Computational Nano-materials Design and Realization for Semiconductor Nano-spintronics

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1. Introduction

Based upon the recent development of the first-principles calculation method to go beyond the LDA for magnetic properties of dilute magnetic semiconductors (DMS) in ZnO, GaN, GaAs etc, it has been recognized that the magnetic percolation effect is disastrous to the high temperature ferromagnetism in DMS in particular for low concentrations. The exchange interactions calculated from first-principles are strong for nearest neighbors, but those interactions are short ranged and can not play an important role for realizing high-T_C because the solubility of magnetic impurity into DMS is too low to achieve magnetic percolation.

2. Computational Materials Design and Results

To overcome above difficulty and realize room temperature ferromagnetism, we focus on the spinodal nano-decomposition to increase the magnetic interactions and co-doping to increase the solubility in DMS, and propose a new method by controlling the spinodal decomposition with high blocking temperature can be realized leading for ferromagnetic behavior at high temperature.

We design the realistic new materials using the different exchange mechanisms such as Zener's double exchange interaction, Zener's *p–d* exchange interaction and anti-ferromagnetic as well as ferromagnetic super-exchange interactions in DMS by *ab initio* calculations. We obtain a universal trend for the exchange interactions with band filling or applied gating voltages. Typical examples are (Ga,Mn)N and (Ga,Mn)As. In the case of (Ga,Mn)N, Zener's double exchange interaction in the partially occupied Mn_{3d} deep-impurity-band in the band gap dominates the ferromagnetism because the N_{2p} levels are more deeper than the Mn_{3d} levels. On the other hand, in the case of (Ga,Mn)As, Zener's *p-d* exchange interaction in the partially occupied valence band dominates the ferromagnetism because As_{4p} levels are more shallower than Mn_{3d} levels.

We show that self-organized spinodal nano-decomposition (*Dairiseki-Phase*), supporting magnetic network over the three dimensional (3D) DMS, offers the functionality to have high Curie temperatures, even if the magnetic exchange interaction is short ranged. We show that spinodal nano-decomposition under layer-by-layer crystal growth condition (2D) leads to characteristic quasi-one dimensional nano-structures (*Konbu-Phase*) with highly anisotropic shape and high Curie temperature (T_C) even for low concentrations in DMS.

We also discuss the design and realization of d^0 ferromagnetism such as MgO, SrO and BaO comparing with the available experimental data.

3. Conclusions

In summary, based upon *ab initio* electronic structure calculation and multi-scale simulation of the spinodal nano-decomposition and calculation of T_C, we can design and realize the high-T_C DMS. We find that two different ferromagnetic mechanisms, Zener's double exchange interaction and Zener's *p–d* exchange interaction, can be available for the computational materials design of DMS. In order to solve the percolation problem in the DMS, spinodal nano-decomposition in two-dimensional crystal growth is very effective for the realization of high blocking temperature in the super-paramagnetic DMS, which we can use for the realistic spintronic devices. In order to realize the high-T_C DMS with increasing the solubility of magnetic impurities, the co-doping method with Li interstitial donor or Cu interstitial donor is very efficient to increase the solubility of Mn impurity in GaAs. We also design the d^0 ferromagnetism such as C, N and metal-vacancy-doped MgO, SrO and BaO, and compared with the available experimental data. We propoed the application to magnetic Re-RAM and M-RAM applications using the MgO or NiO based Re-RAM and M-RAM applications.

4. Open Questions

In order to increase the solubility of transition metal impurities in semiconductors, we have proposed couples of candidate for the co-doping such as Cu or Li-interstitial donors and Mn acceptors, we need experimental verifications. We need experimental verification for the system integration of DMS spintronics based on the spinodal nano-technology as a new class of bottom-up nanotechnology.

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