AMTC Letters
Vol. 2 (2010)

Phase Field Calculations of Domain Selection Following Order-Disorder Transition in FePd under External Field

Nobufumi Ueshima[1], Masato Yoshiya[1,2], Hideyuki Yasuda[1]

[1)] Department of Adaptive Machine Systems, Osaka University, Osaka 565-0871, Japan.
[2)] Nanostructures Research Laboratory, Japan Fine Ceramics Center, Nagoya, 456-8587, Japan

The order-disorder transition in FePd involves the structural change from cubic one (FCC) to tetragonal one ($L1_0$). This change causes the domain formation since any one of three *a*-axes of cubic structure can turn into one *c*-axis of tetragonal structure. Therefore, even if $L1_0$ FePd is formed from FCC FePd which is single-domained, the structure of $L1_0$ FePd would not be single-domained but have three domains having three different crystal orientations. Hereafter, the domain that has *c*-axis in *x*-, *y*-, or *z*-direction is referred to as *X*-, *Y*-, or *Z*-domain, respectively. Since the ordered phase has high magnetic crystalline anisotropy, single-domained structure is desired. Actually, the structure is not single-domained without external field. Applying uniaxial external field is one of attractive means to produce single-domained sample. For example, $L1_0$ FePd which has single-domained structure was produced by applying uniaxial magnetic field [1-3] or compressive stress field [3-4]. While there are discussions regarding the processing for the single-domained structure, it is still unclear as to how the single-domained is formed. In this study, to reveal this, the calculations by Phase Field Model incorporating magnetic field effect have been carried out.

The free energy for the calculations was expressed by the sum of chemical energy, interface energy and magnetic crystalline anisotropy energy. Elastic strain energy and other magnetic energies, such as, dipole interaction energy or exchange interaction energy, were not taken into account. This expression enables the calculations that intentionally exclude the effects of other energies, focusing on the influence of those energy terms included, which is quite difficult to do by means of practical experiments. The initial state of the calculations is following: Temperature is 50 [K] below from transition temperature, Composition is equiatomic, Phase distribution is uniformly disordered one with very small magnitude of random noise, And temperature and composition were fixed throughout the calculation. Then, the evolutions of microstructure have been calculated.

Figure1 shows snapshots of microstructure in the course of its evolution under no magnetic field. The corresponding results under magnetic field of 5 [T] parallel to *x*-axis is shown in Fig. 2. In these figures, black, red, green and blue indicate disordered phase, *X*-, *Y*-, and *Z*-domain, respectively. Comparison of these leads to a realization that more *X*-domain, which has the easy-axis of magnetization parallel to external magnetic field, is formed when non-zero magnetic field is applied. This suggests that the magnetic crystalline anisotropy energy has enough large effect for variant selection.

In the next step, to clarify when the magnetic field is effective, a series of systematic calculations was conducted. In these calculations, the time to begin applying magnetic field was changed from 0 to 10^5 steps while keeping the length of time for the application of magnetic field at 1000 steps. Selected results are shown in Fig. 3. The earlier magnetic field was applied, the more *X*-domains were formed at later stage. This indicates that magnetic field is more effective at earlier stage for domain selection. It is

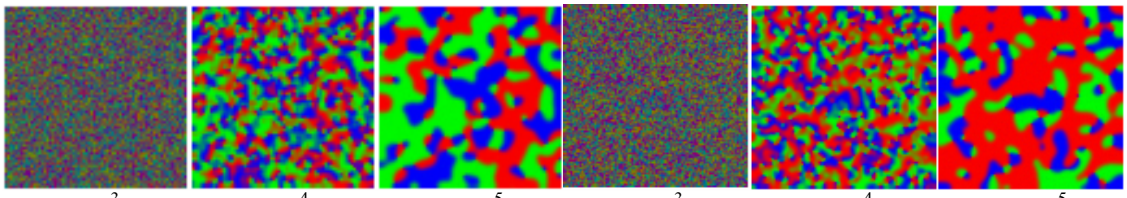
expected that interface energy become dominant at later stage when grain size gets larger, because the difference in the interface energy per unit volume among domains increases through coarsening process due to variation in grain size while the difference in magnetic energy per unit volume remain same.

This indicates that, applying magnetic field at early stage, when the difference in interface energy per unit volume among domains is relatively small, is crucial to keep the interface energy of favorable domain small relative to other domains, and then at later stage, coarsening process driven by interface energy acts favorably on the favorable domains with slightly larger size resulting in greater evolution than other unfavorable domains with smaller size, resulting in dominance of the favorable domain.

References

[1] Sahar Farjami et al.: *Scr. Mater.*, **58** (2008) 811–814.
[2] Sahar Farjami et al.: *Mater. Trans.*, **49** (2008), 9.
[3] K. Tanaka et al.: *Mater. Sci. Eng. A*, **312** (2001) 118-127.
[4] H. Shima et al.: *Phys. Rev. B*, **70** (2004) 224408.
[5] I. Steinbach et al.: *Physica D*, **94** (1996) 135-147.

Acknowledgment: The authors gratefully acknowledge the support of Grant-in-Aid for Scientific Research on Priority Areas “Atomic Scale Modification” (No. 474) from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

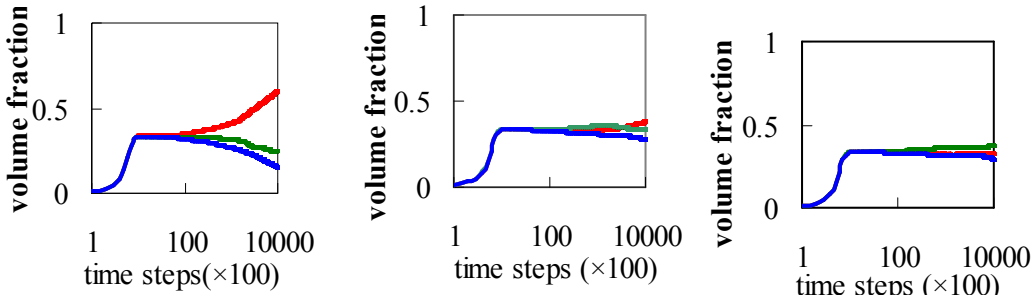


(a) 5×10^3 steps (b) 3×10^4steps (c)1.2×10^5steps

Fig. 1 Phase distribution under no magnetic field

(a) 5×10^3 steps (b) 3×10^4steps (c)1.2×10^5steps

Fig. 2 Phase distribution under magnetic field of 5 [T]



(a) From 0 step (b) From 1000 steps (c) From 10000 steps

Fig. 3 Volume fractions of three variants when magnetic field applied for 1000 steps
In these figures, red, green and blue lines indicate the volume fraction of X-, Y- and Z-domain, respectively.