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Defect-Induced High-T_C Ferromagnetism and Spinodal Nanodecomposition in MgO MASAYOSHI SEIKE, Grad. School of Eng. Sci., Osaka Univ. and Cent. Research Labs., Sysmex Corp., TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Grad. School of Eng. Sci., Osaka Univ. — Based on a first-principles study of the magnetic properties of MgO with Mg vacancies [1,2], we calculated the electronic structures and exchange coupling constants for Monte Carlo Simulation (MCS) of the Curie temperature (Tc). We also performed MCS of the spinodal nanodecomposition based on the calculated chemical pair interactions between the vacancies. In this study, it was found that hole-doping by Mg vacancies leads to a ferromagnetic ground state, invoking long-range magnetic interaction, and that Tc can reach room temperature at sufficient vacancy concentrations of 15 at.% under a homogeneously distributed condition. However, it was also found that the chemical pair interactions between vacancies are significantly attractive and that the system can form super-paramagnetic clusters of vacancies with strong ferromagnetic coupling in the clusters. These results suggest that, by the spinodal nanodecomposition, the Tc or blocking temperature (T_B) can be enhanced and reach room temperature at smaller vacancy concentrations compared with those estimated for room-temperature ferromagnetism under the homogeneous distribution condition.

[1] M. Seike, et al. Jpn. J. Appl. Phys. 50, 090204 (2011).
[2] K. Sato, et al. Rev. Mod. Phys. 82, 1633 (2010).

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