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Anisotropy Energy, Spin-Atomic Vibration Interaction, and Spin-Flip Hamiltonian of a Single Atomic Spin in a Crystal Field SATOSHI KOKADO, Faculty of Engineering, Shizuoka University, Japan, KIKUO HARIGAYA, Nanosystem Research Institute, AIST, Japan, AKIMASA SAKUMA, Graduate School of Engineering, Tohoku University, Japan — We derive the anisotropy energy $V_{\rm A}$, the spin-atomic vibration interaction $V_{\rm SA}$, and the spin-flip Hamiltonian $V_{\rm SF}$ of a single atomic spin system, "Fe^{2+} ($3d^6$) in a crystal field of tetragonal symmetry" [1,2]. We here apply the perturbation theory to a model with the spin-orbit interaction and the kinetic and potential energies of electrons. The model also takes into account the difference in vibration displacement between an effective nucleus and electrons, Δr. We first find conditions to enhance a coefficient $|D|$ of $V_{\rm A}=-|D|S_Z^2$, where D is an anisotropy constant and S_Z is the Z component of a spin operator. Second, we show that $V_{\rm SA}$ appears for $\Delta r \neq 0$, while $V_{\rm SF}$ is present independently of Δr. Also, the magnitudes of the coefficients of $V_{\rm SA}$ can be larger than those of the conventional spin-phonon interaction depending on vibration frequency.

[1] S. Kokado *et al.*, J. Phys. Soc. Jpn. **79**, 114721 (2010).
[2] S. Kokado *et al.*, phys. stat. solidi (c) **7**, 2612 (2010).

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