Computational nano-materials design and realization for semiconductor spintronics: Control of defect and spinodal nano-decomposition

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Semiconductor spintronics, in which one tries to use the spin degree of freedom of electrons in semiconductor technology, is one of the candidates for next generation electronics. So far dilute magnetic semiconductors (DMS) systems have been investigated intensively as a spintronics material. The purpose of this lecture is to show perspective on spintronics materials by proposing some ideas to answer the most important question in material science for semiconductor spintronics, namely, how we can realize high-TC DMS. To understand materials design of high-TC DMS proposed in this lecture, firstly, I discuss electronic structure of transition metal (TM) impurities in semiconductors. As fundamental mechanisms of magnetic interactions in DMS, double exchange, $p - d$ exchange and super exchange mechanism are introduced, and it is pointed out that relative importance of these mechanisms depends on the occupancy of d-states of TM impurities and calculated chemical trend of the magnetism in III-V and II-VI DMS is discussed [1]. Next, I discuss magnetic properties of DMS at finite temperature. To calculate $T_C$, I will explain how to map the first-principles total energy results on classical Heisenberg model to estimate magnetic properties. Accuracy in estimating $T_C$ depends strongly on the approximations used. It will be shown that the mean field approximation is not justified particularly in the double exchange systems for low concentrations. Here, I emphasize that the magnetic percolation is the biggest problem that prevents us from realizing high-$T_C$ [1]. Then, I propose two scenarios for realizing high-$T_C$ DMS. The first one uses spinodal decomposition. Thermodynamics consideration based on calculated total energies of DMS tells us that strong inhomogeneity is in general induced in DMS and clusters with high concentration of TM (thus high-$T_C$), whose structure is coherent to host matrix, are formed. If the cluster size is large enough, due to the super-paramagnetic blocking phenomena the system shows hysteresis even at high temperature [2]. The other way is a co-doping method. When we dope TM impurities in semiconductors, by introducing compensating donor impurity at the same time the solubility of TM impurities increases owing to the reduction of mixing energy. If we use interstitial donors for the co-dopants, we can remove the co-dopants by low-temperature annealing after the crystal growth to recover the ferromagnetism [3].
To realize the above two proposals, I will emphasize that the understanding on the defect properties in DMS is very important. In addition to the above two scenarios, it is still important to discover new materials which is useful for spintronics. I will present our recent materials design of LiZnAs-based [4] and IV-VI semiconductor-based materials [5].

References