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Materials design of dilute magnetic semiconductors based on the control of spinodal decomposition

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Recently, spinodal decomposition phenomena attract much attention in the fabrication of dilute magnetic semiconductors (DMS). Many experimental results indicate that the magnetic properties of DMS are strongly affected by the occurrence of spinodal decomposition [1], thus people are now interested in controlling the magnetic properties of DMS by tuning the spinodal decomposition. In this talk, I will discuss spinodal decomposition in DMS based on the first-principles calculation. The electronic structure of DMS is calculated by using the Korringa-Kohn-Rostoker coherent potential approximation method. Based on the calculated mixing energy I will discuss phase diagrams of DMS systems and their chemical trends. By using the calculated chemical pair interactions between magnetic impurities in DMS, the self-organization of nano-structures in DMS of the nano-structures are simulated by using the Monte Carlo method. The simulation results indicate that we can control super-paramagnetic blocking temperature by optimizing the size of the nano-structures by changing the crystal growth condition [2]. Next, I will propose co-doping method to control solubility limit of magnetic impurities in DMS. From the total energy calculations, it is shown that the solubility of magnetic impurities is strongly enhanced under the existence of interstitial donors [2]. However, due to the compensation of holes by the co-dopants, the ferromagnetism is suppressed. Based on the kinetic Monte Carlo simulations, we propose low temperature annealing method to remove interstitial co-dopants for recovering the ferromagnetism. By combining the co-doping and the low temperature annealing, we can fabricate DMS with high concentration of magnetic impurities which should show high-Tc. This work is based on the collaboration with H. Fujii, L. Bergqvist, P. H. Dederichs and H. Katayama-Yoshida.

[1] A. Bonanni, Semicond. Sci. Technol. 22 (2007) R41.
[2] K. Sato et al., Rev. Mod. Phys. Phys. accepted.