Computer Simulation of Phase Decomposition in Magnetic Materials Based on the Phase-field Method

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During the last decade, the phase-field method has emerged across many fields in materials science as a powerful tool to simulate and predict complex microstructure evolution, (e.g., dendrite growth, spinodal decomposition, Ostwald ripening, crystal growth, recrystallization, martensitic transformation, dislocation dynamics, electromigration, crack propagation, and so on). Since phase-field methodology can model complex microstructure changes quantitatively, it is possible to search for the most desirable microstructure by using this method as a design simulation, i.e., through computer trial-and-error testing. In order to carry out this methodology, the flexible quantitative modeling method for complex microstructure changes using the phase-field method must first be established.

In this study, as the typical examples for the modeling of the complex microstructure changes using phase-field method, I will demonstrate the recent simulation results for the diffusion controlled phase transformations and microstructure developments in magnetic materials, for example, 1) the spinodal decomposition in Fe-Cr-Co hard magnetic alloys under external magnetic field, 2) Cu-cluster formation in amorphous Fe-Si-Cu alloy during isothermal aging, 3) FePt nano-granular structure formation during sputtering and the order-disorder phase transition of FePt nano particles, 4) Twin macrostructure developments in Ni$_2$MnGa ferromagnetic alloy under external stress and magnetic field, 5) the phase transformation and microstructure changes in Co-Sm-Cu hard magnetic materials, etc. Furthermore, I will discuss the relation between the calculated microstructure morphology and the magnetic hysteresis loop through the micromagnetics calculation.