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Solubility control in dilute magnetic semiconductors by using the co-doping method KAZUNORI SATO, HITOSHI FUJII, ISIR, Osaka University, LARS BERGQVIST, PETER H. DEDERICHS, IFF, FZ-Juelich, HIROSHI KATAYAMA-YOSHIDA, Osaka University — To overcome low solubility limit of magnetic impurities in dilute magnetic semiconductors (DMS) and realize room temperature ferromagnetism, we propose a co-doping method to increase solubility of magnetic impurities in DMS [1]. We calculate electronic structure of (Ga, Mn)As, (Ga, Mn)N, (Ga, Cr)N and (Zn, Cr)Te with interstitial impurities, such as Li, Na and Cu, from first-principles by using the Korringa-Kohn- Rostoker coherent potential approximation (KKR-CPA) method. From the total energy results, it is shown that the mixing energy of magnetic impurity becomes negative and the solubility of magnetic impurities is strongly enhanced under the existence of interstitials [1]. In general, the co-dopants compensate hole carriers, thus the system becomes paramagnetic. However, owing to the large diffusivity of these interstitial impurities, we can anneal out the co-dopants after the crystal growth to recover the ferromagnetism. As an example, kinetic Monte Carlo simulations for the diffusion of interstitial co-dopants in DMS will be shown. [1] K. Sato et al., Jpn. J. Appl. Phys. 46 L1120 (2007)

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