第81回応用物理学会秋季学術講演会 講演予稿集 (2020 オンライン開催)

Role of dopants to exchange interaction and magnetocrystalline anisotropy in antiferromagnet NiO

Graduate school of Engineering, Mie University[1], Department of Physics, Institut Teknologi Bandung, Indonesia[2], Institute for Chemical Research, Kyoto University[3]

○(M2) K. Miyamae[1], A.-M. Pradipto[2], T. Moriyama[3], and K. Nakamura[1]

E-mail: 419M618@m.mie-u.ac.jp

The use of optoelectronics in the terahertz region has been attracting attention in recent years as an important technology for future large-capacity communication and sensing technology. One candidate of the promising materials is known to be antiferrimagnets, such as doped NiO, since antiferromagnetic resonance has terahertz region frequency arising from two factors, exchange and anisotropic magnetic fields [1]. Here, in order to clarify systematically the role of dopants to the exchange interaction and the magentocrsystaline anisotropy in NiO, we performed first principles calculations for doped NiO with impurities of Mn, as a magnetic element, and Li and Mg, as non-magnetic elements. Calculations were carried out based on generalized gradient approximation by using the full-potential linearized augmented plane wave method [2]. The electron correlation effect at Ni sites in NiO was treated in the DFT+U scheme with an effective on-site Coulomb interaction parameter U_{eff} [3], and the atomic positions were fully relaxed by atomic force calculations. The exchange interaction parameters, *J*s, were estimated by fitting calculated total energies to the Heisenberg Hamiltonian, and the magnetocrystalline anisotropy energy, E_{MCA}, were calculated based on Force theorem by using second variation SOC method [2]. The results predict that when the non-magnetic elements (Li and Mg) are doped, the *J* value of the next nearest neighbor tends to decrease compared to that in the pure NiO, while for the magnetocrystalline anisotropy, the E_{MCA} increases over that of the pure NiO by doping Mn. Details discussion of the dopant effects to the exchange interaction and magnetocrystalline anisotropy will be presented.

[1] Z. Wang *et al*., Appl. Phys. Lett. **112**, 252404 (2018).
[2] K. Nakamura *et al*., Phys. Rev. B **67**, 14405 (2003).
[3] K. Nawa *et al*., Phys. Rev. B **97**, 035117 (2018).