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Design of dilute magnetic semiconductors with room temperature ferromagnetism by controlling spinodal decompostion[1]

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Owing to the recent development of the first-principles method for calculating magnetic properties of dilute magnetic semi-conductors (DMS), it has been recognized that the magnetic percolation effect is disastrous to the high temperature ferro-magnetism in DMS in particular for low concentrations [1]. 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 impurities into DMS is too low to achieve magnetic percolation. To overcome this difficulty and realize room temperature ferromagnetism, we focus on the spinodal decomposition in DMS, and suggest that by controlling the spinodal decomposition high blocking temperature can be realized leading to ferromagnetic behaviour at high temperature [2]. We calculate electronic structure of DMS from first-principles by using the Korringa- Kohn-Rostoker coherent potential approximation (KKR-CPA) method. Then, chemical pair interactions and magnetic exchange interactions between magnetic are calculated. We use the Monte Carlo techniques to simulate spinodal decomposition of DMS and to estimate the magnetic properties of them [3]. The computer simulations for the magnetization process of the decomposi-tion phases indicate that we can control super-paramagnetic blocking temperature by optimizing the size of the clusters by changing the crystal growth condition. This simulation suggests the material design of high blocking temperature DMS by controlling the spinodal decomposition [2].As another approach for realizing high-Tc DMS we propose co-doping method to increase solubility limit of transition metal impurities in DMS [4]. This work is based on the collaboration with H. Katayama-Yoshida and T. Fukushima.

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