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Monte Carlo Simulation Study of Atomic Structure of alnico Permanent Magnets MANH CUONG NGUYEN, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, U.S. DOE — Lattice Monte Carlo simulation based on quinternary cluster expansion energy model is used to investigate nano-scale structure of alnico alloy, which is considered as a candidate material for rare-earth free high performance permanent magnets, especially for high or elevated temperature applications such as electric motor for vehicles. We observe phase decomposition of the master alnico alloy into FeCo-rich magnetic ($\alpha 1$) and NiAl-rich matrix ($\alpha 2$) phases. Concentrations of Fe and Co in $\alpha 1$ phase and Ni and Al in $\alpha 2$ phase are higher for lower annealing temperature. Ti is residing mostly in the $\alpha 2$ phase. The phase boundary between $\alpha 1$ and $\alpha 2$ phases are quite sharp with only few atomic layers. The $\alpha 1$ phase is in B2 ordering with Fe and Al occupying the α-site and Ni and Co occupying the β-site. The $\alpha 2$ phase is in L21 ordering with Al occupying the 4a-site. The phase composition profile again annealing temperature suggests that lower annealing temperature would improve the magnetism of $\alpha 2$ and diminish the magnetism of $\alpha 2$ phase, hence improve shape anisotropy of $\alpha 1$ phase rods and that of alnico.

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