixed at 800 [K], which is below transition temperature. Values of phase field were randomly distributed at the initial state. Calculation has been carried out under magnetic field of 6 [T] along to x-axis. Hereafter, an easy axis of magnetization, x-axis, and the other in $L1_0$-FePd, y-axis, are referred to as x-, y-variant, respectively

Figure 1 shows snapshots of microstructure evolution. In these figures, black, red and green region represent FCC-FePd, x-variant and y-variant, respectively. That is, red region is magnetically preferable. Twin structure can be seen in Figure 1 and the magnetically preferable variant became dominant. Figure 2 shows the time dependence of volume fraction of each phase. It is found that the volume fraction of x-variant increases with time as the volume fraction of interface decreases. Then, we defined the driving force of variant selection as the difference between the driving force to increase x-variant and the driving force to increase y-variant, followed by extraction of the component of it at interface region. The time evolution of the driving force upon the variant selection at the interface region is shown in figure 3. It is found that magnetic, interface and strain energies are dominant to drive variant selection at initial, middle or final stage of phase evolution, respectively. This means magnetic field is effective only at the initial stage. In order to confirm this, magnetic field was applied only for the initial 200 steps. The result became almost indistinguishable from figure 1 or figure 2. This indicates that it is important to apply magnetic field at initial stage to obtain single-variant FePd.

In summary, variant selection mechanism of FePd was analyzed by Phase Field Modeling. Our analysis indicates that high magnetic field should be imposed at the beginning of the variant evolution for variant selection. This indicates that Phase Field analysis have a potential to improve process not by trial and error or brute force methods but by analytical prediction.

References

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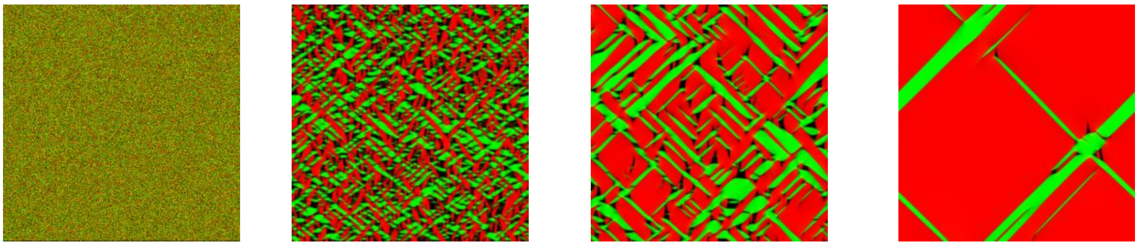

FIG. 1. Time evolution of microstructure under magnetic field of 6 [T]. Black, red and green regions represent FCC FePd, *x*-variant and *y*-variant, respectively. Twin structure forms and magnetically favorable variant (Red region) become dominant.

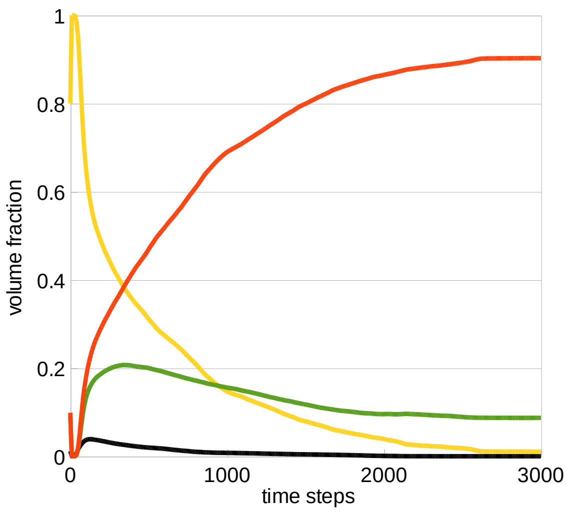

FIG. 2. Time evolutions of volume fraction. Red, green, yellow and black lines represent *x*-variant, *y*-variant, interface and FCC FePd, respectively. It is found that variant selection proceeds as the interface diminishes.

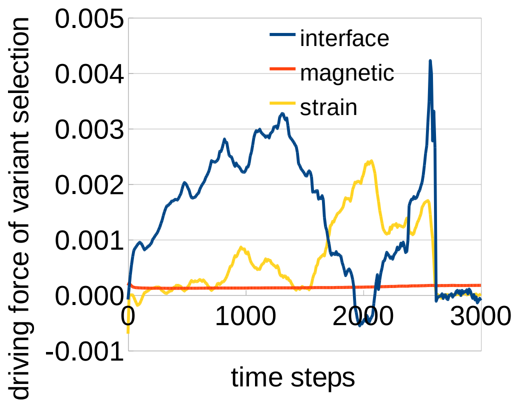

FIG. 3. Time evolutions of interface region component of driving force of variant selection. Blue, yellow and red lines represent interface, strain and magnetic energy contributions, respectively. It is found that magnetic, interface and strain energy contribution is dominant at initial, middle or final stage, respectively.