Computational thermodynamics and microstructure simulations applied to grain boundary engineering in Nd-Fe-B sintered magnet

T. Koyama[1] and T. Abe[2]
[1] Department of Materials Design Innovation Engineering, Nagoya University, Nagoya 464-8603, Japan
[2] Research Center for Structural Materials, National Institute for Materials Science, Tsukuba 305-0047, Japan

To control the coercivity of the Nd hard magnet efficiently, we should understand the thermal stability of constituent phases and the microstructure changes observed in the hard magnets during their thermal processes. Since the CALPHAD method and the phase-field method have been recognized as promising approaches to realize the phase stability and microstructure developments in the engineering materials recently,[1)] we applied these methods for understanding the nature of the grain boundary phase and the microstructure developments in Nd-Fe-B hard magnet.
Figure 1 demonstrates the two-dimensional simulation result on the microstructure changes of Fe-15.3 at %Nd-5 at %B-0.2 at %Cu alloy with isothermal aging at 873K. Upper and lower figures are the phase field and the composition field, respectively. The white, black and gray parts in the phase-field are the $Nd_2Fe_{14}B$ phase (T_1 phase), the liquid phase, and the Nd solid phase, respectively, and each number indicated by *t* ' is a dimension less aging time. The degree of red color in the composition field means the local Nd concentration in the microstructure. At early stage, the Nd solid phase starts dissolving, and a liquid phase appears at grain boundary region. With aging, the Nd solid phase gradually disappears, and the Nd-rich liquid phase penetrates along grain boundary region, then the characteristic morphology of microstructure that the T_1 grains are uniformly covered with thin film of liquid phase appears. It has been elucidated experimentally that the Cu addition lowers the melting point of the liquid phase, because a eutectic reaction exists in the Cu-Nd binary phase diagram. By increasing the thermodynamic stability of liquid phase by Cu addition, the volume fraction of the liquid phase also increases, and then, it can be understood that the characteristic morphology is stabilized. Furthermore, when we focused on the final composition field carefully, the brightness of red color at the tri-junction region of T_1 grains differs from that at the grain boundary region between T_1 grains. This is because of the phase separation in the liquid phase, i.e., $L \rightarrow L_1 + L_2$. Since a phase separation of liquid phase has been reported in the calculation of the Fe-Cu-Nd phase diagram, the liquid phase separation induced by Cu addition is not an unusual phenomenon. When we imagine the coarsening process of the liquid phases, the L_1 phase should move over the L_2 phase; in other words, the movements of the L_1 and L_2 phases will interfere with one another during coarsening. The phase separation of liquid phase can contribute to stabilize the characteristic morphology (uniform coating of the T_1 grains by the liquid phase) temporally.

Reference

1) T. Koyama, Y. Tsukada, T. Abe and Y. Kobayashi, J. Japan Inst. Met. Mater., **81** (2017) 43-48.

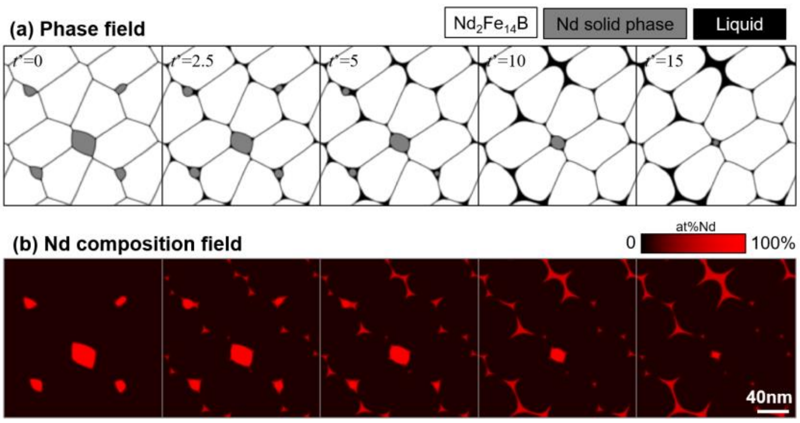

Fig.1 Phase-field simulation of the microstructure changes in Fe-15.3 at %Nd-5 at %B-0.2 at %Cu alloy with isothermal aging at 873K.

Acknowledgement: This work was partly supported by the project in Elements Strategy Initiative Center for Magnetic Materials (ESICMM) founded by Ministry of Education, Culture, Sports, Science and Technology, Japan.